Metal and Material Physics Division
Fachverband Metall- und Materialphysik (MM)

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Overview of Invited Talks and Sessions

(Lecture rooms H 0106, H 0107, TC 006, and TC 010; Poster C and E)

Invited Talks

MM 1.1	Mon	9:30–10:00	TC 006	**Beyond Hall-Petch: Mechanism based description of dislocation grain-boundary interactions** — •Christoph Kirchlechner, Nataliya Malyar, Juan Li, Nicolas Peter, Christian Liebscher, Jean-Sebastien Micha, Gerhard Dehm
MM 9.1	Mon	15:00–15:30	TC 006	**Deciphering fracture patterns: what crack paths teach us about the mechanics and physics of fracture** — •Laurent Ponson
MM 18.1	Tue	9:30–10:00	TC 006	**Hydrogen storage in individual metal nanoparticles** — •Andrea Baldi, Tarun Narayan, Fariah Hayee, Ai Leen Koh, Robert Sinclair, Jennifer Dionne
MM 28.1	Wed	9:30–10:00	TC 006	**Accurate and fast machine learning n-body force fields** — Aldo Glielmo, Claudio Zeni, James Kermode, •Alessandro De Vita
MM 49.1	Thu	9:30–10:00	TC 006	**Analysis of amorphous structures by transmission electron microscopy** — •Martin Peterlechner
MM 59.1	Thu	15:00–15:30	TC 006	**Dilatometric Techniques for Atomic Scale Analysis of Defects and Processes in Solids** — •Wolfgang Sprengel

Invited talks of the joint symposium SYID

See SYID for the full program of the symposium.

SYID 1.1	Mon	9:30–10:00	H 0105	**Data driven R&D for Materials: Cognitive Discovery** — •Alessandro Curioni
SYID 1.2	Mon	10:00–10:30	H 0105	**Rational design and synthesis of Pt-based catalysts for fuel cell applications** — •Younan Xia
SYID 1.3	Mon	10:30–11:00	H 0105	**2D, or not 2D? Materials discovery, data provenance, and workflow reproducibility.** — •Nicola Marzari
SYID 1.4	Mon	11:00–11:30	H 0105	**Generating and assessing data from combinatorial and high-throughput experiments for the design of new materials** — •Alfred Ludwig
SYID 1.5	Mon	11:30–12:00	H 0105	**Novel materials discovery: big-data-analytics methods and infrastructure for building maps of materials** — •Luca Ghiringhelli

Invited talks of the joint symposium SYMS

See SYMS for the full program of the symposium.

SYMS 1.1	Mon	15:00–15:30	H 0105	**Stochastic numerical algorithms: from molecular dynamics to big data analytics** — •Benedict Leimkuhler
SYMS 1.2	Mon	15:30–16:00	H 0105	**A Generally-Applicable Machine-Learning Scheme for Materials and Molecules** — •Michele Ceriotti
SYMS 1.3	Mon	16:00–16:30	H 0105	**Girsanov reweighting for path ensembles and Markov state models** — •Bettina G. Keller, Luca Donati, Carsten Hartmann

SYMS 1.4	Mon	16:45–17:15	H 0105	**Liquid State Theory Meets Deep Learning and Molecular Informatics** — •Alpha Lee
SYMS 1.5	Mon	17:15–17:45	H 0105	**Computational high-throuhgput screening of drug-membrane thermodynamics** — •Tristan Bereau

Invited talks of the joint symposium SYDM

See SYDM for the full program of the symposium.

SYDM 1.1	Thu	15:00–15:30	H 0105	**Bending, pulling, and cutting wrinkled two-dimensional materials** — •Kirill Bolotin
SYDM 1.2	Thu	15:30–16:00	H 0105	**Ultrafast valley and spin dynamics in single-layer transition metal dichalcogenides** — •Alejandro Molina-Sanchez
SYDM 1.3	Thu	16:00–16:30	H 0105	**Interlayer excitons in layered semiconductor transition metal dichalcogenides** — •Steffen Michaelis de Vasconcellos
SYDM 1.4	Thu	16:45–17:15	H 0105	**Exploring exciton physics in liquid-exfoliated 2D materials** — •Claudia Backes
SYDM 1.5	Thu	17:15–17:45	H 0105	**A Progress Report on Electron Transport in MXenes; A New Family of 2D Materials** — •Michel Barsoum

Invited talks of the joint symposium SYAM

See SYAM for the full program of the symposium.

SYAM 1.1	Fri	9:30–10:00	H 0105	**Bringing Dino-Birds to life – Synchrotron X-ray fluorescence and Raman imaging of ancient materials** — •Uwe Bergmann
SYAM 1.2	Fri	10:00–10:30	H 0105	**Linear and Nonlinear Optical Properties of Cultural Heritage Materials** — •Marta Castillejo
SYAM 1.3	Fri	10:30–11:00	H 0105	**Morphology and topology of multiscale pore networks: Imaging structural alteration and hydric invasion** — •Pierre Levitz
SYAM 1.4	Fri	11:15–11:45	H 0105	**Painting cracks: a way to reveal physical properties of matter** — •Ludovic Pauchard
SYAM 1.5	Fri	11:45–12:15	H 0105	**Finite element analysis and biomechanical interpretation of fossil material properties** — •Emily Rayfield

Sessions

MM 1.1–1.1	Mon	9:30–10:00	TC 006	**Invited talk Kirchlechner**
MM 2.1–2.5	Mon	10:15–11:30	H 0106	**Battery Materials**
MM 3.1–3.8	Mon	10:15–13:15	H 0107	**Topical session (Symposium MM): Hydrogen in Materials**
MM 4.1–4.4	Mon	10:15–11:30	TC 006	**Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales**
MM 5.1–5.8	Mon	10:15–13:15	TC 010	**Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)**
MM 6.1–6.10	Mon	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)**
MM 7.1–7.5	Mon	11:45–13:00	H 0106	**Battery Materials**
MM 8.1–8.5	Mon	11:45–13:15	TC 006	**Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales**
MM 9.1–9.1	Mon	15:00–15:30	TC 006	**Invited talk Ponson**
MM 10.1–10.5	Mon	15:45–17:00	H 0106	**Battery Materials**
MM 11.1–11.3	Mon	15:45–17:00	H 0107	**Topical session (Symposium MM): Hydrogen in Materials**
MM 12.1–12.5	Mon	15:45–17:15	TC 006	**Topical Session (Symposium MM): Fundamentals of Fracture**
MM 13.1–13.8	Mon	15:45–18:45	TC 010	**Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)**
MM 14.1–14.9	Mon	15:00–17:15	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)**

MM 15.1–15.5	Mon	17:30–18:45	H 0106	**Battery Materials**
MM 16.1–16.5	Mon	17:30–19:00	H 0107	**Topical session (Symposium MM): Hydrogen in Materials**
MM 17.1–17.5	Mon	17:30–19:00	TC 006	**Topical Session (Symposium MM): Fundamentals of Fracture**
MM 18.1–18.1	Tue	9:30–10:00	TC 006	**Invited talk Baldi**
MM 19.1–19.5	Tue	10:15–11:30	H 0106	**Battery Materials**
MM 20.1–20.8	Tue	10:15–13:00	H 0107	**Topical session (Symposium MM): Hydrogen in Materials**
MM 21.1–21.4	Tue	10:15–11:30	TC 006	**Topical Session (Symposium MM): Fundamentals of Fracture**
MM 22.1–22.4	Tue	10:15–11:15	TC 010	**Microstructure and Phase Transformations**
MM 23.1–23.5	Tue	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)**
MM 24.1–24.4	Tue	11:45–13:00	H 0106	**Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)**
MM 25.1–25.6	Tue	11:45–13:15	TC 006	**Topical Session (Symposium MM): Fundamentals of Fracture**
MM 26.1–26.5	Tue	11:45–13:00	TC 010	**Microstructure and Phase Transformations**
MM 27.1–27.34	Tue	18:30–19:45	Poster E	**Poster Session I**
MM 28.1–28.1	Wed	9:30–10:00	TC 006	**Invited talk De Vita**
MM 29.1–29.4	Wed	10:15–11:15	H 0106	**Nanomaterials**
MM 30.1–30.5	Wed	10:15–11:30	H 0107	**Interfaces**
MM 31.1–31.4	Wed	10:15–11:30	TC 006	**Topical session (Symposium MM): Fundamentals of Fracture**
MM 32.1–32.4	Wed	10:15–11:15	TC 010	**Microstructure and Phase Transformations**
MM 33.1–33.9	Wed	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)**
MM 34.1–34.4	Wed	11:45–12:45	H 0106	**Nanomaterials**
MM 35.1–35.5	Wed	11:45–13:00	H 0107	**Interfaces**
MM 36.1–36.5	Wed	11:45–13:00	TC 006	**Topical Session (Symposium MM): Fundamentals of Fracture**
MM 37.1–37.5	Wed	11:45–13:00	TC 010	**Microstructure and Phase Transformations**
MM 38.1–38.4	Wed	15:15–16:15	H 0106	**Nanomaterials**
MM 39.1–39.6	Wed	15:15–16:45	H 0107	**Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales**
MM 40.1–40.5	Wed	15:15–16:45	TC 006	**Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century**
MM 41.1–41.6	Wed	15:15–16:45	TC 010	**Liquid and Amorphous Metals**
MM 42.1–42.10	Wed	15:00–17:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)**
MM 43.1–43.4	Wed	17:00–18:00	H 0106	**Nanomaterials**
MM 44.1–44.4	Wed	17:00–18:15	H 0107	**Topical Session (Symposium EPS and MM): Mechanical Properties at Small Scales**
MM 45.1–45.5	Wed	17:00–18:30	TC 006	**Topical Session (Symposium MM): Fundamentals of Fracture**
MM 46.1–46.6	Wed	17:00–18:30	TC 010	**Liquid and Amorphous Metals**
MM 47.1–47.51	Wed	18:30–19:45	Poster C	**Poster Session II**
MM 48	Wed	19:45–20:45	TC 006	**General Assembly of the Metal- and Materials Division**
MM 49.1–49.1	Thu	9:30–10:00	TC 006	**Invited talk Peterlechner**
MM 50.1–50.4	Thu	10:15–11:30	H 0106	**Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales**
MM 51.1–51.6	Thu	10:15–11:45	H 0107	**Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century**
MM 52.1–52.5	Thu	10:15–11:30	TC 006	**Methods in Computational Materials Modelling (methodological aspecst, numerics)**
MM 53.1–53.5	Thu	10:15–11:30	TC 010	**Liquid and Amorphous Metals**
MM 54.1–54.9	Thu	10:30–12:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)**
MM 55.1–55.4	Thu	11:45–13:00	H 0106	**Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales**

MM 56.1–56.5	Thu	11:45–13:15	H 0107	**Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century**
MM 57.1–57.6	Thu	11:45–13:15	TC 006	**Methods in Computational Materials Modelling (methodological aspecst, numerics)**
MM 58.1–58.6	Thu	11:45–13:15	TC 010	**Liquid and Amorphous Metals**
MM 59.1–59.1	Thu	15:00–15:30	TC 006	**Invited talk Sprengel**
MM 60.1–60.3	Thu	15:45–16:45	H 0106	**Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales**
MM 61.1–61.5	Thu	15:45–17:15	H 0107	**Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century**
MM 62.1–62.6	Thu	15:45–17:15	TC 006	**Methods in Computational Materials Modelling (methodological aspecst, numerics)**
MM 63.1–63.5	Thu	15:45–17:00	TC 010	**Transport (Diffusion, conductivity, heat)**
MM 64.1–64.10	Thu	15:00–17:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)**
MM 65.1–65.6	Thu	17:30–19:00	H 0106	**Functional Materials (Actuators, filters, sensors, shape memory)**
MM 66.1–66.5	Thu	17:30–19:00	H 0107	**Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century**
MM 67.1–67.6	Thu	17:30–19:00	TC 006	**Methods in Computational Materials Modelling (methodological aspecst, numerics)**
MM 68.1–68.4	Thu	17:30–18:30	TC 010	**Transport (Diffusion, conductivity, heat)**
MM 69.1–69.5	Fri	9:30–10:45	H 0106	**Structural Materials (Steels, light-weight materials, high-temperature materials)**
MM 70.1–70.5	Fri	9:30–11:00	H 0107	**Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century**
MM 71.1–71.6	Fri	9:30–11:00	TC 006	**Methods in Computational Materials Modelling (methodological aspecst, numerics)**
MM 72.1–72.4	Fri	9:30–10:30	TC 010	**Magnetic Shape Memory Alloys (joint with MA)**
MM 73.1–73.9	Fri	10:30–12:45	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)**
MM 74.1–74.4	Fri	11:15–12:15	H 0106	**Structural Materials (Steels, light-weight materials, high-temperature materials)**
MM 75.1–75.5	Fri	11:15–12:45	H 0107	**Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century**
MM 76.1–76.5	Fri	11:15–12:30	TC 006	**Methods in Computational Materials Modelling (methodological aspecst, numerics)**

Annual General Meeting of the Metal and Material Physics Division

Wednesday 19:45–20:45 TC 006

MM 1: Invited talk Kirchlechner

Time: Monday 9:30–10:00 Location: TC 006

Invited Talk MM 1.1 Mon 9:30 TC 006

Beyond Hall-Petch: Mechanism based description of dislocation grain-boundary interactions — •Christoph Kirchlechner[1], Nataliya Malyar[1], Juan Li[1], Nicolas Peter[1], Christian Liebscher[1], Jean-Sebastien Micha[2], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH — [2]CEA Grenoble

The important role of grain boundaries as an obstacle for dislocation slip has long been recognized. However, until today, there are no quantitative, mechanism based models describing the interaction of a lattice dislocation with one particular grain boundary.

The unique possibilities offered by micro pillar compression complemented by advanced in situ characterization (SEM, TEM, microLaue) is well able to quantitatively answer fundamental questions in dislocation grain boundary interaction: What is the impact of one grain boundary on (i) the observed yield stress and (ii) the measured apparent hardening? (iii) Can we define a meaningful *transmission stress*? (iv) Is the dislocation slip transfer process strain-rate dependent and (v) what is the strain rate dependence quantitatively? Within the talk, these question will be answered for various grain boundaries in copper. The talk will mainly focus on two different high angle grain boundaries one permitting and one preventing dislocation slip transfer and finally a coherent Sigma3 twin boundary.

MM 2: Battery Materials

Advanced Lithium-Ion Batteries

Time: Monday 10:15–11:30 Location: H 0106

MM 2.1 Mon 10:15 H 0106

A thermodynamic description of the battery material LiCoO2 based on ionic and electronic work functions — •Johanna Schepp[1], Stephan Schuld[1], Rene Hausbrand[2], Mathias Fingerle[2], Wolfram Jägermann[2], and Karl-Michael Weitzel[1] — [1]Philipps Universität Marburg, Chemistry Department — [2]TU Darmstadt, Department of Material Science

The release of Li+ from stoichiometric LiCoO2 (LCO) - a typical battery electrode material has been investigated by means of thermionic emission. Analysis of the data leads to an ionic work function of wLi+(LCO) = 4.1 eV. Combination of this value with the electronic work function we-(LCO) = 5.1 eV also measured in this work by photoelectron spectroscopy, and information available from the literature allows to setup for the first time a complete thermodynamic cycle for a LiCoO2 // Li battery. We arrive at an open circuit cell voltage of 2.4 eV in line with available literature information. The proof-of-principle study presented here provides experimental data on the binding energy values, i.e. chemical potentials, of Li+-ions and electrons and thus of Li-atoms in LiCoO2 as battery cathode and is expected to open access to a better understanding and consequently also a better design of battery materials. Current efforts in measuring the long term characteristics of LCO as a function of the composition and the total amount charges exchanged will be discussed.

MM 2.2 Mon 10:30 H 0106

Effect of stress/strain on ionic and electronic conductivity in LiCoO$_2$ cathode material — •Ashkan Moradabadi and Payam Kaghazchi — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195, Berlin

It has been revealed that stress/strain can affect conductivity of materials up to several orders of magnitude [1]. In this study, we have investigated the influence of stress/strain on charge carrier mobilities in bulk LiCoO$_2$ using an ab initio-based “elastic dipole tensor” concept. It is shown that only 1% lateral tensile strain can increase the ionic conductivity in bulk LiCoO$_2$ more than two times [2]. The effect of longitudinal strain on ionic conductivity is even more significant [2]. Moreover, we calculated the electronic conductivity in bulk LiCoO$_2$ using hole-polaron hopping model. Our estimated value for the electronic conductivity is 2.7×10^{-4} S/cm [3] which is in good agreement with experiments (1.0-3.3×10^{-4} S/cm [4]). We find that the effect of stress/strain on ionic conductivity is stronger than that of the electronic one. By comparing the results obtained by this method and those calculated by DFT-NEB, we show that the “elastic dipole tensor” method can be used to estimate conductivity of materials under any given strain field with low computational and time effort.

[1] J. Garcia-Barriocanal *et al.*, Science, 2008, 321, 676-680. [2] A. Moradabadi *et al.*, submitted to Phys. Rev. Mats., 2017, arXiv: 1706.01709. [3] A. Moradabadi *et al.*, Phys. Rev. App., 2017, 7 (6), 064008. [4] Qiu *et al.*, Phys. Chem. Chem. Phys., 2012, 14, 2617-2630.

MM 2.3 Mon 10:45 H 0106

Pressure-dependence of the contact resistance in transport measurements of single secondary particles of Li(Ni$_x$Co$_y$Mn$_{1-x-y}$)O$_2$ — •Markus S. Friedrich[1], Janis K. Eckhardt[1], Simon Burkhardt[1,2], Limei Chen[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Gießen, Germany

Lithium ion intercalating and deintercalating layered structured transition metal oxides, such as Li(Ni$_x$Co$_y$Mn$_{1-x-y}$)O$_2$ (NCM), are of interest for applications in lithium-ion batteries due to the predicted high capacity and the high cycling stability. Most studies on these materials were carried out using composite electrodes which not only contained the active electrode material, but also additives that significantly influence the electrochemical properties of the electrode. A deeper understanding of the intrinsic properties of the active particles is needed, to examine the influence of the electrode-materials structure on energy storage and conversion of the cell system the material is used in. We developed a technique which allowed us to contact single particles of pure NCM with a controlled pressure and to perform electrochemical impedance spectroscopy to gain information about the electronic transport properties of the material. To contact the particles, they were arranged in trap holes, formed by photolithographical structuring of a photoresist, on top of a noble metal coated substrate.

MM 2.4 Mon 11:00 H 0106

Electrochemical Lithiation of crystalline Si investigated by operando NR and EIS — •Arne Ronneburg[1,2], Marcus Trapp[1], Robert Cubitt[3], Luca Silvi[1], Sebastian Risse[1], and Matthias Ballauff[1,2] — [1]Helmholtz-Zentrum Berlin, Institute of Soft Matter and Functional Materials, Hahn-Meitner Platz 1, 14109 Berlin, Ger-many — [2]Humboldt-University Berlin, Institute of Physics, Zum Großen Windkanal 6, 12489 Berlin, Germany — [3]Institute Laue Langevin (ILL), 71 avenue des Martyrs - CS 20156, 38042 Cedex 9 Grenoble, France

Silicon is a promising material for Li-Ion batteries due to its eleven times higher specific capacity compared to graphene. However, Si-anodes suffer from strong capacity fading. Therefore more fundamental understanding of the degradation is needed for further improvement. Neutron scattering is ideally suited for the investigation of the Li/Si system due to the high contrast between the scattering length densities. Si anodes were investigated with operando neutron reflectometry in parallel with electrochemical impedance spectroscopy to elucidate the solid electrolyte interface(SEI) layer growth and decomposition during (de-)lithiation. The lithiation kinetics were investigated over four cycles revealing a successive growth of the lithiated zone and the formation of a SEI-layer within delithiation and its decomposition during lithiation. The correlation of the integrated electric current with the Li fraction in the Si electrode discloses the amount of charge that is needed to dissolve the SEI-layer during lithiation. This necessary investment of charge is a reason for a low coulombic efficiency.

MM 2.5 Mon 11:15 H 0106

First-principles approach to lithium diffusion in silicon — •Vishank Kumar, Davide Di Stefano, Gian-Marco Rignanese, and Xavier Gonze — Institute for Condensed Matter and Nanosciences, European Theoretical Spectroscopy Facility, Université Catholique de Louvain, Chemin des étoiles 8, B-1348 Louvain-la-Neuve, Belgium

The high lithium storing capacity of silicon has drawn a strong interest for its possible application as an anode material in Li-ion batteries. However, the kinetics of lithium diffusion in silicon and in other lithiated phases of silicon, are not yet fully understood. In this study, the transition state theory was used to calculate the temperature dependent diffusion coefficient of Li, in bulk Si and LiSi phase. Quantum mechanical effects were also considered via semi-classical transition state theory. The energy barriers and pre-exponential factors have been obtained from total energy and phonon calculations, respectively, using the density functional theory (DFT). Kinetic Monte Carlo (KMC) simulations were used to calculate the effective diffusion coefficient in LiSi case with multiple vacancy mediated diffusion pathways.

Our results are in good agreement with the experimental data and suggest that quantum mechanical effects are only marginally significant in Li-Si system. The current study shows a theoretical approach, which is computationally efficient and quantitatively accurate, to fill the lack of studies on Li diffusion in lithiated Li_xSi phases.

MM 3: Topical session (Symposium MM): Hydrogen in Materials

Hydrogen interactions with defects

Hydrogen in Materials organized by Astrid Pundt (Institute of Materials Physics, U Göttingen, Germany) and Tilmann Hickel (MPI Eisenforschung, Düsseldorf, Germany).

Time: Monday 10:15–13:15 Location: H 0107

Topical Talk MM 3.1 Mon 10:15 H 0107

Effects of hydrogen on plasticity and fracture in iron—atomic level to mesoscale theory — •Anthony Paxton — King's College London, London, UK

The phenomenon of hydrogen embrittlement involves processes at all time and length scales. At the smallest scales it must be recognised that the proton in magnetic α-Fe acts as a quantum particle even at room temperature [1]. It is necessary to take into account proton quantum effects if one is not to make errors of factors of two or three in calculations involving trapping and diffusion problems. On the other hand the frequently discussed concepts of hydrogen induced localized plasticity (HELP) and hydrogen enhanced decohesion (HEDE) can only be discussed meaningfully at the mesoscale level and above. Here I will describe our recent work in which we have used magnetic tight binding [2] and density functional theory results as inputs into calculations of dislocation velocity and cohesive strength as functions of stress, temperature and hydrogen concentration in magnetic iron [3, 4]. I may also speculate on certain paradoxes surrounding the theory of elastic shielding of dislocations by hydrogen and on how hydrogen may act to localise plasticity.

1. A. T. Paxton and I. H. Katzarov, *Acta Mater.*, **103**, 71 (2016)
2. A. T. Paxton and C. Elsässer, *Phys. Rev. B*, **82**, 235125 (2010)
3. I. H. Katzarov, D. L. Pashov and A. T. Paxton, *Phys. Rev. Materials*, **1**, 033602 (2017)
4. I. H. Katzarov, and A. T. Paxton, *Phys. Rev. Materials*, **1**, 033603 (2017)

Topical Talk MM 3.2 Mon 10:45 H 0107

Hydrogen-assisted failure in Ni-based superalloy 718 studied under in situ hydrogen charging: The role of localized deformation in crack propagation — Zahra Tarzimoghadam[1], •Dirk Ponge[1], Jutta Klöwer[2], and Dierk Raabe[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]VDM Metals GmbH, Altena, Germany

We investigated hydrogen embrittlement (HE) of Ni-base superalloy 718 after different heat treatments by slow strain rate tensile testing under continuous electrochemical hydrogen charging. Hydrogen-assisted cracking mechanisms were studied by electron backscatter diffraction (EBSD) analysis and electron channeling contrast imaging (ECCI). Fracture in hydrogen-charged samples was dominated by localized deformation. Non-uniform hydrogen concentrations and plastic instabilities arise at the impingement of slip bands on grain boundaries and at intersecting slip lines. Transgranular cracking was caused by shear localization assisted by hydrogen-enhanced localized plasticity (HELP) along slip planes. Intergranular cracking was due to grain boundary triple junction cracking, slip-localization at grain boundaries, and delta/gamma interface cracking. Observations on the overaged state confirmed that the delta-phase promotes HE by initializing micro-cracks from delta/gamma interfaces. Hydrogen-enhanced strain-induced vacancy (HESIV) mechanism also assisted the ductile intergranular and transgranular fracture. The failure mechanism is explained based on hydrogen-enhanced formation of strain-induced vacancies, nano-void nucleation and coalescence during deformation.

30 min. break

MM 3.3 Mon 11:45 H 0107

Ab-initio study of the role of kappa carbides as potential hydrogen traps in advanced high-strength steels — •Poulumi Dey[1], Tobias A. Timmerscheidt[2], Dimitri Bogdanovski[2], Jörg von Appen[2], Tilmann Hickel[1], Richard Dronskowski[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany

Hydrogen embrittlement is one of the major challenges for Fe based materials such as high-Mn steels. Addition of Al to high-Mn steels is known to reduce their sensitivity to hydrogen-induced delayed fracture which motivated us to investigate possible trapping effects related to the presence of Al in the grain interior employing density-functional theory (DFT). The role of Al-based kappa carbide precipitates is investigated to understand the relevance of short-range ordering effects. As H tends to occupy the same positions as C in these precipitates, the interaction and competition between both interstitials is studied via DFT-based simulations. Our study reveals that the interstitials tend to increase the lattice parameter leading to a net increase of the trapping capability despite the fact that the individual H-H/C-H chemical interactions are generally repulsive. An increased Mn content is shown to enhance H trapping due to attractive short-range interactions. Another short-range ordering that is favorable for H trapping is found at the interface between an Fe-matrix and the carbide. The study further shows that the trapped H atoms subsequently yield a decohesion at the interface, which may be one reason for the observed failure.

MM 3.4 Mon 12:00 H 0107

Atomistic modelling of hydrogen cosegregation at grain boundaries in iron and nickel — •Eunan J. McEniry, Tilmann Hickel, and Joerg Neugebauer — Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The behaviour of hydrogen at structural defects in metallic alloys is well-known to play a key role in the mechanical stability of such materials. As a result, the energetics and kinetics of hydrogen in the vicinity of grain and phase boundaries have been extensively studied via atomistic simulation, in order to understand mechanisms of hydrogen-induced decohesion. The emphasis of this work is the critical interplay of hydrogen with additional elements present in the material.

Using atomistic simulations, we have performed high-throughput calculations of the cosegregation behaviour of H, B, C, and N at selected grain boundaries in Fe and Ni. Due to the large number of configurations that must be considered, we have employed tight-binding approaches to enable the efficient and accurate description of the thermodynamics of light element cosegregation. Having obtained segregation profiles at the chosen grain boundaries as a function of bulk concentration and temperature, we employ both thermodynamic analysis as well as simulated mechanical testing to assess the impact of segregants on the structural stability of the grain boundaries.

MM 3.5 Mon 12:15 H 0107

Hydrogen embrittlement of Tungsten induced by Deuterium Plasma: Insights from Nanoindentation Test — •Xufei Fang[1], Arkadi Kreter[2], Marcin Rasinski[2], Christoph Kirchlechner[1], Steffen Brinckmann[1], Christian Linsmeier[2], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Structure and Nano-/ Micromechanics of Materials, Max-Planck-Str. 1, 40237 Düsseldorf, Germany — [2]Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung - Plasmaphysik, Partner of the Trilateral Euregio Cluster (TEC), 52425 Jülich, Germany

Hydrogen exposure has been found to result in metal embrittlement. We use nanoindentation experiments to study the mechanical properties of single crystalline and polycrystalline tungsten subjected to deuterium plasma. The results exhibit a decrease in the pop-in load and increase in hardness on exposed tungsten sample due to the presence of deuterium. These findings agree with the defactant theory that explains the decrease of the load required for dislocation nucleation. The hardness increase is also discussed based on the solid solution strengthening effect.

MM 3.6 Mon 12:30 H 0107

Hybrid QM/MM study of the effect of hydrogen on dislocation glide in tungsten — •Petr Grigorev and James Kermode — Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry CV4 5AL, United Kingdom

In this study we use a hybrid musltiscale approach, namely quantum mechanics/molecular mechanics (QM/MM) [1], combining an accurate local QM description of the dislocation core atoms with a classical model for the rest of the system. We apply a recently developed QM/MM implementation of the virtual work principle [2] to compute energy barriers. The effect of H atoms in the material on the dislocation core structure together with the energetics of interaction of H with dislocations are investigated. The obtained results are analysed by comparison with pure DFT studies from literature [3, 4, 5] together with machine learning based Gaussian Approximation Potential (GAP) model [5].

[1] N. Bernstein, J. R. Kermode, and G. Csányi, Rep. Prog. Phys. 72, 026501 (2009). [2] T. Swinburne, J. R. Kermode, Phys. Rev. B. 96, 144102 (2017). [3] L. Dezerald, D. Rodney, E. Clouet, L. Ventelon, F. Willaime, Nat. Commun. 7, 11695 (2016) [4] A. Bakaev, P. Grigorev, D. Terentyev, A. Bakaeva, E. E. Zhurkin, Y. A. Mastrikov, Nucl.Fusion 57, 126040 (2017) [5] W. Slachta, A. Bartók and G. Csányi, Phys. Rev. B. 90, 104108 (2014).

MM 3.7 Mon 12:45 H 0107

DFT study of absorption and migration of hydrogen and oxygen in MAX phases — •Daniel F. Urban[1], Francesco Colonna[2], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

MAX phases are ternary metal carbides and nitrides with multi-layered crystal structures and mixed metallic-covalent bonding. They have very good thermal, chemical, and mechanical properties which make them potentially suitable as corrosion protection coatings for high-temperature energy-conversion devices such as solid oxide fuel cells. To assess the capability of MAX phases as diffusion barriers for hydrogen and oxygen, we investigate absorption and migration of H and O atoms in a variety of MAX-phase carbides and nitrides by means of first-principles calculations based on density functional theory. The resulting calculated formation and migration energies indicate that MAX-phase coatings can act as protective diffusion barriers for both hydrogen and oxygen, but with different migration mechanisms [1].

[1] F. Colonna, C. Elsässer, RSC Advances 7, 37852 (2017)

MM 3.8 Mon 13:00 H 0107

New approaches for in-situ nanoindentation of hydrogen charged alloys: insights on bcc FeCr alloys — •Jazmin Duarte Correa, Xufei Fang, Steffen Brinckmann, and Gerhard Dehm — Max-Planck-Institut für Eisenforshung GmbH, 40479 Düsseldorf, Germany

Understanding hydrogen-microstructure interactions in metallic alloys is needed to prevent hydrogen embrittlement. The failure mechanisms that initiate at the atomic scale with hydrogen absorption and interaction with trap binding sites, can be studied independently by nanoindentation; in-situ charging the sample with hydrogen avoids the formation of concentration gradients due to desorption. Two custom electrochemical cells were built for hydrogen charging while nanoindenting the sample: front-side charging with sample and indenter tip immersed into the electrolyte, and back-side charging where the analyzed region is never in contact with the solution. We discuss the advantages and disadvantages of both approaches during the study of the hydrogen effect on homogeneous nucleation of dislocations in bcc FeCr alloys. A reduction in the pop-in load indicating the yield point with the increase of hydrogen content and formation of multiple pop-ins during nanoindentation provided evidence for the decrease in the resolved shear stress and enhanced dislocations nucleation. Although a similar trend is observed for both strategies, a more pronounced effect is noticed by front-side charging, likely due to surface degradation.

MM 4: Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales

Plasticity: Experiments

EPS-Symposium organized by Laurent Pizzagalli (U Poitiers, France), Gerhard Dehm (MPI Eisenforschung, Düsseldorf, Germany), Olivier Thomas (U Aix-Marseille, Marseille, France), and Jörg Neugebauer (MPI Eisenforschung, Düsseldorf, Germany).

Time: Monday 10:15–11:30 Location: TC 006

Topical Talk MM 4.1 Mon 10:15 TC 006

Plasticity in complex crystals * On the role of building blocks in intermetallics and layered compounds — •Sandra Korte-Kerzel[1], Sebastian Schröders[1], Stefanie Sandlöbes[1], James Gibson[1], and William Clegg[2] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen University, Aachen, Germany — [2]Department of Materials Science and Metallurgy, University of Cambridge, UK

Plasticity in most complex crystals remains poorly understood owing to their brittleness and the associated difficulties in mechanical testing. The development of microcompression and its use in conjunction with electron microscopy has been a major step forward and systematic studies are now possible [1]. However, the uncharted phase space in terms of plastic deformation remains vast. In this context, the role of recurring building blocks in complex crystals and how plasticity may be governed by smaller elements in large unit cells is discussed in the light of intermetallic and atomically layered phases. Taking the extraordinary properties of MAX phases [2] and the topologically close packed μ-phase with its Laves building blocks as example, small-scale testing in conjunction with electron microscopy to atomic resolution and density functional theory calculations was used to elucidate the key components of the respective large unit cells.

[1] Korte-Kerzel, S. Microcompression of brittle and anisotropic crystals, MRS Comm 1-12 (2017) [2] Howie, P.R., Thompson, R. J., Korte-Kerzel, S., Clegg, W.J. Softening non-metallic crystals by inhomogeneous elasticity, Sci Rep 7, 11602 (2017)

MM 4.2 Mon 10:45 TC 006

Insights into the deformation behavior of the superplastic alloy Zn22Al at the micro-scale — •Patrick Feldner, Benoit Merle, and Mathias Göken — Friedrich-Alexander-University Erlangen-Nuremberg, 91054 Erlangen, Germany

Due to their remarkable ductility, superplastic metallic alloys are promising candidates to create micro-scale components via micro-forming processes. However, it has not yet been established if the macroscopically observed superplastic behavior also persists at microscopic length scales.

For this reason, the superplastic alloy Zn22Al was characterized at small length scales using nanoindentation at elevated temperatures, pillar compression experiments as well as tensile testing in situ in a TEM.

Coupling the local strain-rate sensitivity with the apparent activation energy, strong evidences for superplastic like flow at the micrometer-scale were found. However, further successively decreasing the size of the plastic zone yields a significant change of the deformation kinetics, which suggests a critical length scale beneath which the superplastic material behavior disappears.

Supported by the deformation and fracture mechanisms observed during thin film tensile testing, a transition from boundary mediated ductility to boundary mediated brittleness is proposed.

MM 4.3 Mon 11:00 TC 006

Plastic Poisson's Ratio of Nanoporous Metals: A Macroscopic Signature of Tension-Compression Asymmetry at the Nanoscale — •Lukas Lührs[1], Birthe Zandersons[1], Norbert Huber[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

At small length scales atomistic simulations suggest a surface-induced tension-compression asymmetry of the strength and flow stress of metallic bodies. As experimental evidence supporting this notion remains to be reported, we investigate the impact of capillary forces on small-scale plasticity.

We study the transverse plastic deformation of macroscopic nanoporous gold under uniaxial compression in electrolyte. This affords in situ variation of the surface state, specifically the surface tension, γ, during plastic flow. We find that decreasing γ results in an increase of the macroscopic plastic Poisson's ratio, ν_P. We show that γ promotes the compression while hindering tensile elongation of individual ligaments. Transverse deformation during compression of the network structure is partly caused by the stretching of ligaments oriented perpendicular to the load axis. Here, the surface-induced tension-compression asymmetry acts to reduce ν_P. Finite element simulations support experimental observations and confirm the significant contribution of the surface tension to small-scale plasticity.

[Nano Lett., 2017, 17 (10), 6258-6266]

MM 4.4 Mon 11:15 TC 006

Electro-plastic deformation studies of Al-Cu eutectic alloys — •Doreen Andre, Stefanie Sandlöbes, and Sandra Korte-Kerzel — Institut für Metallkunde und Metallphysik, RWTH Aachen 52056 Aachen, GERMANY

A promising approach of forming materials with poor deformation behaviour, such as metallic-intermetallic composite materials, here an Al-Cu eutectic alloy, is to apply electric pulses during the forming processes. This effect is known as the electro-plastic effect (EPE). The EPE causes a drop in the yield strength resulting in higher formability of materials. However, the underlying physical mechanisms are not fully understood yet. Since the EPE has only been studied on the macroscopic scale until now, we have modified our nanoindenter device such that we can apply electrical pulses during nanoindentation and micro-pillar compression. This enables us to study the effects of electrical pulses during plastic deformation of single-phase and single-crystalline samples of even complex microstructures, hence, providing more detailed insights into the physical nature of the electro-plastic effect. Additionally, high current densities can be achieved due to the small tested sample volumes. Here, we present our experimental set-up and report about first experimental results of a nano-mechanical electro-plastic study on an Al-Cu eutectic alloy.

MM 5: Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)

Sessions: Magnetism I and Magnetism II

EPS-Symposium organized by Chuchun Fu (CEA-Saclay, Gif-sur-Yvette, France), Thomas Hammerschmidt (Ruhr-Universität Bochum, Germany), Tilmann Hickel (MPI Eisenforschung, Düsseldorf, Germany), and Véronique Pierron-Bohnes (IPCMS CNRS-Unistra, Strasbourg, France).

Time: Monday 10:15–13:15 Location: TC 010

Topical Talk MM 5.1 Mon 10:15 TC 010

First principles many-body calculations for rare earth-based materials: present status and open challenges — •Silke Biermann — Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France

Rare earth compounds are at the heart of a wide range of modern materials applications, ranging from permanent magnets to pigments, and reliable and efficient first principles descriptions of their properties are highly desirable in view of the development of rational design techniques. Strong local Coulomb interactions on the rare earth f-shell, however, make ab initio calculations for such materials challenging.

We will review the present status of dynamical mean field theory-based approaches to the problem and describe recent methodological developments in the field [1,2,3].

[1] P. Seth, P. Hansmann, A. van Roekeghem, L. Vaugier, S. Biermann, Physical Review Letters 119 056401 (2017). [2] Pascal Delange, Silke Biermann, Takashi Miyake, Leonid Pourovskii, Phys. Rev. B 96, 155132 (2017). [3] S. Panda, L. Pourovskii, S. Biermann, in preparation.

MM 5.2 Mon 10:45 TC 010

Continuous transition from antiferro- to ferromagnetic state via moment canting in $Ni_{2-x}Co_xMnAl$ — •Michael Leitner[1], Pascal Neibecker[1], Matthias Opel[2], Xiao Xu[3], Ryosuke Kainuma[3], and Winfried Petry[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [3]Department of Materials Science, Tohoku University, Sendai 980-8579, Japan

The magnetic structure of materials is often discussed only in terms of the classical concepts of ferromagnetism and antiferromagnetism, however, interesting phenomena can be expected when a system is driven to the boundary between these regimes by adjusting external parameters. B2-ordered $Ni_{2-x}Co_xMnAl$ is a case in point: Ni_2MnAl, a potential ferromagnetic shape-memory material, displays antiferromagnetism [1], while NiCoMnAl, predicted to be a halfmetal, is ferromagnetic [2].

We have studied this system for $0 \leq x \leq 0.8$. Temperature-dependent neutron powder diffraction proves an antiferromagnetic ordering for $x < 0.4$, while the macroscopic magnetization shows an increasing longitudinal component for all $x > 0$. We argue that this constitutes a continuous, spatially homogeneous transition from antiferro- to ferromagnetism via canted spins, which is reproduced by a simple Heisenberg model.

[1] M. Acet et al., *J. Appl. Phys.* **92**, 3867 (2002)

[2] P. Neibecker et al., *Phys. Rev. B* **96**, 165131 (2017)

MM 5.3 Mon 11:00 TC 010

Modeling the high-temperature paramagnetic state of magnetic materials from first-principles - coupling of lattice vibrations and disordered magnetism — •Björn Alling[1,2] and Irina Stockem[1,2] — [1]Linköping University, Sweden — [2]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

The paramagnetic state of magnetic materials lack global magnetization and long range order between moments. However, in most cases there still exist important local magnetic moments. Also, lattice vibrations are important for properties and stability of materials at high temperature. Simultaneous presence of disorder of magnetic and vibrational nature poses a severe challenge for first-principles theory.

I present our recently developed method combining atomistic spin dynamics with ab-initio molecular dynamics (ASD-AIMD) treating the magnetic and vibrational degrees of freedom on an equal, first-principles based footing. It allows us to explicitly study the coupled dynamics of magnetism and lattice in the paramagnetic state.

We use it to study paramagnetic CrN. Phonon life times are obtained from the AIMD part of the simulations. At 300 K, we see dramatically lower phonon lifetimes as compared to an adiabatic, fast-magnetism, approximation. Further, the phonon lifetime does not decrease in the normal manner with increasing temperature which could explain anomalys thermal conductivity observed experimentally for many materials in the paramagnetic state. These results underline the importance of allowing for a dynamical coupling between magnetism and lattice vibrations in theoretical studies of the paramagnetic state.

MM 5.4 Mon 11:15 TC 010

Lattice relaxations in paramagnetic materials from first principles — •Davide Gambino[1] and Björn Alling[1,2] — [1]Department of Physics, Chemistry, and Biology (IFM) Linköping University, SE-58183 Linköping, Sweden — [2]Max-Planck-Institut für Eisenforschung GmbH, D-402 37 Düsseldorf, Germany

The first-principles calculation of many material properties starts with the relaxation of the atomic positions of the system under investigation. This procedure is routine for nonmagnetic materials, as well as for magnetically ordered compounds. However, when it comes to magnetically disordered systems, it is not clear what geometry one should take into account. Here we propose a method for the structural relaxation of magnetic materials in the paramagnetic regime within the disordered local moment (DLM) picture in the framework of density functional theory (DFT). The method can be easily implemented using any ab initio code.

We consider as a test case Fe vacancy in bcc Fe in the paramagnetic regime: as a result, the nearest neighbors to the vacancy relax inwards of about 0.16 Angstrom (-5% of the ideal bcc nearest neighbor distance), which is twice as large as the relaxation in the ferromagnetic case, and the vacancy formation energy calculated on these positions results to be 1.60 eV, which corresponds to a reduction of about 0.1 eV compared to the formation energy calculated on ferromagnetic-relaxed positions. Our results are in good agreement with recent DFT+DMFT calculations and with experimental values. Other systems under investigations are interstitial defects in bcc Fe and FeCr random alloys.

15 min. break

Topical Talk MM 5.5 Mon 11:45 TC 010

We need perfect defects - challenging the Brown's paradox in permanent magnetism — •Oliver Gutfleisch — TU Darmstadt, Materialwissenschaft

It is common understanding that among the intermetallic phases used for high performance permanent magnets, practically none can fully realize its potential based on the intrinsic magnetic properties. Even if the grain size of the fully-dense magnet is close to the single domain size, the coercivity Hc is usually one order of magnitude smaller than the anisotropy field Ha - this situation is known as Brown's paradox. The presence of crystallographic defects of various kinds, of secondary phases, of surface imperfections as well as magnetic inhomogeneities leads to local magnetic softening. On the other hand, a perfect single crystal shows 'no' coercivity whatsoever. Looking at nucleation-type NdFeB (1,2) and pinning type SmCo (3) magnets we will revisit the Brown's paradox and discuss possible ways of overcoming it.

1 Helbig et al., Experimental and Computational Analysis of Magnetization Reversal in (Nd,Dy)-Fe-B Core Shell Sintered Magnets, Acta Materialia 127 (2017) 498.

2 Loewe et al., Grain boundary diffusion of different rare earth elements in Nd-Fe-B sintered magnets by experiment and FEM simulation, Acta Materialia 124 (2017) 421.

3 Duerrschnabel et al., Atomic structure and domain wall pinning in samarium -cobalt based permanent magnets, Nature Communications 8:54 (2017).

Topical Talk MM 5.6 Mon 12:15 TC 010

Interplay of moment-volume and electron-phonon coupling in the itinerant electron metamagnet LaFe$_{13-x}$Si$_x$H$_y$ — •Markus Ernst Gruner — Faculty of Physics and Center for Nanointegration, CENIDE, University of Duisburg-Essen, Germany

LaFe$_{13-x}$Si$_x$H$_y$ compounds belong to the most promising systems for room temperature magnetic refrigeration. Here, large adiabatic temperature and isothermal entropy changes in an external magnetic field are obtained at a first-order metamagnetic transition. It is accompanied by a large volume change without change in lattice symmetry, attributed to the competition of different magnetic states of Fe associated with varying atomic volumes. Recently, we detected by first-principles lattice dynamics and nuclear resonant inelastic X-ray scattering characteristic changes in the vibrational density of states at the magnetic transition in LaFe$_{13-x}$Si$_x$, which involves the disappearance of a high-energy peak in connection with an overall softening of phonons in the paramagnetic phase. This contributes to the good magneto- and barocaloric properties of the material, in terms of a cooperative contribution of magnetic, electronic and vibrational degrees of freedom to the entropy change. The softening originates from adiabatic electron-phonon coupling caused by specific changes in the electronic density of states at the Fermi level, which are sensitive to the magnitude of the Fe moment, rather than to magnetic order. Finally, we demonstrate that the same mechanisms are effective in the hydrogenated compound at ambient conditions.

Funding by the DFG within SPP 1599 is gratefully acknowledged.

MM 5.7 Mon 12:45 TC 010

Spin-lattice effects in LaFe$_{11.6}$Si$_{1.4}$ revealed by powder diffraction — •Tom Faske[1], Wolfgang Donner[1], and Markus Hölzel[2] — [1]TU Darmstadt, Materials Science, Structure Research, Darmstadt, Germany — [2]Heinz Maier-Leibnitz Zentrum, Garching, Germany

LaFe$_{13-x}$Si$_x$ ($x = 1.0 - 1.6$) is a promising material class for application in magnetic cooling and has been extensively studied in recent years. For $x \leq 1.6$ it exhibits a first order magneto-structural phase transition around 200 K which becomes second order for $x > 1.6$. The first-order transition is accompanied by a large isothermal entropy change $|\Delta S_{iso}|$ in conjunction with a high adiabatic temperature change $|\Delta T_{ad}|$, which are both important figures of merit for a potential magnetocaloric application.

Here we report on the detailed study of the first-order phase transition of LaFe$_{13-x}$Si$_x$ by means of temperature and magnetic field dependent x-ray and neutron powder diffraction. External magnetic fields increase the Curie temperature by $\approx$ 4 K/T, so that the phase transition could be induced thermally and by applying magnetic fields of up to 5 T during the diffraction experiments. In a narrow magnetic field and temperature range, both phases were present in the diffraction patterns. Subtle structural differences in the two-phase region between the magnetic field and temperature induced phase transitions revealed a change in the entropy transfer of the two systems.

MM 5.8 Mon 13:00 TC 010

Symmetry breaking induce robust monoclinic-distortion and unconventional charge ordering at room temperature in single crystal of Na2.7Ru4O9 — •Arvind Yogi[1,2], C. I. Sathish[1,2], Hasung Sim[1,2], Y. Noda[3], and Je-Geun Park[1,2] — [1]Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 08826, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [3]Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

We discovered by combining the results of SC-XRD, electrical resistivity, specific heat, and susceptibility that Na2.7Ru4O9 with the monoclinic new tunnel type lattice (space group P 21/m) evolves an unprecedentedly charge ordering (CO) at room temperature while retaining of metallicity. The temperature dependent SC-XRD results shows super-lattice peaks q1 (0, 1/2, 0) and q2 (0, 1/3, 1/3), that causes the translation symmetry breaking of the lattice which induces robust monoclinic-distortion at room temperature, is the evidence for the formation of an unconventional charge ordering (CO). Na2.7Ru4O9 show a first-order phase transition in the electrical resistivity with two consecutive transitions at Tc (1) = 365 K and Tc (2) = 345 K for Na2.7Ru4O9 which supports well by magnetization and heat-capacity results. The electron-phonon mediated scattering mechanism is involved in the resistivity. We argue that the origin of unprecedented CO is due to the localized 4d electrons.

MM 6: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)

Exploring, understanding, and describing materials with strong electronic Coulomb correlations remain among the big challenges of modern condensed matter physics. Correlated materials are characterized by an extreme sensitivity to external probes such as pressure or temperature, and slight changes in composition, constraints during the growth process (e.g. by heterostructuring) or off-stoechiometries can significantly alter their properties. While the invited lectures will have a focus on correlated electron materials, the symposium will cover the general field of computational materials science and electronic-structure theory.

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Time: Monday 10:30–13:00 Location: HL 001

MM 6.1 Mon 10:30 HL 001

How Derivative Discontinuities in the Energy Yield Interatomic Steps in the Exact Kohn-Sham Potential of Density-Functional Theory — •Eli Kraisler[1], Matthew J. P. Hodgson[1], Axel Schild[2], and Eberhard K.U. Gross[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [2]Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland — [3]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Israel

Accurate density-functional calculations hinge on reliable approximations to the unknown exchange-correlation (xc) potential. The most popular approximations usually lack features of the exact xc potential that are important for an accurate prediction of the fundamental gap and the distribution of charge in complex systems. Two principal features in this regard are the spatially uniform shift in the potential, as the number of electrons infinitesimally surpasses an integer, and the spatial steps that form, e.g., between the atoms of stretched molecules. Although both aforementioned concepts are well-known, the exact relationship between them remained unclear. In this talk, we establish this relationship and introduce a new concept: the charge-transfer derivative discontinuity, Δ^{CT}. By numerically solving the many-electron Schrödinger equation, we extract the exact Kohn-Sham potential and directly observe its features, particularly the spatial interatomic steps. For the first time, spatial steps in the exact xc potential of a full configuration-interaction (FCI) calculation of a molecule are presented in three dimensions.

MM 6.2 Mon 10:45 HL 001

Steps in the exact Kohn-Sham potential of ensemble density-functional theory for excited states and their relation to the derivative discontinuity — •Matthew J. P. Hodgson[1], Eli Kraisler[1], Michael T. Entwistle[2], Axel Schild[3], and Eberhard K. U. Gross[1,4] — [1]MPI für Mikrostrukturphysik, D-06120 Halle, Germany — [2]Dep. of Physics, Uni. of York, Heslington, YO10 5DD, UK — [3]Lab. für Physikalische Chemie, ETH Zürich, 8093, Switzerland — [4]Fritz Haber Center for Molecular Dynamics, The Hebrew University of Jerusalem, 91904, Israel

An accurate approximation to the exchange-correlation (xc) part of the Kohn-Sham (KS) potential is essential for any density-functional calculation. Understanding the behaviour of the exact xc potential and developing improved approximations to it are crucial. The focus of calculations within density functional theory is usually on the ground state. However, knowledge of how the system responds to an excitation is important. In this talk we present the exact KS potential of an ensemble of the ground state and the first excited state of a 1D diatomic molecule. For this system, upon excitation, a small amount of charge transfers from one atom to the other. In the corresponding exact ensemble xc potential we find two plateaus: one that forms around the nucleus of the acceptor atom, associated with the derivative discontinuity of that atom, and another that forms around the donor atom and corresponds to a new phenomenon which we term the 'charge-transfer derivative discontinuity'.

MM 6.3 Mon 11:00 HL 001

Koopmans-compliant functionals: A reliable and efficient tool for the prediction of spectroscopic quantities — •Nicola Colonna[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], and Nicola Marzari[1] — [1]THEOS and MARVEL, EPFL, Lausanne, Switzerland — [2]Centro S3, CNR-Istituto Nanoscienze, Modena, Italy

Commonly used approximate density functionals produce total energies that do not exhibit the expected piecewise-linear behavior as a function of the particle number, leading to a discrepancy between total and partial electron removal/addition energies and poor predictive capabilities of ionization potentials. Koopmans-compliant functionals enforce a generalized criterion of piecewise linearity in the energy of any approximate density functional with respect to the partial removal/addition of an electron - i.e., with respect to charged excitations - from/to any orbital of the system. When used to purify approximate density functionals, Koopmans' corrections lead to orbital-density dependent functionals and potentials that are able to deliver accurate spectroscopic properties. As an example, ionization potentials of a large set of molecules (the GW100 test set), photoemission spectra of organic donors and acceptors and band gaps of 35 semiconductors and insulators are presented, showing very good agreement with experiment or higher-order theories. Being this a functional framework, the straightforward advantages are that forces and other derivatives are also readily accessible, that the computational costs are much reduced, and the numerical parameters are those typical of DFT calculations.

MM 6.4 Mon 11:15 HL 001

Selfconsitent density embedding - a new class of functionals for DFT — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new technique to find functionals for density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

The proposed density-embedding scheme serves as functional in DFT, which, unlike in usual DFT, can be systematically improved by increasing the size of the active space.

We show convergence toward exact results for 1D systems as well as results for 2D systems.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

MM 6.5 Mon 11:30 HL 001

Pressure dependence of the effective screened Coulomb interactions in transition metal monoxides — •Swarup Kumar Panda[1], Hong Jiang[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, France — [2]College of Chemistry and Molecular Engineering, Peking University, China — [3]Collège de France, Paris, France

In transition metal compounds, the magnitudes of the effective Coulomb interaction parameters (Hubbard U) and their pressure dependence are of utmost importance in any realistic many-body simulations for describing their pressure driven insulator-metal transition. One of the powerful methods for calculating the Hubbard U from first principles is based on linear response theory within the constrained random-phase approximation (cRPA) [1], which provides the full U matrix including off-site elements and its frequency dependence. In this presentation, we apply this method (in its implementation into the Wien2k code [2]) to the transition metal monoxides (FeO, CoO, NiO, and CuO) [3]. Although the pressure induced changes in the bare Coulomb interactions are negligible, the effective screened U grows monotonically with increasing pressure for all of the above monoxides. Finally, I will argue that neither the pressure dependence nor the frequency dependence of U should be ignored in a reliable theoretical description of correlated oxides.

References: [1] Aryasetiawan et al., PRB 70, 195104 (2004) [2] Vaugier et al., PRB 86, 165105 (2012) [3] Panda et al., PRB 96, 045137 (2017)

MM 6.6 Mon 11:45 HL 001

Self-Interaction Corrected SCAN for Molecules: All-Electron Implementation with Numerical Atom-Centered Basis Functions — •Sheng Bi, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The self-interaction error (SIE) is a well-known problem in all semilocal density-functional approximations (DFAs), including the recently proposed "strongly constrained and appropriately normed" (SCAN) functional [1]. The so-called self-consistent Fermi-orbital SIC (FSIC) algorithm proposed by Pederson *et al.* [2] shows promising potential to eliminate the self-interaction error in semilocal approximations, which has been demonstrated for the local-spin-density approximation (LSDA) in a study of molecules.

We present an all-electron implementation of the self-consistent FSIC approach on the SCAN method [1]. Beside a systematic benchmark with respect to a selected molecular test set, we examine the performance of FSIC-SCAN in predicting the geometry of Pentacene, which is a well-documented challenge for standard semilocal DFAs [3]. Finally, we briefly discuss our ongoing work concerned with the implementation of the all-electron FSIC-SCAN approach for solids.

[1] J. Sun, A. Ruzsinszky, and J. P. Perdew, *Phys. Rev. Lett.* **115**, 036402 (2015).

[2] M. R. Pederson and T. Baruah, *Advances In Atomic, Molecular, and Optical Physics* **64**, 153 (2015).

[3] M. R. Pederson, T. Baruah, D. you Kao, and L. Basurto, *The Journal of Chemical Physics* **144**, 164117 (2016).

MM 6.7 Mon 12:00 HL 001

Progress in Fermi-Löwdin orbital self-interaction correction to DFT — •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Mark Pederson[2], and Jens Kortus[1] — [1]TU Freiberg, Institute for Theoretical Physics, Germany — [2]Johns Hopkins University, Department of Chemistry, USA

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. We present the current state of the method and discuss the performance of FLO-SIC DFT applied to atoms and molecules in combination with different exchange-correlation functionals. In addition, this method delivers a description of the chemical bonding as intuitive as Lewis theory that may bridge the gap between DFT and chemical intuition.

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)

[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)

[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)

[4] T. Hahn et. al., J. Chem. Phys., vol- 143, 224104 (2015)

MM 6.8 Mon 12:15 HL 001

First-principles modeling of mixed-valence compounds from extended Hubbard-corrected functionals — •Matteo Cococcioni and Nicola Marzari — Theory and Simulations of Materials and MARVEL, EPFL, Lausanne, Switzerland

Modeling the electronic properties of mixed valence compounds is central to developing many materials of technological relevance. Unfortunately, most approximate implementations of density functional theory (DFT) fail in capturing the localization of valence electrons on low dispersion states (e.g., of d or f kind) and mis-represent many properties of these systems. Quantitatively predictive first-principles calculations thus require, for these systems, the use of corrective functionals able to improve the description of electronic localization. Using the results of a recent study on materials for cathodes of Li-ion batteries this work shows how an extended Hubbard correction to DFT functionals, including on-site (U) and inter-site (V) interactions (named DFT+U+V) improves considerably on simpler approximations for electronic, magnetic and structural properties and correctly describes localized states even in presence of significant inter-site hybridization. The work also demonstrates that evaluating the effective interaction parameters (U and V) consistently with the electronic and crystal structures, and treating them as material-specific quantities, improves the prediction of thermodynamic quantities and of average voltages. Finally, a novel method to compute these interactions from density-functional perturbation theory is shown to guarantee unprecedented efficiency, accuracy and convergence control.

MM 6.9 Mon 12:30 HL 001

A Kohn-Sham type construction on a lattice with the exact kinetic energy density — •Iris Theophilou[1], Michael Ruggenthaler[1], Florian Buchholz[1], Florian Eich[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In this presentation we explore a possible formulation of ground state Density Functional Theory by introducing the kinetic energy density as basic quantity in addition to the density. We presently restrict this formulation to the lattice case, and show that for a few site Hubbard interacting model it is numerically feasible to find an equivalent non-interacting system that yields the same density and kinetic energy density. By finding such a non-interacting system we mean here finding the local/on site potential and the non-local site dependent hopping that will give the target density and kinetic energy density. Our hope is that by including the kinetic energy density we will facilitate the functional construction and also put into grounds already existing approximations based on this quantity.

MM 6.10 Mon 12:45 HL 001

Small-Polaron Formation in Polymorphs of Ga_2O_3 and TiO_2 — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin 14195, Germany

Transparent oxides are key materials for new devices in photovoltaics and electronics. One important factor influencing the behavior of charge carriers in these materials is the interaction with polar phonon modes. We focus on materials with strong electron-phonon coupling, where small polarons are formed. Although, density-functional theory (DFT) is often used for calculating polaron properties, there are two challenges: Sensitivity of the calculated properties to the errors in exchange-correlation treatment, and finite-size effects in supercell calculations. We have developed an approach [1] to address these issues. The polaron properties are obtained using a modified neutral potential-energy surface from DFT [2]. Based on Pekar′s model [3], we correct for the proper elastic long-range behavior of the polaron in a supercell. With this approach, the influence of the crystal structure on the polaron properties is investigated for rutile and anatase TiO_2, and for the monoclinic β– and orthorhombic ε–Ga_2O_3. We find that in rutile TiO_2 only small electron polarons are stable, while only small hole polarons are found in anatase. On the contrary, small hole polarons exist in both Ga_2O_3 polymorphs but have significantly different binding energies.

[1] S. Kokott, arXiv:1710.03722 (2017)

[2] B. Sadigh et al., Phys. Rev. B **92**, 75202 (2015)

[3] S. I. Pekar, Zh. Eksp. Teor. Fiz. **16** 335 (1946)

MM 7: Battery Materials

Advanced Magnetic Resonance

Time: Monday 11:45–13:00 Location: H 0106

MM 7.1 Mon 11:45 H 0106

NMR studies on ion dynamics in solid electrolytes for Li-ion batteries — •Edda Klotz[1], Stefan Spannenberger[2], Michael Haaks[1], Bernhard Roling[2], and Michael Vogel[1] — [1]Condensed Matter Physics, TU Darmstadt, Germany — [2]Department of Chemistry, University of Marburg, Germany

In order to improve safety, lifetime, and energy density in batteries, all-solid state ion batteries are of great significance in modern-day research. One of their key components are solid electrolytes with high ionic conductivities. In this area, various materials based on Li^+-ions as well as Na^+-ions have been investigated and found to have the potential to outperform the liquid electrolytes currently used in ion batteries.

The improvement of those materials depends directly on understanding the ion dynamics that determine the ion conductivity. By combining various NMR techniques such as spin-lattice relaxation, stimulated-echo and line-shape analysis, we are able to investigate local ion dynamics in a broad time range. Additionally, self-diffusion coefficients are determined using static field gradient NMR (SFG). We apply those methods to investigate the effects of ceramization in glassy Li-ion conductors [1]. We show that local dynamics and macroscopic diffusion can be consistently described by the same broad distributions of activation energies.

[1] Haaks et al., Phys. Rev. B 96, 104301 (2017)

MM 7.2 Mon 12:00 H 0106

Theoretical simulation of Li solid-state NMR in battery research — •Simone Köcher[1,2], Josef Granwehr[1], Rüdiger-A. Eichel[1], Karsten Reuter[2], and Christoph Scheurer[2] — [1]IEK-9 - Fundamental Electrochemistry, Forschungszentrum Jülich, Jülich, Germany — [2]Chair for Theoretical Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

Nuclear Magnetic Resonance (NMR) spectroscopy is a powerful tool to gain detailed understanding of the ionic mobility in battery materials. Notwithstanding, configurational disorder and ionic dynamics increase the complexity and ambiguity of experimental spectra of Li ion electrode materials. Support by independent first-principles based calculations is indispensable to achieve an unambigious interpretation. For correlating theoretically calculated magnetic resonance parameters with experiments, an accurate reference scale of different lithium compounds is required. We establish this reference scale through density-functional theory (DFT) calculations of chemical shifts for ideal periodic lithium salts with a focus on the influence of geometry, relativistic effects and computational method on the calculated chemical shieldings. For the novel high-capacitance electrode material $Li_4Ti_5O_{12}$ (LTO), we discuss ^{6}Li magic angle spinning (MAS) NMR and ^{7}Li spin-alignment echo NMR studies. The impact of ionic motion and configurational space is studied.

MM 7.3 Mon 12:15 H 0106

Nuclear Magnetic Resonance measurements on layered chalcogenides LiCu*Ch* (*Ch* = Se, Te) — •Lena Spillecke[1], Martin Valldor[1], Daria Mikhailova[1], Lars Giebeler[1], Kwing-To Lai[2], Hans-Joachim Grafe[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Department of Physics, The Chinese University of Hong Kong, Shatin, Hong Kong, Republic of China

Nuclear Magnetic Resonance (NMR) measurements were performed on the two novel chalcogenide compounds LiCuCh (Ch = Se, Te). These layered transition metal compounds are isostructural to anti-PbClF and, thus, also isostructural to the superconducting LiFeAs compound. Several Li containing transition metal compounds have recently become a focus of research interest because of their expected performance in electrochemical battery cells. Hence, temperature dependent measurements of the spin-lattice (T_1) and spin-spin (T_2) relaxation times on the ^7Li and the ^{63}Cu-site of the LiCuCh compounds were performed to investigate ^{7}Li mobility and structural changes. In LiCuTe the diffusion of ^{7}Li-atoms set in at a temperature of 302K, corresponding to an activation energy of 0.49 eV. The activation energy can be extracted separately from T_1, T_2 and linewidth measurements. Furthermore, LiCuTe and LiCuSe show two inequivalent ^{7}Li-sites which can be recognized from two differing spin-lattice relaxation times as well as from two observable peak-positions in the NMR-spectra, which is unexpected based on x-ray diffraction data.

MM 7.4 Mon 12:30 H 0106

In-operando EPR spectroscopy of lithium ion batteries — •Arvid Niemöller, Peter Jakes, Svitlana Eurich, Anja Paulus, Hans Kungl, Rüdiger-A. Eichel, and Josef Granwehr — Forschungszentrum Jülich GmbH, Institut für Energie- und Klimaforschung (IEK-9), 52425 Jülich, Germany

Redox mechanisms in battery cathode materials are challenging to be identified. Despite investigations using a wide range of different experimental techniques, exact mechanisms on atomic scales are still not well understood for many classes of materials. In-operando electron paramagnetic resonance (EPR) is a recently introduced technique with the potential to shed new light on oxidation states of transition metal ions in battery cathode materials. An electrochemical flat cell was developed that matches the requirements of the EPR spectrometer. It was used to cycle a LiNi0.5Mn1.5O4 (LNMO) spinel cathode vs. lithium metal over 500 hours, proving the functionality and stability of the cell setup. EPR spectra show a broad LNMO EPR signal with weak amplitude that was recorded with sufficiently high sensitivity to unravel oxidation mechanisms in the cathode material during battery cycling. These results are compared with ex-situ SQUID measurements. In addition, the EPR linewidth varied continuously with the state of charge, suggesting the formation of a solid solution for slow cycling and a mixed model of solid solution and two-phase formation for fast cycling rates. Long-term EPR experiments complement the electrochemical measurements, allowing us to deduce a model for long-term material degradation of LNMO during battery cycling.

MM 7.5 Mon 12:45 H 0106

Conduction EPR spectroscopy with applied current — •Léonard Kröll[1], Arvid Niemöller[1], Peter Jakes[1], Josef Granwehr[1,2], and Rüdiger-A. Eichel[1,3] — [1]Institute of Energy and Climate Research - Fundamental Electrochemistry (IEK-9), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Technische und Makromolekulare Chemie (ITMC), RWTH Aachen University, 52056 Aachen, Germany — [3]Institut für physikalische Chemie (IPC), RWTH Aachen University, 52074 Aachen, Germany

The EPR signal evolution of a metallic lithium sample under a direct current (DC) has been investigated. The data show a significant change of the EPR signal. The Dysonian signal splits up at a threshold value resulting in two peaks with lower intensities.

Theoretical considerations show that the observation arises from the magnetic field induced by the DC. This field B_j interacts with the magnetization generating spins in two ways depending on the position of the spins in the sample. Firstly, B_j in- or decreases the main field B_0 leading to two peaks. Secondly, the interaction field B_1, which induces the spin flips, is modified. The direction of the DC determines if the on- or the off-resonance part of B_1 is increased by B_j. In the first case the spin flipping process is strengthen, whereas in the second case it is not affected. Both factors together leads to an asymmetry in the signal originated by the direction of the DC.

In order to allow a comparison of the measured with the calculated data, the effect of the diffusion of the spin carrying electrons in the metal has to be incorporated. The results are shown within this work.

MM 8: Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales

Plasticity: Modelling

Time: Monday 11:45–13:15 Location: TC 006

Topical Talk MM 8.1 Mon 11:45 TC 006

Deformation twinning in nanostructured metallic systems: molecular dynamics study — •Sandrine Brochard, Romuald Béjaud, and Julien Durinck — Institut PPRIME - Poitiers-Futuroscope - France

At the nanoscale, mechanical twinning seems to be promoted, as shown e.g. in thin films or nanocrystalline materials. This trend is also true for metallic nanolayered composites obtained by severe plastic deformation processes. In such materials, interfaces may act as partial dislocation and deformation twin sources, and the interfaces structure is expected to have a key role in twin propagation and thickening.

In this study, we investigate how different interface types influence the main stages of mechanical twinning. Because of the small length and times scales at which the elementary plasticity mechanisms involved occur, molecular dynamics simulations prove to be relevant and efficient tools.

Heterophase interfaces in a bimetallic Cu/Ag system, as well as a coherent twin boundary (CTB), are examined in a similar thin film geometry. A reference case with no planar defect inside the thin film is also considered. For both systems with "heterotwin" heterophase interface and CTB, the deformation twins are smaller, consistent with the low permeability of these interfaces to dislocations. But twins are more numerous, which is correlated to Lomer dislocation nucleation. For the Cu/Ag film with a "cube on cube" type interface, our simulations reveal the specific role of the misfit dislocation mesh in twin extension from the interface.

MM 8.2 Mon 12:15 TC 006

Multi-scale modeling of dislocations behavior in molybdenum — •Sergei Starikov[1,2] and Vasily Tseplyaev[1] — [1]Joint Institute for High Temperatures, Moscow, Russia — [2]ICAMS, Ruhr-Universität Bochum, Germany

Various types of computer simulation were performed for study of dislocations behavior in molybdenum. Molybdenum is typical body-centered cubic metal and such study allows to understand basic properties of plasticity in bcc metals. Multi-scale approach consists from combination of different methods which one calculates properties at various scales. We used three different models: development of an interatomic potential on the basis of ab-initio calculations; molecular dynamics simulations; dislocation dynamics. Such multi-scale approach allows us to investigate the dislocation properties in molybdenum and compare the simulation results with the available experimental data. Particular attention is given to the link between models at various scales and calculations of macroscopic features (like stress-strain curve).

MM 8.3 Mon 12:30 TC 006

Atomistic simulations of the mechanical behavior of semiconductor and metallic nanoparticles — Dimitrios Kilymis[1], Sélim Bel Haj Salah[1], Céline Gérard[1], Jonathan Amodeo[2], and •Laurent Pizzagalli[1] — [1]Institut Pprime, CNRS UPR 3346, Université de Poitiers, Poitiers, 86962, France — [2]MATEIS, CNRS UMR 5510, INSA-Lyon Université 1, Villeurbanne, 69621, France

We present the results of molecular dynamics simulations of the mechanical properties of semiconductor and metallic nanoparticles. The aim of the study is to investigate the first stages of plasticity during uniaxial compression while focusing on the influence of the shape (spherical, or facetted, or cubic geometries) and size (from 10 to 50 nm). The nanoparticles are deformed at a constant velocity using flat punch indenters, along different orientations in most of cases. We fully characterize the onset of plasticity, both in terms of yield point and of mechanisms, and examine how those depend on the size and the shape of the nanoparticle. The influence of temperature is also considered. In the case of semiconductor nanoparticles, original plasticity mechanisms are identified, including V-shaped dislocations and an hexagonal phase transition of limited extent. Conversely, for metallic systems, the first plasticity mechanisms are similar to the ones usually activated in bulk. In both cases, it is found that both size and shape effects are significant for the investigated systems.

MM 8.4 Mon 12:45 TC 006

Effect of hard amorphous shell on gold nanowire during mechanical cycling — •Maxime Guillotte, Laurent Pizzagalli, and Julien Godet — Pprime Institute, CNRS, University of Poitiers - France

In order to evaluate the role of a hard amorphous silicon (a-Si) shell on the deformation of a soft crystalline gold core, we have investigated the mechanical properties under tensile and compressive cycling of the Au@a-Si core-shell nanowire (NW) by molecular dynamics simulations. We used an existing parametrization of the MEAM potential that has been optimized to better reproduce the mechanical properties of gold and silicon as well as the Au-Si interactions. The comparison of the mechanical tests performed on pristine Au NW and Au@a-Si core-shell NW reveals that the hard amorphous shell is able to confine the plasticity inside de core. In consequence, the localized plasticity and the expansion of nano-twin are reduced. The confinement of the dislocations in the core also leads to a homogeneous plastic deformation of the core-shell nanowire at almost constant flow stress equal to the yield stress up to a strain of 50%. This behavior is characteristic of an elastic/perfect-plastic mechanical regime. During the cycling tests, it also seems that the hard amorphous shell is is at the origin of the recovery of the FCC core.

MM 8.5 Mon 13:00 TC 006

Plasticity of silicon at small scale and low temperature: an experimental and numerical study — •Michael Texier[1], Amina Merabet[1], Firas Abed El Nabi[2], Christophe Tromas[2], Sandrine Brochard[2], Laurent Pizzagalli[2], Ludovic Thilly[2], Jacques Rabier[2], Anne Talneau[3], Olivier Thomas[1], and Julien Godet[2] — [1]IM2NP, UMR7334 CNRS - Univ. Aix-Marseille, Marseille, FR — [2]Pprime, UPR3346 CNRS - Univ. Poitiers, Futuroscope, FR — [3]C2N, Univ. Paris Sud, Orsay, FR

Mechanical properties of silicon have been widely studied in the last decades, but recent studies evidenced that silicon nano-objects behave differently than bulk materials when submitted to mechanical stress. Indeed, for dimensions below a few hundreds of nanometres, a brittle-to-ductile transition (BDT) occurs at room temperature and its origin remains undetermined. Although essential for the Si-based nanotechnologies, the understanding of the microscopic mechanisms responsible for this behavioural change requires to compare results obtained from well-controlled deformation experiments at smallest scales with realistic numerical simulations. In this work, both experimental and numerical nano-compression tests were carried out on similar Si nanopillars. Results obtained from simulations and HRTEM analyses of the deformed specimen disrupt the established description of undissociated-dislocations-mediated plasticity of silicon at low temperatures. This study allows deeply reinterpreting the experimental data recently reported in the literature, and highlights the intricate relationship between BDT, dislocation interactions, and size effect.

MM 9: Invited talk Ponson

Time: Monday 15:00–15:30 Location: TC 006

Invited Talk MM 9.1 Mon 15:00 TC 006

Deciphering fracture patterns: what crack paths teach us about the mechanics and physics of fracture — •Laurent Ponson — Institut Jean le Rond d'Alembert, CNRS, Paris - France

Cracks follow intriguing trajectories that seem to hide a mysterious secret. Ancient Chinese civilization interpreted the tortuous path of cracks in turtle shells as an oracle to foresee the future. Nowadays, fractography, the study of fracture surfaces, is a broadly used engineering technique that aims at tracing back the history of a failure and determining its root causes. For 30 years, the study of fracture patterns has taken a new turn: could we learn from the morphology of cracks the fundamental laws of fracture? During this presentation, I will present some remarkable advances in the understanding of fracture patterns and I will explain how they challenge the current theory of fracture and, in fine, contribute to improve it. I will first discuss how to decipher triangular patterns observed on fracture surfaces of polymeric solids and why it contributed to understand on how tensile cracks behave in presence of shear. Then, I will focus on crack roughness that is the fingerprint of the interaction of cracks with the microstructure of materials. I will present how their statistical properties reveal basic crack growth mechanisms, leading us to revisit, and even reconcile, the concepts of ductile and brittle failure. Last but not least, I will discuss some implications for engineering sciences. Even though the analysis of fracture patterns still does help to foresee the future, it can now be used to trace back the history of the failure and characterize material properties with unprecedented accuracy and reliability.

MM 10: Battery Materials

Theory

Time: Monday 15:45–17:00 Location: H 0106

MM 10.1 Mon 15:45 H 0106

Exploring structure and conductivity of the lithium superionic conductors $Li_{10}GeP_2O/S_{12}$: a first-principles molecular dynamics study — •Giuliana Materzanini[1], Leonid Kahle[1], Aris Marcolongo[1,2], and Nicola Marzari[1] — [1]Theory and Simulations of Materials (THEOS), EPFL, Lausanne, Switzerland — [2]IBM RSM Zurich Research Laboratory, Zurich, Switzerland

With the aim of finding superior lithium-ion conducting solids to replace the highly reactive liquid electrolytes typically used in rechargeable batteries, Lisicon-type materials (with orthorhombic or monoclinic cells) have been extensively studied in the last decades. Recently, following the experimental discovery of a highly conductive tetragonal phase for the thio-Lisicon $Li_{10}GeP_2S_{12}$, a theoretical study predicted the same phase for $Li_{10}GeP_2O_{12}$ to be poorly conducting. In this work we address the conductivity of $Li_{10}GeP_2O_{12}$ and $Li_{10}GeP_2S_{12}$ through Car-Parrinello molecular dynamics, tuned to achieve an optimal thermalization between the heavy species and the light Li ions. The simulations feature extended thermostatted thermalization followed by microcanonical evolution. Last, NPT variable cell dynamics simulations within the Parrinello-Rahman scheme were also performed to complete exploration of the configurational space, since in these superionic materials there is not a corresponding unique ground state structure. A thorough analysis of the conducting performance for the oxide and the sulphide is presented.

MM 10.2 Mon 16:00 H 0106

Superionic diffusion through frustrated energy landscape — •Davide Di Stefano[1], Anna Miglio[1], Koen Robeyns[1], Yaroslav Filinchuk[1], Marine Lechartier[2], Anatoliy Senyshyn[3], Hiroyuki Ishida[4], Stefan Spannenberger[5], Denise Prutsch[6], Daniel Rettenwander[6], Martin Wilkening[6], Bernhard Roling[5], Yuki Katoh[2], and Geoffroy Hautier[1] — [1]Université catholique de Louvain, Louvain-la-Neuve, Belgium — [2]Toyota Motor Europe NV/SA, Zaventem, Belgium. — [3]Technische Universität München, Garching, Germany — [4]Toray Research Center, Inc., Otsu, Japan — [5]ilipps-Universität Marburg, Marburg, Germany — [6]Graz University of Technology, Graz, Austria

Solid-state materials with extremely high ionic diffusion are necessary to many technologies including all-solid-state Li-ion batteries. Despite the efforts made towards the identification of crystal structures leading high lithium diffusion, only a handful crystalline structure families have been reported as Li superionic conductors.

In this work, we demonstrate that LiTi2(PS4)3, or LTPS, shows exceptional Li-ion diffusion about an order of magnitude higher than current state-of-the-art superionic conductors. By means of extensive theoretical studies through ab initio molecular dynamics (backed up by several experimental characterization), we also rationalize the exceptional performances of this new superionic conductor through the concept of frustrated energy landscape.

Our work sheds light on a new family of superionic conductors and also offers a new design principle for discovering new ones.

MM 10.3 Mon 16:15 H 0106

Modeling Li_3OCl glass-electrolytes for all-solid-state Li ion batteries — •Hendrik H. Heenen[1], Johannes Voss[2], Christoph Scheurer[1], Alan C. Luntz[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]SLAC National Accelerator Laboratory, USA

All-solid-state Li ion batteries are facilitated by using glass superionic electrolytes that combine very high Li ion conductivity and mechanical ductility. One material that has attracted much excitement is the recently reported glass-amorphous Li_3OCl. Already a superionic conductor in its crystalline form, a glass transition increases its room temperature conductivity by an order of magnitude to an outstanding 25 mS cm^{-1} [1]. The elevated mobility likely originates from a lowered density of the liquid-like glass structure for which the ion transport mechanism has however not yet been elucidated. Based on a classical force-field [2] we explore Li_3OCl glass structures in simulation cells large enough to account adequately for long-range disorder. Via systematic melt-quench procedures qualitatively different glass ensembles are created allowing for structural heterogeneity. We use molecular dynamics simulations to analyze the ion mobility with emphasis on clarifying the influence of the structural relaxation associated with the glass transition.

[1] M.H. Braga, *et al.*, J. Mater. Chem. A **2**, 5470 (2014)
[2] R. Mouta, *et al.*, Chem. Mater. **26**, 7137 (2014)

MM 10.4 Mon 16:30 H 0106

Understanding Cation-Disordered Cathode Materials — •Alexander Urban — University of St Andrews, Scotland, UK — University of California, Berkeley, USA

Cation-disordered transition-metal (TM) oxides have recently emerged as a new class of high-energy-density cathode materials for Li-ion batteries [1]. We previously showed that the practical capacity of disordered cathodes can be well estimated using percolation theory [2] and that high-throughput (HT) first principles calculations can be used to screen for novel materials in well-defined composition spaces [3]. However, apart from HT calculations, the discovery of novel disordered materials has mostly been guided by intuition.

Here, we combine a normal-mode analysis of TM site distortions with a tight-binding model and density-functional theory calculations to identify a specific electronic-structure mechanism that affects cation disorder in TM oxides. We show that d^0 TM species (Ti^{4+}, Nb^{5+}, Mo^{6+}, etc.) promote disordering, whereas TMs with other d-band fillings, especially d^6 TMs (e.g., Co^{3+}), destabilize the disordered phase [4]. This mechanism explains the stability of the known disordered cathodes and provides a simple guideline for the design of novel disordered compositions.

[1] Lee, Urban, Li, Su, Hautier, Ceder, *Science* **343** (2014) 519–522. [2] Urban, Lee, Ceder, *Adv. Energy Mater.* **4** (2014) 1400478. [3] Ur-

ban, Matts, Abdellahi, Ceder, *Adv. Energy Mater.* **6** (2016) 1600488. [4] Urban, Abdellahi, Dacek, Artrith, Ceder, *Phys. Rev. Lett.* **119** (2017) 176402.

MM 10.5 Mon 16:45 H 0106

Interfacial challenges in solid-state Li-ion batteries: Towards multiscale simulations of working interfaces — •Simon P. Rittmeyer[1], Josef Granwehr[2], Christoph Scheurer[1], and Karsten Reuter[1] — [1]Theoretische Chemie, TU München — [2]IEK-9, Forschungszentrum Jülich

The concept of an all-solid-state battery promises gains in safety and durability beyond the current generation of Li-ion batteries. While solid-state electrolytes with sufficient ion conductivity measured under idealized conditions have recently been introduced, a thorough microscopic understanding of the involved ion transport processes, in particular at and across the interface regions associated with grain boundaries, is still lacking. In a recent electrochemical impedance spectroscopy (EIS) and microscopy (LSM, SEM, AFM) study [1], mobilities in the highly conductive LATP battery material could be correlated with bulk and interfacial structural motifs. Rational material improvement based on explicit ion dynamics simulations, however, requires detailed atomistic structures for bulk and interfaces not directly accessible from these experiments. We thus present our recent combined experimental and theoretical efforts based on a newly parametrized polarizable force field for LATP. Following the spirit of *ab initio* structure prediction, this allows us to develop an atomistic structural model of the corresponding interface regions. We further give a perspective on how to improve our sampling scheme by introducing high-resolution TEM images into an experiment-assisted score function.
[1] A. Mertens *et al.*, Solid State Ionics **309**, 180 (2017).

MM 11: Topical session (Symposium MM): Hydrogen in Materials

Hydrogen interactions with materials surfaces (catalysts)

Time: Monday 15:45–17:00 Location: H 0107

Topical Talk MM 11.1 Mon 15:45 H 0107

Hydrogen transportation across palladium surfaces: Microscopic mechanism and control — •Markus Wilde, Satoshi Ohno, and Katsuyuki Fukutani — Institute of Industrial Science, The University of Tokyo, 153-8505 Tokyo, Japan

The ingress of H_2 into and the release of H_2 from the interior of H-absorbing metals, widely utilized in metal hydride storage, H_2 purification, and Pd-catalyzed C=C hydrogenation [1], still lacks atomic-level understanding. We here clarify the H_2 absorption mechanism at Pd single crystal surfaces through a unique combination of H depth profiling with ^{15}N nuclear reaction analysis [2] and thermal desorption spectroscopy. We resolve the long-standing paradox that although chemisorbed surface H is predominantly transferred into the Pd interior, the large potential energy difference between surface H and H in the Pd bulk does not materialize in the activation energy for H_2 absorption [3]. In contrast to Pd(100) and Pd(111), both defects and regular terrace sites of Pd(110) are active for H_2 absorption, implying that the H_2 absorption kinetics are sensitive to the surface 'openness'. Moreover, by manipulating the surface structure of Pd(110) through CO-induced (de-)reconstructions, we demonstrate the possibility to control the desorption dynamics of Pd-dissolved hydrogen in a wide range of temperatures (160-375 K) [4].

[1] M. Wilde, et al., Angew. Chem. Int. Ed. 47 , 9289 (2008) [2] M. Wilde, K. Fukutani, Surf. Sci. Rep. 69, 196 (2014) [3] S. Ohno, et al., J. Chem. Phys. 140, 134705 (2014) [4] S. Ohno, et al., J. Phys. Chem. C 119, 11732 (2015).

Topical Talk MM 11.2 Mon 16:15 H 0107

Hydrogen interaction with metal substrates studied from first principles — •Axel Gross — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

The interaction of hydrogen with metals is of great technological importance in different areas such as hydrogen storage or H_2 production and heterogeneous catalysis. First-principles electronic structure calculations based on density functional theory (DFT) represent a reliable tool to elucidate atomistic details of the structures and processes resulting upon the hydrogen-metal interaction, but also to identify the underlying electronic factors determining the interaction strength. In this talk, I will illustrate this using several examples.

The subsurface penetration of hydrogen on precovered surfaces has been studied using ab initio molecular dynamics simulations [1] showing that concerted processes can significantly ease the absorption of hydrogen. It will furthermore be shown how the interaction of hydrogen with metal surfaces can be tuned by changing the structure and/or composition of bimetallic surfaces [2]. Finally, I will also briefly sketch the important role of metal-hydrogen interactions at electrochemical interfaces relevant for energy storage and conversion [3].
[1] S. Sakong, C. Mosch, A. Lozano, H.F. Busnengo, and A. Groß, ChemPhysChem **13**, 3467 (2012).
[2] S. Sakong, J.M. Fischer, D. Mahlberg, R.J. Behm and A Groß, Electrocatal. **13**, 530 (2017).
[3] A. Groß, F. Gossenberger, X. Lin, M. Naderian, S. Sakong, and T. Roman, J. Electrochem. Soc. **161**, E3015 (2014).

MM 11.3 Mon 16:45 H 0107

First-principles study of hydrogen related defects in titanium dioxide — •Mohsen Sotoudeh[1], Marian Bongers[2], Vladimir Roddatis[2], Jakub Čížek[3], Carsten Nowak[2], Martin Wenderoth[4], Peter Blöchl[1,2], and Astrid Pundt[2] — [1]Institute for Theoretical Physics, Clausthal University of Technology, Leibnizstr. 10, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Department of Low-temperature Physics, Charles University in Prague, V Holešovičkách 2, 18000 Praha 8, Czech Republic — [4]IV. Physikalischen Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Titanium dioxide (rutile) under hydrogen loading has been studied using first-principles calculations. In particular, we studied the defect electrochemistry near the interface with a metal. Defects related to oxygen vacancies and hydrogen have been investigated for different Fermi-levels. The band-gap underestimation in density-functional theory has been corrected. The nature of the electronic structure of the defects have been explored in detail. The defect concentration near the interfaces and their changes under hydrogen loading have been investigated. The calculated defect concentrations and the defect electronic structure explain experimental EELS spectra measured under hydrogen loading. We provide a mechanistic picture of the underlying chemical processes.

The work has been supported by the DFG through SFB 1073, projects B03, C03 and C06 as well via the Heisenberg grant PU131/9-2.

MM 12: Topical Session (Symposium MM): Fundamentals of Fracture

Joint session of Mechanical Properties at Small Scales and Fundamentals of Fracture: Small Scale Fracture Experiments

Fundamentals of Fracture organized by Erik Bitzek (U Erlangen-Nürnberg, Germnany), Sandra Korte-Kerzel (RWTH Aachen University, Germany) and Peter Gumbsch (Fraunhofer Institute for Mechanics of Materials, Freiburg, Germany)

Time: Monday 15:45–17:15 Location: TC 006

Topical Talk MM 12.1 Mon 15:45 TC 006

Microscale Fracture Testing: State of the Art and Future Challenges — •David Armstrong — University of Oxford, Oxford, UK

Over the last 15 years there has been a large increase in the use of microscale fracture tests. This is linked to the increase in availability of focused ion beam systems allowing the manufacture of increasingly complex test geometries and improvements in nanoindetation equipment allowing the testing of smaller and more complex structures. In addition the development of high temperature nanoindentation systems allows for microscale studies of the effects of temperature on fracture behaviour.

This paper will give an overview of the current state of the art in the area of microscale fracture. Specific examples that will be used to demonstrate this will include microscale measurements brittle to ductile transition in tungsten alloys and a comparison of micro and microscale fracture of oxidised grain boundaries in nickel alloys.

Finally some future directions will be suggested for research and to stimulate discussion.

MM 12.2 Mon 16:15 TC 006

Damage in DP Steel - statistical in-situ analysis of brittle and ductile mechanisms prior to the onset of fracture — •Carl F. Kusche[1], Martina Freund[1], Tom Reclik[1], Ulrich Kerzel[2], Talal Al-Samman[1], and Sandra Korte-Kerzel[1] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen, Germany — [2]Lehrstuhl für Operations Research, RWTH Aachen, Germany

For the last years, analysing deformation damage in dual-phase steels has been a well-discussed topic; this is largely due to the ongoing rise in demand for high-strength steels with good ductility, allowing for a further optimization in weight reduction.

To reveal the micromechanical mechanisms of damage, the currently undergone methods of post-mortem analysis as well as in-situ methods deliver an incomplete picture; the first being unable to deliver data for the evolution of damage while classically, in-situ methods being spatially limited to the observation of few damage events. The novel approach in this work combines in-situ observation with an automated recognition and classification of micromechanical damage mechanisms. An algorithm based on machine learning is developed to achieve this methodical expansion, allowing the analysis of large deformed areas while at the same time maintaining spatial resolution. The in-situ experiment is enhanced by the possibility of generating statistically relevant data characterizing the mechanisms of fracture in brittle phases and ductile void formation on the microscale. Thus, exposing the evolution of predominant damage mechanisms during deformation yields a holistic approach to deformation damage.

MM 12.3 Mon 16:30 TC 006

The brittle-ductile transition of tungsten single crystals at the micro-scale — •Johannes Ast, Jakob Schwiedrzik, Juri Wehrs, Johann Michler, and Xavier Maeder — Empa, Swiss Federal Laboratories for Materials Science and Technology, Feuerwerkerstrasse 39, 3602 Thun, Switzerland

Notched micro-cantilevers were prepared by focused ion beam (FIB) milling in a tungsten single crystal. This material has nearly perfect elastic isotropy, a limited amount of activated slip systems and detailed knowledge of the macroscopic fracture behaviour is available. The cantilevers have dimensions of 25 μm in length, 5-7 μm in thickness and crack length to thickness ratios a/w of ca. 0.4. Loading rate and temperature are known to influence the fracture behaviour decisively in bcc metals. Therefore displacement-controlled fracture tests were performed inside a scanning electron microscope in the temperature range between -90°C and 500°C. Applying the J-Integral technique to plot continuous crack resistance curves, the fracture toughness and brittle-to-ductile transition (BDT) temperatures, which depend on the applied loading rate, were determined. This allows a thorough investigation of the activation energy of the BDT at the micro-scale.

MM 12.4 Mon 16:45 TC 006

Influence of pre-deformation on the microscale fracture toughness of bcc-materials — •Stefan Gabel, Merle Benoit, and Mathias Göken — Dapartment of Materials Science and Engineering Institute I - General Materials Properties, Erlangen, Germany

The ductility of bcc-Materials is often insufficient for structural applications at low temperatures. The transition to brittle fracture below a critical temperature is likely caused by two possible mechanisms. Either the dislocation mobility is limited or the nucleation sources cannot be activated. In order to find out, semibrittle materials with dislocation gradients were investigated with microcantilevers.

In order to apply achieve a specific initial dislocation density, indentations were made on a sample surface. The resulting plastic strain field in the material was analyzed by FEM in order to identify areas with homogeneous deformation for fracture tests. The cantilevers for the fracture tests had a diameter of 3000 nm and were milled with a FIB. Testing was achieved by two different approaches. On the one hand an in situ setup with a micromanipulator was used to directly observe crack growth and tip blunting. On the other hand an ex-situ nanoindenter setup was used, which offered better displacement resolution and a larger load range.

The measurements show the dependence of the transition in the fracture behavior on the availability and activity of dislocations sources. Nevertheless the fracture toughness is also dependent on the mobility of dislocations at different temperatures.

MM 12.5 Mon 17:00 TC 006

In Situ TEM and SEM Fracture Experiments at RT — •Inas Issa and Daniel Kiener — Department Materials Physics, Montanuniversitat Leoben, Austria

Among high strength and elastic limit that materials gain when decreasing their volumes to the sub-micron range, they exhibit large plastic deformation under high load. Mechanisms proposed are mainly size, among other parameters, dependent. Fewer studies are dedicated on the investigation of the *intrinsic* size effect on the strengthening of materials, i.e. fracture experiments at RT in the nanoscale. A good knowledge of the critical size for materials strengthening and for BDT of brittle materials, allows better design guideline of more fracture resistant, tough materials and avoid brittle failure of semiconductors used in many advanced microelectronic devices. We present in situ TEM fracture experiments at RT on metallic and semiconductors single crystals nanobending beams of thickness ranging from [70-400] nm. Dislocations activities and characters at the notche zone are investigated. Size effect on notch blunting and increase of fracture toughness is observed. Notches are introduced in TEM and others using Fib. Thus, a comparative study on the notches size effect on fracture toughness measurements is performed. In situ SEM fracture tests on similar but larger metallic samples are performed and on ultrafine grains ones. Thus, the influence of interfaces on the crack propagations is also studied.

MM 13: Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)

Sessions: Magnetism III and Magnetism IV

Time: Monday 15:45–18:45 Location: TC 010

Topical Talk MM 13.1 Mon 15:45 TC 010

Ferromagnetic Nuclear Resonance for studying defects in multilayers and nanocomposites : Structure and magnetic properties — •Christian Mény — IPCMS, 23 rue du loess 67034, Strasbourg, France

Nuclear Magnetic Resonance in Ferromagnets (also called Ferromagnetic Nuclear Resonance, FNR) is a rather unknown technique. However it can give very unique information in the study of defects in ferromagnetic films, multilayers, and nanocomposites. The yield of FNR experiments is twofold. On one hand the FNR spectrum reflects the distribution of hyperfine fields in the sample and thus gives information about the different chemical configurations and site symmetries in the sample,their structure and their defects (stacking faults, impurities, grain boundaries...). On the other hand the evolution of the spectral shape against the FNR radio frequency field strength probes the magnetic stiffness of the electronic moments around the nucleus site thus providing information comparable to that given by ferromagnetic resonance measurements. Therefore, combining both yields makes it possible to correlate the inhomogeneous magnetic properties of a sample to its different structural components and defects. A general presentation of FNR will be given in the first part of the presentation; the second part will be focused on the study of defects in nanostructures.

Reference: Y.F. Liu, , C. Meny; Sampling the structure and chemical order in assemblies of ferromagnetic nanoparticles by Nuclear Magnetic Resonance. Nat. Commun.7, 11532 (2016); and references therein.

MM 13.2 Mon 16:15 TC 010

First-principles study of interface energies in Fe-Al superalloy nanocomposites — •Ivana Miháliková[1,2], Anton Slávik[1,2], Martin Friák[1,2], David Holec[3], Nikola Koutná[1,2,4], Monika Všianská[1,5,6], and Mojmír Šob[5,1,6] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [4]Institute of Materials Science and Technology, TU Wien, Vienna, Austria — [5]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [6]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Fe-Al nanocomposites with a superalloy-type of microstructure possess a great potential as an alternative to the currently used steel grades in high temperature applications. We employ *ab initio* calculations to analyze relations between ordering tendencies of Al atoms in the disordered Fe-18.75at.%Al phase on one hand and thermodynamic, structural and magnetic properties of Fe-Al-based nanocomposites on the other. The Fe-18.75at.%A supercells without 1st and 2nd nearest neighbor Al-Al pairs have a lower energy than those mimicking an ideal disorder (a special quasi-random structure, SQS). The same thermodynamic preference is found also in the case of coherent interfaces with {001}, {011} and {111} crystallographic orientations between Fe$_3$Al compound and Fe-Al phases with different atomic distributions.

MM 13.3 Mon 16:30 TC 010

***Ab initio* study of magnetic states in superalloy nanocomposite phase Fe$_2$AlTi** — •Anton Slávik[1,2], Ivana Miháliková[1,2], Martin Friák[1,2], David Holec[3], Monika Všianská[1,4,5], and Mojmír Šob[4,1,5] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversitaet Leoben, Leoben, Austria — [4]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

The Fe$_2$AlTi intermetallic compound is one of Heusler L2$_1$-structure materials possessing interesting magnetic properties. We study thermodynamic, electronic, structural and elastic properties of different magnetic states in Fe$_2$AlTi by *ab initio* fixed-spin-moment calculations. A spin-polarized ferrimagnetic state with the magnetic moment of 0.925 μ_{B} per formula unit is found to be a stable energy minimum at T=0 K. Interestingly, a non-magnetic state has its total energy only by 10.6 meV/atom higher and, consequently, the lowest energy state is found very sensitive to different perturbations. We discuss this weak stability in the case of fairly high statistical probability of occurrence of the non-magnetic state, trigonal strains (to which Fe$_2$AlTi has a compression-tension asymmetric response), off-stoichiometry and point defects as well as interfaces within Fe-Al-Ti superalloy nanocomposites.

MM 13.4 Mon 16:45 TC 010

Energetics of non-stoichiometric stacking faults in Fe-Nb alloys: An ab initio study — •Ali Zendegani[1], Michaela Šlapáková Poková[2], Christian Liebscher[2], Frank Stein[2], Alvin Noe Collado Ladines[3], Thomas Hammerschmidt[3], Ralf Drautz[3], Fritz Körmann[1], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Charles University, Prague, Czech Republic — [3]ICAMS, Ruhr-Universität Bochum, Bochum, Germany

The microstructure in structural materials plays an essential role for their mechanical properties. In Fe-Nb alloys a hardening via TCP phases (e.g. Laves Fe2Nb and Fe7Nb6) can be achieved. At the same time, various types of stacking faults occur during deformation. In the present work, we investigate the correlation of both features in the C14 Fe2Nb Laves phase. For this purpose, density functional theory calculations are combined with thermodynamics concepts. Particular care has been taken to take atomic relaxation effects and magnetic degrees of freedom into account. We proof that excess Nb will segregate to these planar defects and result in a local phase transformation next to it. The energetics of these structures are compared to the phase separation as predicted by the bulk phase diagram. Comparing our results with high-quality TEM measurements has revealed that some of the complex crystal structures next to basal and pyramidal stacking faults are in a constrained state.

30 min. break

Topical Talk MM 13.5 Mon 17:30 TC 010

Improving the finite-temperature description of magnetic materials — •Anders Bergman — Department of Physics and Astronomy, Uppsala University,Uppsala, Sweden

State-of-the-art simulations based on electronic structure theory and atomistic models have now evolved to a point where computer-guided materials design has become a realistic option for many classes of materials. In this talk we will introduce improvements to the standard description of finite-temperature magnetism with the aim of increasing the predictive capability of these simulations further.

We present an extended atomistic spin model obtained by augmenting the Heisenberg Hamiltonian to take longitudinal fluctuations of the magnetic moments into account. This is done by parametrisation from a first-principles basis, interpolating from low-temperature ferromagnetic and high-temperature paramagnetic reference states. The method gives a good agreement of Curie temperatures and paramagnetic properties compared with experiments as well as similar, earlier theoretical models.

Introducing quantum statistics into atomistic simulations has been shown to improve the observed temperature dependence of the magnetisation and of the magnetic specific heat. This allows for a more realistic modelling of the magnetic contribution to the free energy and thus a better description of phase-stabilities and related properties. We present how the quantum statistics can be modelled with varying levels on complexity and demonstrate the method for both elemental systems and magnetic alloys.

MM 13.6 Mon 18:00 TC 010

Interplay between magnetic and energetic properties in FeMn alloys from first principles — •Anton Schneider[1], Chu Chun Fu[1], Cyrille Barreteau[2], and Frédéric Soisson[1] — [1]CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191 Gif-sur-Yvette, France — [2]CEA, DRF, Service de Physique de l'Etat Condensé, F-91191 Gif-sur-Yvette, France

Iron-based alloys play a central role in several technological applications. In these alloys, the magnetism has an important impact on thermodynamic and kinetic behaviors, and on the properties of point defects. Especially, iron-based alloys may exhibit complex magnetic structures if the magnetic ordering tendency of the alloying element in its pure phase differs from that of iron.

Iron-Manganese bcc alloys are studied using Density Functional Theory (DFT) in order to elucidate the correlation between the magnetic structures, and the energetics of Mn atoms and clusters in the presence of vacancies and interstitial impurities. The FeMn alloys exhibit well distinct magnetic interactions between the Fe atoms and the Mn solutes depending on local chemical environments, which are rationalized in terms of electronic structures. Both low-energy magnetic collinear and non-collinear states are investigated.

The DFT results are then used to parameterize new Heisenberg-like models, in the presence of vacancies, aiming at investigating the finite-temperature magnetic effects employing Monte Carlo simulations. A particular attention is given to the role of magnetic short-range order on the vacancy formation energy, as a function of temperature.

MM 13.7 Mon 18:15 TC 010

Machine Learning assisted Heisenberg model for systems with ill-defined pairwise magnetic interactions — •Osamu Waseda, Omkar Hegde, and Tilmann Hickel — MPIE

Magnetic interactions are important for the stability of structural phases as well as for various thermophysical effects such as magnetocalorics. In order to determine their free energy contribution in Fe-based materials, the Heisenberg model has been used as a handy method for decades. Despite its simplicity, there is little experience with the application of this model to systems containing various types of atoms and/or structural defects, as their interaction parameters cannot be defined straightforwardly. In this study, data sets for Fe-Mn systems containing structural defects are created from spin-polarized DFT calculations. They are then translated into the Heisenberg parameters via Ridge regression. Finally, the contribution of the magnetic interactions to the specific heat is determined through Monte Carlo simulations.

MM 13.8 Mon 18:30 TC 010

Numerical simulation of spin fluctuations in materials science: magnetic bond-order potentials and hybrid Monte Carlo — •Ning Wang, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Bochum, Germany

The finite-temperature properties of many magnetic materials are to a large degree influenced by spin fluctuations. The numerical simulation of these effects, however, faces several obstacles. In particular, the modelling of the magnetic interactions at the quantum-mechanical level should be neither oversimplified nor too computationally expensive. Furthermore, an efficient numerical sampler is required in order to treat the high-dimensional integration problem of the thermal expectation values. Our modelling approach are analytic bond-order potentials based on tight-binding. To treat the sampling problem, we extended the hybrid Monte Carlo sampler so that it will also work for the classical spin system. We furthermore developed an auxiliary-Hamiltonian method in order to improve the sampling efficiency. With this methodology, we simulate the magnetic phase transitions in BCC iron and determine the magnetic free energy difference between the BCC and FCC states of iron.

MM 14: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Monday 15:00–17:15 Location: HL 001

MM 14.1 Mon 15:00 HL 001

Non-adiabatic Dynamics in Single-Electron Tunneling Devices with Time-Dependent Density Functional Theory — •Niklas Dittmann[1,2,3], Janine Splettstoesser[2], and Nicole Helbig[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [2]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Gothenburg, Sweden — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

The recent advance of various single-electron sources in solid-state setups has sparked interest in the investigation of electronic transport at the single-particle level. In our recent work (N. Dittmann, J. Splettstoesser, N. Helbig, arxiv:1706.04547), we put forward time-dependent density-functional theory to calculate the dynamics of interacting electrons in single-electron tunneling devices. As a physical system, we analyze a single-electron source which is built by a quantum dot tunnel-coupled to a nearby electron reservoir and driven by a time-dependent gate voltage. By using analogies with quantum-transport theory, we extract a time-nonlocal exchange-correlation potential for a Hubbard U on-site interaction on the quantum dot. The time nonlocality manifests itself in a dynamical potential step, which we explicitly link to physical relaxation time scales of the electron dynamics. Finally, we discuss prospects for simulations of larger mesoscopic systems.

MM 14.2 Mon 15:15 HL 001

Dissipative exchange-correlation functional in QED-TDDFT — •Camilla Pellegrini[1], Ilya Tokatly[2,3], and Angel Rubio[2,4] — [1]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — [3]IKERBASQUE, Basque Foundation for Science, 48001 Bilbao, Spain — [4]Max Planck Institute for the Structure and the Dynamics of Matter, Luruper Chausse 149, 22761 Hamburg, Germany

Time-dependent density functional theory has been recently extended to treat many-electron systems coupled to quantized electromagnetic modes. Here we discuss the implications of this approach for the theory of open quantum systems. In particular we show that in the limit of continuous spectrum of photon modes, QED-TDDFT naturally leads to time-dependent density functional theory for dissipative systems coupled to the Caldeira-Leggett bath. We consider the application to the Ohmic spin boson model and show that the developed approximation to the exchange-correlation functional describes the natural linewidth of the electronic linear density response function.

MM 14.3 Mon 15:30 HL 001

Electric and magnetic response properties of solids from the current density — •Rubén Rodríguez Ferradás[1], Pina Romaniello[2], and Arjan Berger[1] — [1]LCPQ, University of Toulouse, France — [2]LPT, University of Toulouse, France

The evaluation of the macroscopic polarization and magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities [1-5]. In this work we show the advantage of calculating electric and magnetic response properties of solids using the current density as basic variable. An efficient approach to calculate the current density is time-dependent current-density-functional theory. We will show results for optical properties of solids using a recently developed functional [6]. We will also discuss how the magnetization can be described within this framework.

[1] F. Kootstra, P.L. de Boeij, and J.G. Snijders, J. Chem. Phys. 112, 6517.

[2] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 71, 155104 (2005).

[3] P. Romaniello and P.L. de Boeij, Phys. Rev. B 71, 155108 (2005).

[4] J.A. Berger, P. Romaniello, R. van Leeuwen, and P.L. de Boeij, Phys. Rev. B 74, 245117 (2006).

[5] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 75, 035116 (2007).

[6] J.A. Berger, Phys. Rev. Lett. 115, 137402 (2015)

MM 14.4 Mon 15:45 HL 001

Coupling Maxwell's equations to the time-dependent Kohn-Sham equations: near-field effects and electromagnetic backreaction — •Rene Jestaedt[1], Micael Oliveira[1], Angel Rubio[1,2,3], and Heiko Appel[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, USA — [3]Nano-bio Spectroscopy Group and ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain

Induced currents in large molecular and condensed matter systems are non-negligible and can affect the conductivity and the optical properties of the system. In the present work, we have implemented the real-time propagation of Maxwell's equations in Riemann-Silberstein representation to use standard unitary propagation techniques in the TDDFT code octopus [1]. The Maxwell and the Kohn-Sham system are coupled via a predictor-corrector method to obtain a self-consistent time-evolution of the total system [2]. Explicitely solving the microscopic Maxwell's equations also allows us to determine the optical properties of the system directly from the Maxwell fields. We show near-field effects of a full Maxwell-matter and matter-Maxwell coupling for plasmon excitations in metallic nanoparticles [2,3] and for ring-currents in organic molecules [2].
[1] Alejandro Varas et al., J. Phys. Chem. Lett. 2015, **6**, 1891-1898 / [2] R. Jestädt et al., (to be submitted) / [3] X. Andrade et al., Physi. Chemistry Chem. Physics 2015, **17** 31371-31396

MM 14.5 Mon 16:00 HL 001

Enhanching excitation energy and charge transfer with strongly correlated light-matter interaction — •Christian Schäfer[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

Förster excitation energy and charge transfer are fundamental processes of chemical reactions and connected to interesting quantities such as correlation. Often this correlation is taken as fixed property of the system.

In the current work, we present how the coupling to cavity photons in a minimal realistic molecular system can drastically alter transfer characteristics, e.g. renders the excitation transfer to be distance independent [1,2]. The photonic interaction can imprint fermionic correlation on arbitrary distances.

The exact real-space description is suited to describe transfer and correlation in a unprejudiced ab-initio picture and allows us to extend our insights beyond common quantum-optical approximations.

[1] X. Zhong et al., Angew Chem Int Ed Engl. **56(31)**, 9034 (2017). [2] M. Slootsky et al., PRL **112**, 076401 (2014).

MM 14.6 Mon 16:15 HL 001

Effects of electronic correlations on the magnetic properties of organometallic molecules — •Sumanta Bhandary and Silke Biermann — Centre de Physique Thèorique, Ecole Polytechnique, 91128 Palaiseau, France

The realm of molecular spintronics relies on the external accessibility of molecular magnetic states. In correlated organometallic complexes, a delicate balance between the crystal field, Coulomb repulsion and dynamical hybridization between metal center and organic ligands dictates the electronic and magnetic properties and often poses challenges for an accurate theoretical modelling. We have employed density functional theory (DFT), the GW approach and Anderson's impurity model (AIM) technique to study the ground state electronic and magnetic properties of transition metal-based porphyrin and phthalocyanine molecules, both in the gas phase [1] as well as while adsorbed on surfaces. Our study reveals that the dynamical correlation effects are important in order to accurately estimate spin-transition energies, magnetic anisotropy energies as well as the ground state electronic configurations in the molecular complexes. We have explored the manipulation of surface molecule interactions to externally influence the electronic and magnetic properties of the molecular system.

[1] S. Bhandary, M. Schüler, P. Thunström, I. di Marco, B. Brena, O. Eriksson, T. Wehling, and B. Sanyal, Phys. Rev. B **93**, 155158 (2016).

MM 14.7 Mon 16:30 HL 001

Structural, electronic and optical properties of cubic and tetragonal $SrTiO_3$: a DFT study including many-body effects — •Vijaya Begum, Markus E. Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg.

$SrTiO_3$ (STO) is of fundamental interest as a substrate material in oxide electronics. The bulk undergoes a phase transition from the cubic to a tetragonal structure at T=105 K accompanied by characteristic antiferrodistortive rotations of the TiO_6 octahedra. We present a systematic comparison of the performance of the gradient corrected exchange correlation functional (GGA), the strongly constrained and appropriately normed (SCAN) meta-GGA and the hybrid functional HSE06 with respect to the electronic, structural and optical properties of cubic and tetragonal STO. For the tetragonal structure, SCAN gives a significantly improved description of the structural properties, comparable to HSE06, at a computational cost similar to GGA. The experimental band gap can be reproduced within SCAN with an on-site Hubbard term ($+U$), whereas within GGA the gap is underestimated even for very high U values. We calculate the optical spectrum for both phases, including many-body effects and excitonic corrections within the GW+Bethe-Salpeter equation approach, and compare this to previous theoretical results for the cubic phase [PRB 87, 235102 (2013)] and experiment [PRB 93, 075204 (2016)]. Funding by the DFG within SFB1242, project C02 is gratefully acknowledged.

MM 14.8 Mon 16:45 HL 001

Unveiling the mysterious magnetic state of superconducting iron under pressure — •Matteo d'Astuto — Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — IMPMC, UMR CNRS 7590, Sorbonne Universités-UPMC University Paris 06, MNHN, IRD, 4 Place Jussieu, F-75005 Paris, France

Compressed iron undergoes a transition from bcc to hcp crystal structure with a loss of ferromagnetism. The magnetic state of the hcp phase has been debated for many decades and experiments give seemingly contradictory results. Mössbauer measurements find no magnetism, however x-ray emission spectroscopy finds remnant magnetism and Raman mode splitting suggests symmetry breaking due to antiferromagnetism. These paradoxical results are consistent with either a paramagnetic state with spin fluctuations faster than Mössbauer timescales or an antiferromagnetic state, afmII, which is undetectable with Mössbauer spectroscopy. We performed neutron powder diffraction measurements in the hcp phase and do not observe afmII order down to 1.8 K, while confirming the existence of a local magnetic moment in the hcp phase with x-ray emission spectroscopy and find it is intrinsic to this phase (1). This local magnetic moment disappears at 30–40 GPa, exactly the same pressure region where superconductivity disappears.

(1) B. W. Lebert, T. Gorni J.-P. Rueff, S. Klotz, M. Casula, A. Juhin, J. M. Ablett, F. Baudelet, T. Straessle, T. Hansen, A. Polian, P. Munsch, G. Le Marchand, Z. Zhang, M. d'Astuto, article in preparation.

MM 14.9 Mon 17:00 HL 001

Frist-principle and experimental characterisation of the electronic properties of CaGaSiN3 and CaAlSiN3: impact of chemical disorder — •Jan Minar[1], Ondrej Sipr[2], Robin Niklaus[3], Jonas Hausler[3], and Wolfgang Scgnick[3] — [1]New Technologies Research Center, University of West Bohemia, Pilsen, Czech Rep., — [2]FZU, Academy of Sciences, Czech Rep — [3]Department of Chemistry, University of Munich, Munich, Germany

We report a detailed investigation of the electronic, mechanical and optical properties of the recently discovered nitridogallosilicate CaGaSiN3 which has potential as a LED-phosphor host material. We focus on chemical disorder effects, originating from the Ga/Si site, and compared them to those of isostructural CaAlSiN3. We calculate the elastic moduli and the Debye temperature in terms of quasi harmonical approximation. Spectral properties like the joint density of states (JDOS) are evaluated and the absorption, reflectance and energy loss function are obtained from the dielectric function. The optical band gap of CaGaSiN3 from experiment is compared to the electronic band gap in terms of electronic DOS and band structure calculations. All properties are evaluated for different ordering models of Ga/Si while the experimentally observed substitutional disorder is accounted for by utilizing the Coherent Potential Approximation (CPA). We conclude a shrinking of the band gap for both CaGaSiN3 and CaAlSiN3 due to atomic disorder, which is unfavorable for potential phosphor applications [1]. R. Niklaus, J. Minar, J Häusler, W. Schnick, Physical Chemistry Chemical Physics 19 (13), 9292 (2017)

MM 15: Battery Materials

Advanced Characterization

Time: Monday 17:30–18:45 Location: H 0106

MM 15.1 Mon 17:30 H 0106

Neutron imaging of Li-ion batteries with fission and thermal neutrons — •Samantha Zimnik[1,2], Michael Knapp[1,3], Malgorzata Makowska[2,4], Martin Johann Mühlbauer[1,2], and Helmut Ehrenberg[1,3] — [1]Institute for Applied Materials (IAM), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — [3]Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU), Helmholtzstrasse 11, 89081 Ulm, Germany — [4]University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany

Neutron imaging provides outstanding sensitivity to light elements, leading to high contrasts between hydrogen containing materials and metals. Combining imaging with fission and thermal neutrons at a single setup will benefit from the even more selective contrast for hydrogen provided by fission neutrons, while thermal neutrons will serve to reach higher spatial resolution for structure materials surrounding the hydrogen containing materials. Therefore an upgrade of the instrument is currently ongoing to make both neutron energy ranges available at a single setup and benefit from their respective advantages to follow the electrolyte distribution of lithium-ion batteries during operation. The thermal neutron beam option is funded by BMBF in the frame of research project 05K16VK3.

MM 15.2 Mon 17:45 H 0106

Neutrons confirm longer lifetime for Li-ion cells with a befitting anode — •Neelima Paul[1], Johannes Wandt[2], Stefan Seidlmayer[1], Sebastian Schebesta[3], Martin J. Mühlbauer[1,4,5], Oleksandr Dolotko[1], Hubert A. Gasteiger[2], and Ralph Gilles[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85747 Garching — [2]Chair of Technical Electrochemistry, Technische Universität München, 85748 Garching — [3]VW-VM Forschungsgesellschaft mbH & Co. KG, 73479 Ellwangen — [4]Institute for Applied Materials, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen — [5]Helmholtz-Institute Ulm for Electrochemical Energy Storage, P.O. Box, 76021 Karlsruhe

Long battery life is important for stationary storage systems which typically use cells consisting of LFP cathode and a graphite anode similar to needle coke (NC) anode. Such LFP/NC cells typically lose 23% of relative capacity after 4750 cycles and 11% under storage. We report that changing the anode material from NC with a flaky morphology, to a mesocarbon microbeads (MCMB) anode with a spherical morphology can drastically increase the longitivity of batteries. In situ neutron diffraction shows that LFP/MCMB cells lose only 8 % of relative capacity under similar cycling conditions and suffer no capacity loss on storage. It also proves that the entire capacity loss is dominated by the loss of cyclable lithium; no other aging mechanisms like structural degradation or deactivation of anode or cathode materials are observed, highlighting the excellent structural stability and superior quality of the investigated cells.

MM 15.3 Mon 18:00 H 0106

Antimatter meets defects: positron annihilation spectroscopy combined with two-component density functional theory to investigate $Li_4Ti_5O_{12}$ (LTO) — •C. Grosu[1,2], M. Schuderer[2], P. Jakes[1], C. Hugenschmidt[3], R.A. Eichel[1], K. Reuter[2], and C. Scheurer[2] — [1]IEK-9, FZJ Jülich — [2]Chair for Theor. Chemistry, TU Munich — [3]Heinz Maier-Leibniz Zentrum, TU Munich

LTO is a well-established anode material with several advantageous electrochemical properties. These depend sensitively on the crystallographic structure and are influenced by the presence of defects within the structure. In fact, defects are purposefully introduced into the structure by tailored synthesis and sintering protocols to increase LTO's electronic conductivity. Little is known to-date about the true nature of these defects and their exact mechanistic influence. Positron annihilation (PA) is one of the few techniques available to study defect distribution and chemical nature in solid materials experimentally. We perform positron lifetime calculations for bulk spinel LTO using two different self-consistent schemes within the framework of two-component density functional theory. An increased annihilation lifetime on the order of 200 ps is obtained for a positron in a neutral or formally negative defect. In contrast, for positrons in positively charged vacancies we compute lifetimes very close to the 180 ps as for defect-free LTO, likely rendering this type of defect invisible for PA. We discuss these findings in combination with lifetimes and positron coincidence Doppler broadening spectroscopy recently measured at the Garching positron source.

MM 15.4 Mon 18:15 H 0106

Multidimensional operando Analysis of Lithium/Sulfur Cells with X-ray Radiography — •Sebastian Risse[1], Benjamin Kent[1], Arne Ronneburg[1], André Hilger[2], Nikolay Kardjilov[2], Ingo Manke[2], and Matthias Ballauff[1,3] — [1]Institute of Soft Matter and Functional Materials, Helmholtz-Zentrum Berlin, 14109 Berlin — [2]Institute of Applied Materials, Helmholtz-Zentrum Berlin, 14109 Berlin — [3]Institute of Physics, Humboldt University of Berlin, 10099 Berlin

Lithium/sulfur (Li/S) batteries have a fivefold higher theoretical gravimetric energy density (2680 Wh/kg) than state-of-the-art lithium ion batteries. In addition, the abundant raw materials qualify this electrochemical storage system as one of the most promising candidates for the post-lithium-ion-era. However, the strong fading of electrochemical storage capacity with increasing cycle number is still a major obstacle to a broad technical use despite decades of research. Operando techniques are very suitable tools to gain mechanistic understanding of degradation processes. Especially the simultaneous combination of several independent measurements (multidimensional) while the Li/S cell is in operation allows deep insights into the degradation mechanisms. Here we present results of a novel setup where five different measurements are simultaneously performed. EIS, UV-vis spectroscopy, temperature and X-ray radiography were performed over ten cycles while the cell was galvanostically charged and discharged. Changes on the macroscopic scale can be correlated to characteristic signals in the EIS and UV-vis spectroscopy as well as the capacity fading curve.

MM 15.5 Mon 18:30 H 0106

Electronic structure of intercalated MXene: towards next generation supercapacitor — •Ameer Al-Temimy[1,2], Babak Anasori[3], Sneha Choudhury[1], Jian Ren[1,2], Yury Gogotsi[3], and Tristan Petit[1] — [1]Methods for Material Development, Helmholtz-Zentrum Berlin für Materialen und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [2]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Department of Materials Science and Engineering & A.J. Drexel Nanomaterials Institute, Drexel University, Philadelphia, PA 19104, USA

MXenes are a new class of 2D materials consisting of transition metals carbides and nitrides that demonstrated extraordinary features for electrochemical energy storage.

We have investigated MXene (Ti3C2) in water using soft X-ray absorption spectroscopy (XAS) at the O K-edge and Ti L-edge before and after urea intercalation. The samples were characterized as dried state in vacuum and in aqueous dispersion solution using a flow cell system.

The intercalation impact of urea molecules between the MXene planes and the effect of aqueous dispersion on their electronic structure will be discussed.

This study demonstrates that XAS performed directly in aqueous media is a powerful method for the characterization of energy-related materials.

MM 16: Topical session (Symposium MM): Hydrogen in Materials

Hydrogen storage materials

Time: Monday 17:30–19:00 Location: H 0107

Topical Talk MM 16.1 Mon 17:30 H 0107

Development of Hydrogen Storage Materials and Systems — •Martin Dornheim — Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

In recent years a huge number of novel light weight hydrides has been discovered with many of them showing a rather promising prospect for the use in hydrogen storage. Results attained by different characterisation techniques such as in-situ XRD, small angle X-ray scattering, EXAFS and XANES, volumetric Sieverts* type measurements, in-situ neutron radiography etc. on different hydrides and hydride composites will be presented. Insights about reaction mechanisms, sorption behaviour, cycling stability of light weight hydrides and Reactive Hydride Composites, the influence and optimisation of compaction on such materials to pellets and the behaviour of such pellets under in-situ conditions are given. The possibility for scale-up of the synthesis as well as the kinetic and cycle behaviour of larger sample batches considering for example the effect of temperature inhomogeneities on the performance and cycle life time of the storage materials will be discussed. An overview about methods and achieved results on the scale-up of synthesis and testing of different hydrides will be given.

MM 16.2 Mon 18:00 H 0107

Understanding the effect of nanostructured additives on hydride systems by means of electron transmission microscopy — •Julián Puszkiel[1,2], María Victoria Castro Riglos[3], Caludio Pistidda[1], Hujun Cao[1], Thi-Thu Le[1], Antonio Santoru[1], Thomas Klassen[1,4], and Martin Dornheim[1] — [1]Helmholtz Zentrum Geesthacht (HZG), Department of Nanotechnology, Geesthacht, Germany. — [2]Department of Physicochemistry of Materials, Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) and Centro Atómico Bariloche, S.C. de Bariloche, Argentina — [3]Department of Metalphysics, Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET) and Centro Atómico Bariloche, S.C. de Bariloche, Argentina — [4]Helmut Schmidt University, Hamburg, Germany

One of the main limitations for the implementation of hydrogen as energy carrier is the lack of an efficient and safe hydrogen storage system. Hydrogen storage in solid state through the formation of hydride compounds is a potential alternative to address this problem. In recent years, much effort has been devoted to improve the kinetic behavior of promising Li-Mg-B-H and Li-Mg-B-N-H destabilized hydride systems. In this work, nanosized additives added to 2LiBH4+MgH2 and 6Mg(NH2)2+9LiH+ LiBH4 are characterized via transmission electron microscopy (TEM). The aim is to understand the role of in situ formed nanostructured additives on the kinetic behavior of the investigated hydride systems. The information gained by TEM is helpful to optimize solid state hydrogen storage system for practical applications.

MM 16.3 Mon 18:15 H 0107

Grain Boundary Diffusion in the Magnesium-Hydrogen system - Harrison regimes C in action — •Magnus Hamm and Astrid Pundt — Institute for Material Physics, Georg-August University, Göttingen, Germany

Magnesium acts as storage material for hydrogen in a future hydrogen energy based economy because of its high reversible hydrogen capacity of up to 7,6 wt% [1]. However the slow kinetics its high desorption temperature provide a significant barrier to it's commercial use [2]. This kinetic limitation may be improved by the presence of grain boundaries. Grain boundary (GB) diffusion differs from bulk diffusion in crystals. For interstitial diffusion it can be either slower or faster, depending on the solvent concentration [4][5]. Magnesium seems to offers an ideal model system to study the dominant influence of the GBs in diffusion measurements as discussed in a recent publication [6]. The knowledge gained from finite-element-(FEM) simulations [6] will be used to evaluate diffusion coefficients of hydrogen in magnesium. The diffusion coefficients were measured by gasvolumetry and resistivity measurements. Combining experimental with FEM and analytical models results allows to show how grain boundaries can influence the kinetics in the Mg-H system.

Financial support provided via the projects PU131/10-1 and PU131/10-2 is gratefully acknowledged.

[1] Dornheim, R. et al., Scr. Mat. 56 (2007) [2] Bogdanović, B. et al., J. Alloys Compd. 282 (1999) [3] [4] T. Muetschele and R. Kirchheim, Scr. Metall. 21, (1987) [5] M. Hamm and A. Pundt, IJHE 42(2017)

MM 16.4 Mon 18:30 H 0107

Development of the atomistic model for study of hydrogen behavior in magnesium — •Daria Smirnova[1,2] and Sergei Starikov[1,2] — [1]Joint institute for high temperatures, Moscow, Russia — [2]ICAMS Ruhr University Bochum, Bochum, Germany

We report a new attempt to simulation of binary Mg-H system. For this purpose, we constructed a new angular-dependent many-body interatomic potential. The potential functions were fitted towards the ab initio data computed for a large set of reference structures representing various phases of magnesium and its hydrides. We performed molecular dynamic simulations illustrating that the structure and properties (i.e. melting temperatures, defects and stacking faults energies, elastic properties) of magnesium are reproduced with a good accuracy. In addition, the potential describes hcp-bcc phase transition occurring in magnesium at high pressures. The interatomic potential is also appropriate for study of magnesium hydrides existing at different pressures: alpha-MgH2 and gamma-MgH2. We also estimated characteristics of the hydrogen diffusion in magnesium. The results are proven to correlate with the existing experimental and theoretical data. We assume that the created interatomic potential can be applied for predictions dealing with hydrogen diffusivity and magnesium and magnesium hydrides. Also, it can provide an insight in mechanisms of phase transitions and characteristics of dislocations in magnesium.

MM 16.5 Mon 18:45 H 0107

Hydrogenation, dehydrogenation of α-tetragonal boron and its transition to δ-orthorhombic boron — Naoki Uemura[1], Koun Shirai[1], •Jens Kunstmann[2], Evgeny A. Ekimov[3], and Yuliya B. Lebed[4] — [1]Osaka University, Japan — [2]TU Dresden, Germany — [3]HPPI RAS, Troitsk, Russia — [4]NR RAS, Troitsk, Russia

α-tetragonal boron (α-T) was recently added to the list of known boron allotropes. Experiments show that upon annealing of hydrogenated α-T boron (B_nH_m) the H release occurs non-continuous, in two steps, where the second one is associated with a structural change from α-T to δ-orthorhombic boron (δ-O) and full H release [1]. Our free energy calculations based on density functional theory reproduce the experimental trends well, explain the origin of the two-step transition, and show that the difference between α-T and δ-O boron lies in the ordering of interstitial boron atoms occupying *4c* sites of the crystal structure. The latter implies an order-disorder transition. [1] Ekimov et al., J. Mater. Res. 31, 2773 (2016).

MM 17: Topical Session (Symposium MM): Fundamentals of Fracture

Joint session: Mechanical Properties at Small Scales and Fundamentals of Fracture: Small Scale Fracture Experiments and Ceramics

Time: Monday 17:30–19:00 Location: TC 006

MM 17.1 Mon 17:30 TC 006

Micromechanical testing of glasses at room temperature - the effect of strain rate in micropillar compression and impact nano-indentation — •Christoffer Zehnder[1], Hanno Rempel[1], Jan-Niklas Peltzer[1], James S.K.-L. Gibson[1], Doris Möncke[2], and Sandra Korte-Kerzel[1] — [1]IMM, RWTH Aachen University, Germany — [2]Vaxjö University, Sweden

It is well known that the mechanical properties of glasses are closely related to their atomic structure. The exact structure-property-relationship, however, is only poorly understood even for fundamental mechanisms like shear and densification and their influence on the transition between plastic deformation and fracture. Nanomechanical test methods like micropillar compression and impact nano-indentation can help fill this gap. In this study a sodium-boro-silicate glass is quenched to different temperatures to induce changes in the atomic structure. Micropillar compression was used to introduce plastic deformation into these glasses at room temperature in an uniaxial stress state. By increasing the strain rate it is shown that deformation shifts from stable crack growth to brittle failure. Impact nano-indentation showed a hardness plateau for high strain rates. Changing the glass structure leads to a shift of the corresponding strain rates to different values. These findings are analysed against the background of the glass structure and occurrence of shear and densification is discussed.

MM 17.2 Mon 17:45 TC 006

In situ fracture tests of brittle interfaces at the microscale — Giorgio Sernicola, Ben Britton, and •Finn Giuliani — Imperial College, London, UK

The fracture toughness of ceramics is often dominated by the structure of their grain boundaries. Our capacity to improve the performance of ceramic components depends on our ability to investigate the properties of individual grain boundaries. This requires development of new fracture testing methods providing high accuracy and high spatial resolution. Our approach uses a double cantilever geometry to obtain stable crack growth and we calculate the fracture energy under a constant wedging displacement. The tests are carried out within an SEM, this has two benefits: the sample is well aligned for a controlled test and images are recorded during the test for later analysis. Crucially this allows us to use beam deflection and crack length rather than critical load to measure fracture toughness. Our tests have proved it is possible to initiate and stably grow a crack in a controlled manner in ceramic materials for several microns. This approach has been validated on SiC where it gives a good approximation of the surface energy and then extended to SiC bi-crystals along with Ni-alumina interfaces where crack blunting and bridging mechanism can be observed and measured.

MM 17.3 Mon 18:00 TC 006

Micro-Mechanical Testing of Transition Metal (Oxy)Nitride Coatings — •James Gibson, Shahed Rezaei, Holger Ruess, Oliver Hunold, Stephan Wulfinghoff, Jochen Schneider, Stefanie Reese, and Sandra Korte-Kerzel — RWTH Aachen

Transition metal (oxy)nitride coatings are used in polymer forming operations for a combination of outstanding wear resistance and chemical compatibility with the polymer materials. Varying the chemical composition and deposition parameters for the coatings will optimise mechanical properties by a combination of chemistry and microstructural optimisation. By developing a representative model for these materials, these materials can be rapidly and efficiently prototyped and improved.

The effect of thin film composition and temperature on the elastic, plastic and fracture properties of transition metal nitride and oxynitride coatings was invested by nanoindentation and micro-cantilever bending. Vanadium and titanium aluminium nitride and oxynitride coatings were manufactured by high-power impulse magnetron sputtering on silicon substrates. Notched micro-cantilever beams were used to determine values of fracture toughness. Tests were carried out to 500C in-situ using a Nanomechanics inSEM system. Results are explained via DFT modelling of the coating chemistry, and integrated into a cohesive-zone element finite element model.

MM 17.4 Mon 18:15 TC 006

Onset of damage and anisotropic fracture behaviour of LiTaO3 and LiNbO3 single crystals — •Manuel Gruber[1], Raul Bermejo[1], Peter Supancic[1], Maxim Popov[2], Alexander Leitner[3], and Daniel Kiener[3] — [1]Institut fuer Struktur- und Funktionskeramik, Montanuniversitaet Leoben, Austria — [2]Materials Center Leoben Forschung GmbH, Leoben, Austria — [3]Department of Materials Physics, Montanuniversitaet Leoben, Austria

The requirements on new materials used in mobile communications are governed by the constantly growing data transfer rates. Single crystal piezoelectric materials, e.g. LiTaO3 and LiNbO3, have qualified as good candidates for accurate and efficient frequency filters and are thus also considered for the newest 5G mobile network standards. To optimize the functionality of the filters, a particular orientation and surface conditioning of the single crystal substrate must be ensured. This can affect the structural integrity of the functional material in response to external thermo-mechanical loading.

In this work, the onset of surface damage was assessed using nanoindentation techniques and could be correlated to weaker cleavage planes, where traces of plastic deformation (twinning) together with cracks on the contact surface were observed. Strength and fracture toughness of LiTaO3 and LiNbO3 were measured using biaxial bending on wafer samples of different orientations and in-situ SEM bending of notched micro-cantilevers loaded with a nanoindenter-tip, respectively. Experiments were supported by atomistic modelling, which could validate the experimental observations by calculating cleavage fracture energies.

Topical Talk MM 17.5 Mon 18:30 TC 006

Crack dynamics in brittle crystals: the varying cleavage energies. — •Dov Sherman and Merna Shaheen Mualim — School of Mechanical Engineering, Tel-Aviv University, Tel-Aviv, Israel

We investigated cracks dynamics in quasi-statically loaded silicon crystal on two low energy cleavage systems,(110)[1-10] and (111)[11-2]. The experiments were performed in air and under Ar at atmospheric pressure (low oxygen) to imitate vacuum, at low and high driving forces. The experimental energy speed relationships were compared with Freund equation of motion to extract the varying cleavage energies. An important variable in these experiments was the gradient of the energy release rate, dG0/da, denoted Theta. We show that at low Theta(<0.5 J/m2/mm), the cleavage energy is environmental, cleavage system, and crack speed dependent. At high Theta (>0.5 J/m2/mm), however, the stress corrosion cracking mechanisms vanished for both cleavage systems. The cleavage energy at initiation and propagation remain the same, but linearly increases as Theta increasing. We also specified the range of crack speed where crack dynamics is governed by the Griffith barrier. We indicate on an important physical fact in this investigation, i.e., the curvature of the crack front that giving rise to bond breaking mechanisms in form of kinks along the crack front. Crack propagation by kinks is governed by Theta, with complex advance or formation energies that determines the macroscopic cleavage energy. We therefore connect between the macroscopic cleavage energy and the microscopic crack front bond breaking mechanisms.

MM 18: Invited talk Baldi

Time: Tuesday 9:30–10:00 Location: TC 006

Invited Talk MM 18.1 Tue 9:30 TC 006
Hydrogen storage in individual metal nanoparticles — •Andrea Baldi[1,2], Tarun Narayan[2], Fariah Hayee[2], Ai Leen Koh[2], Robert Sinclair[2], and Jennifer Dionne[2] — [1]DIFFER - Dutch Institute for Fundamental Energy Research, Eindhoven, The Netherlands — [2]Stanford University, Stanford, USA

Many energy- and information-storage processes rely on phase transformations of nanomaterials in reactive environments. Compared to their bulk counterparts, nanostructured materials exhibit fast charging and discharging kinetics, resistance to defects formation, and thermodynamics that can be modulated by size effects. However, in ensemble studies of these materials, it is often difficult to discriminate between intrinsic size-dependent properties and effects due to sample size and shape dispersity. Here, we use a wide range of in-situ transmission electron microscopy techniques to reconstruct the absorption of hydrogen in individual palladium nanocrystals. Using electron energy-loss spectroscopy, dark-field imaging and electron diffraction, we shed light on the role of surface energy, crystallographic defects, and lattice strain on the thermodynamics and kinetics of phase transformation in these nanostructured systems (1-3). Our results provide a general framework for studying phase transitions in individual nanocrystals and highlight the importance of single-particle approaches to the characterization of functional nanomaterials.

(1) Baldi et al., Nature Materials 13, 1143-1148 (2014); (2) Narayan et al., Nature Materials 15, 768-774 (2016); (3) Narayan et al., Nature Communications 8, 14020 (2017).

MM 19: Battery Materials

Post Lithium-Ion Batteries

Time: Tuesday 10:15–11:30 Location: H 0106

MM 19.1 Tue 10:15 H 0106
Material and electrode design for sodium-ion batteries — •Yang Xu, Min Zhou, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Academic and industry interest in sodium-ion batteries (SIBs) has been resurrected in recent years, driven by the increasing market of electric vehicles and portable electronics. Sodium is one of the most abundant elements in the earth's crust and has similar chemical properties to lithium, indicating that sodium chemistry could be applied to a similar battery system to the Li counterpart. It is believed that cost-effective SIBs are an ideal replacement to lithium-ion batteries, but it requires further improvement of performance. We conduct our study of SIBs from a fundamental point of view, e.g., crystal structures, molecular structures and electrode structures, aiming at high capacity, cyclability and rate capability. Our material design has greatly promoted the performance of both inorganic (metals and oxides) and organic electrode materials, by controlling their atomic orderliness and utilizing defect chemistry. Our electrode design has proposed highly ordered nanoarrays as advanced electrode architectures to enhance surface ion availability, charge transport and electrode stability. We present here our recent work to demonstrate the material and electrode design, with the emphasis on metallic Sb and oxide-based anodes as well as organic carbonyl compounds. The design strategies could also be applicable in potassium-ion batteries.

MM 19.2 Tue 10:30 H 0106
Low-cost K0.220Fe[Fe(CN)6]0.805 as Cathode Material for Potassium-ion Batteries — •Chenglin Zhang, Yang Xu, Min Zhou, Long Liu, and Yong Lei — Institute für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany

Benefiting from the abundance of potassium, close redox potential to lithium, and similar electrochemistry to lithium system, potassium-ion batteries (PIBs) have attracted increasing attention as an important alternative to lithium-ion batteries. Since development of PIBs is just at its infancy stage, suitable electrode materials are rather limited. We demonstrated Prussian blue K0.220Fe[Fe(CN)6]0.805 nanoparticles as a potential cathode material. It delivered a capacity of 74.5 mAh/g at 50 mA/g and a high discharge voltage of 3.1~3.4 V as well as excellent cycling stability with retention over 98% after 50 cycles. Ex-situ XRD, Raman, and XPS characterizations confirmed that the C-coordicated FeIII/FeII couple is the redox-active site and responsible for K+ storage. Furthermore, we presented a PIB full-cell by coupling the nanoparticles with commercial carbon materials. The full-cell delivered a capacity of 68.5 mAh g-1 at 100 mA g-1 and retained 93.4% of the capacity after 50 cycles. Our work highlights the potentials of future commercialization of PIBs owing to the low cost and sustainability of both electrode materials.

[1] C. Zhang, Y. Xu, M. Zhou, L. Liang, H. Dong, M. Wu, Y. Yang, Y. Lei, Adv. Funct. Mater. 2017, 1604307.

MM 19.3 Tue 10:45 H 0106
Sodium intercalation into graphite: A DFT study — •Holger Euchner[1], Anji Reddy Munnangi[1], Helen Maria Joseph[1], and Axel Gross[1,2] — [1]Helmholtz Institute for Electrochemical Energy Storage, Helmholtzstraße 11, 89081 Ulm — [2]Institute of Theoretical Chemistry, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm

In contrast to graphite, disordered carbon exhibits high Na intercalation capacity and therefore may be regarded as a promising candidate for anode materials in Na ion batteries. Despite the ongoing research with respect to carbon based anodes, the underlying mechanism for Na intercalation is still strongly debated and far from being understood.

In this contribution, we present density functional theory based lattice dynamics and band structure calculations for different stages of Na intercalation in model structures of ordered and disordered graphite. Combining these calculations with data from in situ Raman scattering of Na intercalation in coconut shell derived hard carbon – and interpretation in terms of double resonant Raman scattering – allows us to provide detailed insights into the Na intercalation in disordered carbon.

MM 19.4 Tue 11:00 H 0106
Alkali metal insertion into TiO2 based ternary oxides — •Marketa Zukalova — J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, v.v.i. Dolejškova 3, CZ-18223 Prague 8, Czech Republic

The TiO2-based nanomaterials have triggered great excitement, because of their interesting structural characteristics and potential applications in energy conversion and storage. Among others, monoclinic modification of titanium dioxide (TiO2B) and Li4Ti5O12 spinel were investigated as lithium and sodium storage anode materials, Na2Ti3O7 was reported as the lowest voltage oxide material for sodium-ion batteries anode. Numerous Li insertion studies into TiO2-based materials revealed a dependency of its electrochemical behavior on morphology (particle size, surface area). In our work we demonstrate the excellent performance of sol-gel made nanocrystalline Li4Ti5O12 and Na2Ti3O7 during alkali metal insertion. Nanocrystalline Li4Ti5O12 exhibits the best performance for Na storage, its charge capacities reach 156 mAhg-1 and are twice as high as those of reference Aldrich LTS. The sol gel made Na2Ti3O7 exhibits discharge capacities of 109, 86 and 63 mAh g-1 at charging rates 1, 2 and 5C respectively, with 100% coulombic efficiency and zero capacity drop over 50 cycles after initial conditioning.

MM 19.5 Tue 11:15 H 0106
Calculation of Phase Stability and Point Defect Properties in the Perovskite $LaFeO_3$ — •Daniel Mutter[1], Daniel F. Urban[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

Solid oxide fuel cell (SOFC) and solid oxide electrolyzer cell (SOEC) devices, which transform chemical into electrical energy and vice versa, have the potential to make a significant contribution to the efforts of overcoming future problems of the energy economy. An optimal functionality of the electrodes in such devices requires a high catalytic activity at their surfaces, i.e. the capability for chemisorption and dissociation of O_2 molecules, charge transfer to O^{2-}, and incorporation of O^{2-} ions into vacant anion sites of the crystal structure. Promising materials regarding these requirements are perovskites (ABO_3), with La, Ba or Sr ions on the A sites, and transition-metal ions (Mn, Fe, Co) on the B sites. Using density functional theory calculations with a Hubbard-U correction, we aim to shed light on the correlation between stoichiometry, point defect concentrations and experimental synthesis conditions in the perovskite $LaFeO_3$ (LFO). The stability region of LFO in the phase diagram and point defect concentrations were calculated taking into account image charge corrections. Employing defect equilibrium reactions and applying the charge neutrality condition, point defect concentrations were obtained for varying elemental chemical potentials, i.e., synthesis conditions. The sensitivity of the results on the choice of the Hubbard-U parameter will be discussed.

MM 20: Topical session (Symposium MM): Hydrogen in Materials

Hydrogen absorption in nano-materials

Time: Tuesday 10:15–13:00 Location: H 0107

Topical Talk MM 20.1 Tue 10:15 H 0107
Sensing Hydrogen with (Single) Nanoparticles — •Christoph Langhammer — Chalmers University of Technology, Göteborg, Sweden

Using particles as signal transducers in a hydrogen sensor offers the ultimate miniaturization limit of the single nanoparticle. At the same time, metallic nanoparticles exhibit localized surface plasmon resonance, which provides unique opportunities for optical sensing. In this talk, I will discuss the concept of (single nanoparticle) nanoplasmonic hydrogen sensing on two examples:

A plastic-plasmonic optical hydrogen sensor platform using PdAu alloy nanoparticles embedded in a polymer matrix acting as molecular sieve, which enables deactivation-resistant hysteresis-free hydrogen detection with unprecedented sub-second response time at room temperature, and with sub-5 ppm detection limit.

Single nanoparticle plasmonic hydrogen sensing as a tool to unravel size-and shape effects in the thermodynamics and hysteresis of metal-hydrogen interactions in individual Pd nanocrystals with different size and shape, as well as to understand the role of grain boundaries in the hydrogenation process of individual polycrystalline Pd nanoparticles.

MM 20.2 Tue 10:45 H 0107
Thermodynamic and elastic properties of palladium-hydrides from first principles — •Beatrix Elsner, Gregor Feldbauer, and Stefan Müller — Hamburg University of Technology, Institute of Advanced Ceramics, Denickestr. 15, D-21073 HH

Palladium and Pd-based alloys exhibit a huge potential for widespread applications ranging from hydrogen storage to catalytic processes. Because of its ability to reversibly embed a significant amount of hydrogen into interstitial sites, palladium is often characterized as a "hydrogen sponge". With increasing amount of absorbed hydrogen, the mechanical properties of palladium-hydride (PdH_x) are affected, e.g. it becomes more susceptible to brittle fracture. In order to understand such phenomena in more detail, the thermodynamic stability and elastic properties of PdH_x are here investigated via ab initio methods. Dispersion-corrected density functional theory (DFT) calculations are performed to obtain the energetics as well as the elastic properties of PdH_x for hydrogen concentrations up to 100%. The significant effect of phonon contributions is considered within the harmonic approximation. Using the DFT results as input data, cluster-expansion Hamiltonians for the phase formation energy as well as for the elastic properites are constructed to scan exhaustively the entire configuration space of PdH_x. This approach allows us to identify the most favorable configurations (ground states) as well as to identify trends for the elastic properties, such as a decrease of the shear constant c_{44} with increasing hydrogen concentration.

MM 20.3 Tue 11:00 H 0107
Tunable elasticity of nanoporous palladium by hydrogen insertion — •Shan Shi[1,2], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht — [2]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg, Hamburg

Nanoporous metals with large specific surface area fabricated by dealloying are well-defined model systems for studying the mechanical behavior of nanostructured metals via conventional mechanical testing approaches. It has been demonstrated that mechanical properties such as macroscopic strain and stiffness of nanoporous gold could be tuned via changing the surface state. Most recently, a synthesis protocol for uniform and strong bulk samples of nanoporous Pd has been established. The material is readily equilibrated with H at controlled chemical potential. We have demonstrated that hydrogen electrosorption could result in more than 3% reversible strain variation with np Pd. Here, we explore the elasticity change of np Pd during hydrogen absorption/desorption. It concluded that hydrogen induced over 30% compliance change with np-Pd. Furthermore, the relationship between experimentally measured elastic coefficient and hydrogen content agrees quantitatively with the theory of open system elasticity by Larché and Cahn.

30 min. break

MM 20.4 Tue 11:45 H 0107
Strain Response of Nanoporous Palladium upon Hydrogenation: Contributions of Hydride Phases, Stresses and Strain Rate — •Markus Gössler, Eva-Maria Steyskal, and Roland Würschum — Inst. of Mater. Phys., TU Graz, Austria

Nanoporous (np) palladium is an interesting candidate to study hydrogen and hydride phases in nanoporous systems [1]. The high surface stresses in nanoscaled structures can affect hydrogen interactions substantially, including the formation of metal hydrides. A novel method to achieve particularly fine porosities is electrochemical dealloying, a selective dissolution process from an alloy. In this work the strain response of dealloyed np Pd samples upon electrochemical hydrogenation was studied, using an in-situ dilatometric technique [2]. Unexpected yielding of np Pd during hydrogen desorption could be associated with an enhancement of plasticity, based on the activation of an additional pathway for plastic deformation. There are indications that hydrogen solutes interact with dislocations upon hydrogen desorption at high strain rates which are discussed by analogy with the well-known mechanism of dynamic strain aging. The impact of the np-structure related surface stress on the behaviour of the strain curve will be elucidated. Acknowledgement: This work is financially supported by the Austrian Science Fund (FWF): P30070-N36.

[1] M. Hakamada et al., J.Phys.Chem.C **114** (2010) 868. [2] E.-M. Steyskal et al., Beilst.J.Nanotech. **7** (2016) 1197.

MM 20.5 Tue 12:00 H 0107
Mechanical stress upon hydrogen absorption in Nb-Fe Films — •Philipp Klose, Magnus Hamm, Vladimir Roddatis, and Astrid Pundt — Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Hydrogen absorption in thin films adhered to rigid substrates results in compressive mechanical in-plane stresses.[1,2,3] These stresses can lead to changes in the material's properties. While the in-plane film stress increases linearly on the hydrogen content for low hydrogen concentrations, deviations from the linearity appear at the yield stress [3,4]. The yield stress inversely depends on the film thickness.[5] For hydrogen loaded Niobium films, linearity is maintained to 1 H/Nb, for films below 6 nm and mechanical stress of up to -10 GPa is achieved.[5]

The yield stress can also be affected by alloying.[6] In this presenation we study the stress-development upon hydrogen loading in niobium-iron films of differing compositions. Films of different thickness were prepared by argon-cathode beam sputtering. Electrochemical hydrogen loading was performed during in-plane stress and in-situ XRD-measurements. By alloying the yield stress is shifted to much higher values. This will be discussed with respect to the Hall-Petch relation and the lattice coherency.

This work is financially supported by the DFG via project PU131/12-1. [1] J. Weissmuller et al. , Phil. Mag. Lett. 80 (2000), [2] S. Wagner et al., Appl. Phys. Lett. 92 (2008), [3] U. Laudahn et al., JALCOM (1999), [4] A. Pundt et al., Phys. Rev. B 61.15 (2000), [5] Hamm, M., et al. APL 106 (2015), [6] P. Klose et al. IJHE (2017).

MM 20.6 Tue 12:15 H 0107

Depth-resolved hydrogen content measurement using Laser-induced Ablation-Quadrupole Mass Spectrometry (LIA-QMS) — •Jannis Oelmann, Sebastijan Brezinsek, Cong Li, and Christian Linsmeier — Institut für Energie und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Deutschland

Monitoring the quantitative sample's material composition is important for both- industrial process control as well as for post mortem analysis in research and industrial development. Still there is a lack of diagnostics, providing depth resolved information without using standard samples, although those cannot be used in several cases. We present a new method for measuring volatile sample species, using residual gas analysis with quadrupole mass spectrometry after picosecond laser-induced ablation.

A layer-wise sample analysis in the order of $\mathcal{O}(100$ nm$)$ is achieved by using the third harmonic ($\lambda = 355$ nm) of a Nd:YVO$_4$ laser with a pulse duration of $\tau = 35$ ps and pulse energies up to $E = 50$ mJ for material ablation. To show the capability of the method, results for well characterized multilayer thin film solar cells (μc-Si:H and a-Si:D on ZnO:Al) are shown and compared to standard techniques like Thermal Desorption Spectroscopy (TDS). Additionally, hydrogen content measurements of graphite samples from the fusion test reactor Wendelstein 7-X (W7-X) are shown to study the impact of heat flux on the graphite limiter tiles on hydrogen retention, which is essential for an in-depth understanding of the plasma wall interaction processes.

MM 20.7 Tue 12:30 H 0107

Sensitive 3D Microscopy of H and D in Metals using MeV Protons. — •Patrick Reichart and Günther Dollinger — LRT2, Universität der Bundeswehr München, Neubiberg, Germany

At the Munich microprobe SNAKE (Superconduction Nanoscope für Applied nuclear (Kern–) physics Experiments) a coincidence detection system has been installed to analyze proton-proton scattering events with up to 25 MeV incident protons. This allows to quantitatively analyze atomic H distributions in three dimensions with micrometer resolution. Due to transmission geometry the sample or foil thickness is limited to maximum 50 μm e.g. for W or 150 μm for Si.

The technique is the only nuclear microscopy method with low enough irradiation damage, i.e. not altering the H distribution before sufficient signal is detected. Sub-ppm sensitivity has been achieved for light materials like diamond, worse sensitivity of few ppm is demonstrated in heavy metals like Fe or W. We present a selection of previous studies of H in materials e.g. H in nominally anhydrous minerals of the earth mantle, H adsorption in thin metal films, H retention in irradiated tungsten that is of large interest for potential diverter material in future fusion reactors.

We also demonstrate that sensitive D detection is possible by using a deuteron beam and detect deuteron-deuteron coincidences. This gives the possibility to study adsorption, retention as well as diffusion processes of H in materials by isotope marking.

MM 20.8 Tue 12:45 H 0107

Hydrogen influence on diffusion in nickel from first-principles calculations — •Döme Tanguy[1], Yu Wang[1,2], and Damien Connétable[2] — [1]University Lyon 1, Villeurbanne, France — [2]ENSIACET, Toulouse, France

The diffusion coefficient of vacancy-hydrogen clusters (VH$_n$), at equilibrium, in Ni is evaluated. The key is a good separation of timescales between H diffusion and the metal-vacancy exchange so that cluster diffusion can be treated as an uncorrelated random walk and that H is always in equilibrium before the vacancy-metal exchange. Then, the diffusion coefficient is a sum over jump paths of the equilibrium probability of being in a specific VH$_n$ configuration times the corresponding activation terms. The influence of H on the energy barriers for the metal-vacancy exchange are calculated ab initio. It is shown that vacancies are drastically slowed down by H. Nevertheless, at equilibrium, VH$_n$ clusters always induce a speed up of metal diffusion, because of the overall enrichment in vacancies. The implications concerning H induced damage, in particular in regards to Ni-Cr oxidation and GB embrittlement, are discussed. Details in Phys. Rev. B 91 094106.

MM 21: Topical Session (Symposium MM): Fundamentals of Fracture

Interface Fracture and Atomistic Aspects I

Time: Tuesday 10:15–11:30 Location: TC 006

Topical Talk MM 21.1 Tue 10:15 TC 006

Comparison of interfacial fracture properties in molecular dynamics simulations: A primer on selecting grain boundary sets — •Remi Dingreville[1], Doruk Aksoy[2], and Douglas Spearot[2] — [1]Sandia National Laboratories — [2]Department of Mechanical Engineering, University of Florida

All grain boundaries are not equal in their predisposition for fracture due to the complex coupling between lattice geometry, interfacial structure, and mechanical properties.

This presentation will describe a methodology to isolate the role of grain boundary structure on interfacial fracture properties using atomistic simulations. Instead of commonly constructing sets of grain boundary models within the misorientation/structure space by simply varying the misorientation angle around a fixed misorientation axis, the proposed method creates sets of grain boundary models by means of isocurves associated with important fracture-related properties of the adjoining lattices. Such properties may include anisotropic elastic moduli, the Schmid factor for primary slip, and the propensity for simultaneous slip on multiple slip systems. This approach eliminates the effect of lattice properties from the comparative analysis of interfacial fracture properties and thus enables the identification of structure-property relationships for grain boundaries. As an example, this methodology is implemented to study crack propagation along Ni grain boundaries. Segregated H is used as a means to emphasize the role of the grain boundary structures while keeping lattice properties fixed.

MM 21.2 Tue 10:45 TC 006

Intergranular fracture prediction via multi-scale simulations — •Bertrand Sicaud[1,3], Laurent Van Brutzel[2], and Maxime Sauzay[1] — [1]DEN- Service de Recherches Métallurgiques Appliquées (SRMA), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France — [2]DEN- Service de la Corrosion et du Comportement des Matériaux dans leur Environnement (SCCME), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France — [3]Universités Paris-Sorbonne - UPMC, 75005 Paris, France

Observations of intergranular fracture initiation during slow strain rate tests highlight two relevant mechanisms occuring at grain boundaries (GB): stress concentrations induced by the impact of slip bands and selective internal oxidation in water environment.

The pile-up theory modeling a slip band as a slip plane of negligible thickness in a continuum elastic medium is generaly used with the Griffith criterion. However this approach leads to large underestimation of the remote stress to GB fracture.

Slip band of finite thickness (20-200 nm) inducing more realistic singularities are investigated by using crystalline finite element calculations. A new approach using quantized fracture mechanics in conjunction with a double criterion permits to deduce a model of intergranular crack initiation. This multi-scale analytical model is used with molecular dynamics results of oxide grain boundaries decohesions for assessing the oxidation embrittlement of the interface. An extensive application of the model is carried out for numerous materials. Predictions are in good agreement with experimental results.

MM 21.3 Tue 11:00 TC 006

Exploring the mechanisms of Pellet-Cladding Interaction with atomistic simulation — •Adam Plowman, Conor Gillen, Alistair Garner, Philipp Frankel, and Christopher Race — University of Manchester, Manchester, United Kingdom

Failure of fuel rods in light water nuclear reactors via the Pellet-Cladding Interaction (PCI) is thought to be driven by Stress Corrosion Cracking (SCC), induced by aggressive fission products such as iodine. Empirical observations of PCI together with a limited mechanistic understanding of the phenomenon has led to stringent limits on operational parameters. An improved understanding of PCI would allow these limits to be relaxed and enable reactors to respond to energy demand changes more quickly, without compromising safety. Flexible power manoeuvring is critical to successfully combining nuclear power with fluctuating sources of renewable energy. In tandem with new experimental observations, we are using atomistic simulation to improve our mechanistic understanding of PCI. We present a systematic study of zirconium grain boundary properties, including cleavage energies, undertaken using density functional theory. We have further studied the thermodynamics of impurities (including iodine) in these boundaries and their effect on grain boundary cohesion. We compare our results with new experimental data on iodine-induced SC cracks in commercial Zr alloys.

MM 21.4 Tue 11:15 TC 006

Predicting mechanical properties of carbide-metal interfaces from first principles — •Elric Barbé[1,2], Chu-Chun Fu[2], and Maxime Sauzay[1] — [1]CEA, DEN, Service de Recherches Métallurgiques Appliquées, F-91191, UPSay, Gif-sur-Yvette Cedex, France — [2]CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191, UPSay, Gif-sur-Yvette Cedex, France

The cavity initiation observed in ductile, brittle and intergranular creep damages is often explained by a fracture of interface between carbide and metallic lattices. Understanding the mechanisms of fracture allows the prediction of the cavity density as a function of applied strain, which law strongly affects the damage evolution. This study focuses on interfaces between a metallic matrix (Fe, Ni) and a representative carbide: M23C6 . Surface, interface and fracture energies are calculated via DFT based on chemical potential analysis. Then, interfacial fractures stresses are estimated by the UBER (Universal Binding Energy Relation) model and compared with good correlation to the results of fully-DFT simulations of tensile test carried out using various methodologies. We investigate the dependence of the interfacial mechanical behavior on chemical compositions, crystallographic structures and magnetic orderings. The predicted fracture stresses of coherent interfaces range between 14 and 20 GPa. Then, the effects of some incoherent interfaces are investigated. The resulting critical stress is about two times smaller, which is consistent with experimental observations showing that interfacial fracture rather occurs at incoherent interfaces. Finally, segregations effects are investigated.

MM 22: Microstructure and Phase Transformations

Transformations at extreme conditions

Time: Tuesday 10:15–11:15

Location: TC 010

MM 22.1 Tue 10:15 TC 010

First-principles calculations of the linear elasticity of quartz and implications for pressure induced amorphization — •Christoph Otzen[1], Silvana Botti[1], and Falko Langenhorst[2] — [1]Institut für Festkörpertheorie und Optik, Jena, Germany — [2]Institut für Geowissenschaften, Jena, Germany

Quartz is a material that is prone to amorphization at high pressures. Numerous studies have been carried out since the discovery of amorphization in the late 1980s to explore mechanisms, structural evolution, and onset of amorphization as a function of static pressure. Quartz displays however a peculiar behavior under shock metamorphism, the process under which a material reacts to dynamic pressure waves with extreme conditions. In this case, quartz develops amorphous lamellae at the nanometer scale with sharp crystalline-amorphous boundaries and most strikingly, in particular crystallographic orientations.

Here, we investigate the directional dependence of some mechanical properties of quartz in the approximation of linear elasticity and compare our results with the orientations of amorphous lamellae to gain insight into their formation mechanism. We tackle the problem by calculating second-order elastic coefficients by means of density functional theory. Our first calculations of stress-strain relations for all directions indicate indeed structural changes over pressure that are consistent with anisotropic amorphization of quartz.

MM 22.2 Tue 10:30 TC 010

Stabilization of body-centred cubic iron under Earth's core conditions — •Sergei I. Simak — Linköping University (LiU), 58183 Linköping, Sweden

The Earth's solid core is mostly composed of iron. However, the stable phase of iron under inner-core conditions remains uncertain. The two leading candidates are hexagonal close-packed (hcp) and body-centred cubic (bcc) crystal structures, but the dynamic and thermodynamic stability of bcc iron under inner-core conditions has recently been challenged. We demonstrate the stability of the bcc phase of iron under conditions consistent with the centre of the core using ab initio molecular dynamics simulations. We find that the bcc phase is stabilized at high temperatures by a novel diffusion mechanism that arises due to the dynamical instability of the phase at lower temperatures[1].

[1] A. B. Belonoshko, T. Lukinov, J. Fu, J. Zhao, S. Davis, and S. I. Simak, "Stabilization of body-centred cubic iron under inner-core conditions", Nature Geoscience 10, 312 (2017).

MM 22.3 Tue 10:45 TC 010

Hall-Petch relations of Cu-Ni alloys and their dependence on severe deformation and annealing — •Friederike Emeis, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Westfälische Wilhelms-Universität Münster, D-48149

The Hall-Petch relationship is widely discussed and used as a microstructural description of different materials. In this talk the existence of different Hall-Petch relationships for the same materials, processed in different ways to achieve a variation of their grain sizes and structures is shown and connected to grain boundary characteristics. Pure Cu and Ni as well as four different compositions of Cu-Ni alloys are processed by severe plastic deformation at room temperature up to different strain levels (unsaturated and saturated severely deformed) and subsequent annealed. It is shown, that the processing and thus the characteristics of grain boundaries have in general the same effect on different materials. Furthermore, the saturated severely deformed microstructure is well described by a polycrystalline Hall-Petch relationship. It is concluded that dynamic recovery and recrystallization change the microstructure in a way that the influence of the grain boundaries on the hardness is as dominant as in a relaxed microstructure.

MM 22.4 Tue 11:00 TC 010

High-pressure torsion induced phase transformations in Cu- and Ti-based alloys — •Askar Kilmametov[1], Yulia Ivanisenko[1], Boris Straumal[1,2], Andrey Mazilkin[1,2], Mario Kriegel[3], Olga Fabrichnaya[3], David Rafaja[3], and Horst Hahn[1] — [1]Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Karlsruhe, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russia — [3]TU Bergakademie Freiberg, Institute of Materials Science, Freiberg, Germany

Severe plastic deformation not only leads to grain refinement but also accelerates mass-transfer and drives phase transformations in Cu-based alloys. Dynamic equilibrium between decomposition of (supersaturated) solid solution and dissolution of precipitates during high pressure torsion (HPT) of diluted Cu-based alloys has been studied. The precipitation of second phase particles from a solid solution and their dissolution take place simultaneously and compete with each other. The formation of high-pressure ω-phase has been studied in Ti-based alloys. A defect-rich ω-phase forms after HPT and persists in the samples also after the pressure release. The amount of retained ω-phase after HPT depends on the alloying element concentration. Based on the XRD and TEM observations, the crystallography and mechanisms of α to ω and β to ω phases transformations (which can be diffusionless as well as controlled by mass transfer) are discussed.

MM 23: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Tuesday 10:30–13:00 Location: HL 001

MM 23.1 Tue 10:30 HL 001

Control and prediction of molecular crystal properties by multilevel strategies — •Jan Gerit Brandenburg — London Centre for Nanotechnology, Department of Physics and Astronomy, University College London, 20 Gordon Street, London, U.K.

Computational material science is a dynamic and thriving area of modern scientific research. Approaches based on the fundamental laws of quantum mechanics are now integral to almost any materials design initiative in academia and industry, underpinning efforts such as the Materials Genome initiative or the computational crystal structure prediction [1]. I will present a hierarchy of quantum chemical methods designed for this purpose, in particular targeting molecular crystals and their property prediction. The methods range from high-level diffusion Monte-Carlo (DMC) to London dispersion inclusive DFT, and thus, cover many orders of magnitudes in computational efficiency [2,3]. I will demonstrate the application to the 6th blind test for organic crystal structure prediction. Comparisons to other state-of-the-art methods indicate both success and remaining challenges in the recent method developments [4].

[1] S. L. Price and J. G. Brandenburg, *Molecular Crystal Structure Prediction*; Elsevier Australia, **2017**.

[2] A. Zen, J. G. Brandenburg, J. Klimeš, A. Tkatchenko, D. Alfè, A. Michaelides, **2017**, *submitted*.

[3] J. G. Brandenburg, E. Caldeweyher, S. Grimme, *Phys. Chem. Chem. Phys.* **2016**, *18*, 15519.

[4] A. M. Reilly, et al. *Acta. Cryst. B* **2016**, *72*, 439.

MM 23.2 Tue 11:00 HL 001

Advances in first-principles and model spin Hamiltonian simulations of point defects in semiconductors for quantum sensors and computing — •Viktor Ivády — Department of Physics, Chemistry and Biology, Linköping University, 581 83 Linköping, Sweden — Wigner Research Center for Physics, Konkoly-Thege Miklós út 29-33, 1121 Budapest, Hungary

First principles simulations play a key role in understanding the physics of point defects in semiconductors, while model spin Hamiltonian approaches are traditionally used to interpret experimental spin dependent observations and describe the spin dynamics of point defects. The development of novel point defect applications, such as quantum bit (qubit) and single photon emitter applications for quantum information processing and quantum sensing, requires detailed understanding of spin-related couplings and addressability of localized defects states in the bath of delocalized electrons that calls for further development and implementation of theoretical tools. Here, I report on my contribution to this field that covers 1) first principles studies for identification of point defect based qubits and single photon emitters , 2) method development for the description of point defects with correlated electron states, 3) implementation of zero-field-splitting calculation for point defect based qubits, 4) development of model spin Hamiltonian approaches for the simulation of optical dynamic nuclear polarization process (ODNP) of point defects, and 5) spin dynamic simulation of existing point defect qubits. As an outlook, I discuss the requirements toward fully-ab initio point defect spin dynamic simulations.

MM 23.3 Tue 11:30 HL 001

Recent advances in first-principles modelling of correlated magnetic materials — •Yaroslav Kvashnin — Department of physics and astronomy, Uppsala University, BOX 516, 75120 Uppsala

Most of modern first-principles electronic structure studies of correlated materials are based on a combination of density functional theory and dynamical mean field theory (DFT+DMFT).

Addressing magnetic materials within DFT+DMFT has certain peculiarities. There are two recipes one can follow: either to account for magnetism within the DFT functional or to introduce it entirely within the self-energy. Both approaches have their flaws and advantages, which are well-known for DFT+U, but are not often discussed for DFT+DMFT. In my talk I will present a systematic comparison of the two methods and demonstrate the evidences favouring the use of non-polarised functionals.

Next, I will demonstrate how the obtained electronic structure information can be used to simulate finite-temperature magnetic properties in real materials. I employ a so-called two-step approach. First, I map the system on a Heisenberg model and extract the effective exchange parameters Jij's from DFT+DMFT. Then the atomistic spin dynamics simulations are used to simulate magnon spectra and predict the magnetic ordering temperatures.

I will demonstrate the power of such an approach by showing a direct comparison with available experimental data for a wide range of different materials.

MM 23.4 Tue 12:00 HL 001

A first-principles approach to hot-electron-induced ultrafast dynamics at metal surfaces — •Reinhard J. Maurer — Department of Chemistry, University of Warwick, Gibbet Hill Road, CV4 7AL Coventry, UK

Low-lying electronic excitations in metals, so-called hot electrons, couple efficiently to molecular adsorbate motion. In doing so, they give rise to a number of curious experimental observations. This includes picosecond-scale energy loss of molecular adsorbate vibration, highly inelastic atomic and molecular scattering from metal surfaces, and light-assisted molecular desorption and chemical transformations, recently coined "hot-electron chemistry". In this talk, I will present a first-principles treatment of hot-electron-induced molecular dynamics based on Density Functional Theory that correctly captures the magnitude and mode-specificity of hot-electron mediated adsorbate-substrate energy transfer [1]. Utilizing our efficient all-electron local-orbital implementation of hot-electron-induced frictional forces based on Time-Dependent Perturbation Theory, [2] I will show how we correctly capture vibrational relaxation in large-scale metal-mounted molecular catalysts as well as the energy loss and coupled electron-nuclear dynamics of small molecular adsorbates in both thermal and laser-heated conditions. [3] We scrutinize our approach in comparison to recent Sum-Frequency Generation (SFG) spectroscopy and molecular beam scattering experiments. [1] Phys. Rev. Lett. 116, 217601 (2016) ; [2] Phys. Rev. B 94, 115432 (2017); [3] Phys. Rev. Lett. 118, 256001 (2017);

MM 23.5 Tue 12:30 HL 001

Temperature effects in spin-orbit physics from first principles — •Bartomeu Monserrat — University of Cambridge, UK — Rutgers University, USA

The spin-orbit interaction drives a number of physical phenomena, including the band inversion in topological insulators and the spin splitting of electronic bands in inversion asymmetric crystals. In this work, we study the effects of finite temperature on such spin-orbit physics, including both thermal expansion and electron-phonon coupling effects [PRB 92, 184301 (2015)].

First, we describe the temperature dependence of the inverted gap in topological insulators. We find that increasing temperature reduces the topological gap in the Bi2Se3 family of materials, and we predict a temperature-induced topological phase transition in Sb2Se3 [PRL 117, 226801 (2016)].

Second, we study the temperature dependence of the spin splitting of electronic bands in both inversion symmetric and asymmetric crystals. We predict a dynamical spin splitting in centrosymmetric crystals and characterise the associated phenomenology in the cubic perovskite CsPbCl3 [arXiv:1711.06274]. In inversion asymmetric crystals, exemplified by the bismuth tellurohalides, we find that increasing temperature suppresses the static spin splitting arising from the Rashba effect [PRM 1, 054201 (2017)].

MM 24: Topical session (Symposium EPS and MM, joint session with MA): Magnetism in Materials Science: Thermodynamics, Kinetics and Defects (joint session MM/MA)

Magnetism V

Time: Tuesday 11:45–13:00 Location: H 0106

Topical Talk MM 24.1 Tue 11:45 H 0106

Grain boundary migration and grain growth in non-ferromagnetic metals under the impact of a magnetic field — •Dmitri A. Molodov — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, 52056 Aachen, Germany

Grain boundary migration can be induced by a magnetic field, if the anisotropy of the magnetic susceptibility generates a gradient of the magnetic free energy density across the boundary. In contrast to curvature driven boundary motion, a magnetic driving force also acts on planar boundaries so that the motion of crystallographically fully defined boundaries can be investigated. The magnetically driven motion of planar symmetric and asymmetric tilt grain boundaries was studied in high purity bismuth and zinc bicrystals. Boundary migration was measured in-situ by means of a polarization microscopy probe and the corresponding migration activation parameters were obtained. The results revealed that grain boundary mobility essentially depends on the misorientation angle and the inclination of the boundary plane.

As it has been demonstrated in a series of experiments on polycrystalline zinc, titanium and zirconium, as well as by computer simulations, grain growth in magnetically anisotropic non-ferromagnetic materials can be substantially affected by a magnetic field. This manifested itself by significant changes in the development of the grain growth texture during magnetic annealing compared to annealing at zero field. The magnetically induced texture changes are caused by the generation of an additional magnetic driving force for grain growth/shrinkage.

MM 24.2 Tue 12:15 H 0106

Stability and magnetic properties of grain boundaries in the inverse Heusler phase Fe_2CoGa and in bcc Fe — •Daniel F. Urban[1], Wolfgang Körner[1], Georg Krugel[1], Anna Lehner[1], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

Grain boundaries (GBs) in the cubic inverse Heusler phase Fe_2CoGa are investigated by means of first principles calculations based on density functional theory. The results are compared to those of corresponding GBs in bcc Fe. Besides the energetic stability, the analysis focuses on the magnetic properties of the GBs. The inverse Heusler phase offers a variety of interesting low energy GBs. It is found that such GBs do not lead to a breakdown of the local magnetic moments at the interface, as observed for some of the GBs in bcc Fe. Instead there is partially even a substantial enhancement near the GB. Nevertheless, the integrated increase in total magnetic moment is very similar for GBs in both materials. The analysis of the ferromagnetic coupling indicates that the coupling across such low energy interfaces is not reduced with respect to the single crystal of Fe_2CoGa, whereas in bcc Fe a weakening or even decoupling of two grains can occur.

MM 24.3 Tue 12:30 H 0106

Magnetic properties of the CrMnFeCoNi high-entropy alloy — Oldřich Schneeweiss[1], •Martin Friák[1,2], Marie Dudová[1], David Holec[3], Mojmír Šob[2,1,4], Dominik Kriegner[5], Václav Holý[5], Přemysl Beran[6], Easo-P. George[7], Jörg Neugebauer[8], and Antonín Dlouhý[1] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversitaet Leoben, Leoben, Austria — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [5]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [6]Nuclear Physics Institute, Academy of Sciences of the Czech Republic, Řež, Husinec, Czech Republic — [7]Institute for Materials, Ruhr University, Bochum, Germany — [8]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

The equiatomic CrMnFeCoNi high-entropy alloy undergoes a paramagnetic-to-spin-glass transition at 93 K and a ferromagnetic transition at 38 K while maintaining its fcc structure down to 3 K (Phys. Rev. B 96 (2017) 014437). We study the local atomic magnetic moments in this material by *ab initio* calculations. We find the Cr magnetic moments aligning antiferromagnetically with respect to a cumulative magnetic moment of their first coordination shell. The magnetic moments of Fe and Mn atoms remain high (between 1.5 and 2 μ_B), while the local moments of Ni atoms effectively vanish.

MM 24.4 Tue 12:45 H 0106

Effect of magnetic transition on grain boundary diffusion of Mn in α-iron — Vladislav Kulitckii, Sergiy Divinski, and •Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Münster, Germany

Grain boundary diffusion of Mn in α-Fe has been studied in both, B- and C-types kinetic regimes in a wide temperature range of 473 to 1173 K. The concentration profiles were measured applying the radiotracer technique with serial sectioning by microtome and using the 54Mn radioactive isotope. As a result, Mn segregation at general high-angle grain boundaries of *-Fe is estimated. The grain boundary diffusivities were found to exhibit a distinct non-linear Arrhenius temperature dependence that in discussed in terms of the impact of the magnetic transition on Mn grain boundary diffusion.

MM 25: Topical Session (Symposium MM): Fundamentals of Fracture

Mesoscale Aspects of Fracture

Time: Tuesday 11:45–13:15 Location: TC 006

MM 25.1 Tue 11:45 TC 006

The Topology and Mechanics of the Formation of Fracture Surface Patterns — •Jay Fineberg[1], Itamar Kolvin[1], and Mokhtar Adda-Bedia[2] — [1]The Racah Institute of Physics, The Hebrew University of Jerusalem — [2]Laboratoire de Physique de l'Ecole Normale Supérieure de Lyon, Lyon, France

Fracture of brittle materials is often accompanied by the formation of structure on crack faces whose origin has long remained obscured. The difficulty lies in observing how microscopic structures are formed by rapidly moving cracks. To overcome this difficulty, we study soft brittle gels where crack speeds are significantly lower than in hard materials. Much below the shear wave speed, cracks form faceted surfaces separated by well-defined steps. At higher velocities, the facets give way to micro-branches, frustrated cracks that branch off the main crack. We directly visualize in real time the leading edge of the crack, the crack front, as it forms surface structure. In the faceting regime, steps induce long-ranged deformation along the crack front. Since surface formation costs energy, steps imply locally increased dissipation. We show that steps are stable due to topological defects of the crack front, that quantitatively link local dissipation increases at facets to crack front deformation and explain step persistence. We also show that crack front curvature may feed back to deflect step paths via nonlinear focusing of crack fronts, causing steps to converge to form a micro-branch. Thus, our results supply the basis for a unified picture of pattern formation on fracture surfaces

MM 25.2 Tue 12:00 TC 006

Crack front segmentation and subcritical instability in mixed-mode I+III fatigue and brittle fracture — Tristan Cambonie[1], Alain Karma[2], and •Veronique Lazarus[3] — [1]Department of Mechanical Engineering Development (GMD), Institut National des Sciences Appliquées, Lyon, France — [2]Physics Department and Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston — [3]UME-IMSIA, UMR 9219 EDF-CNRS-CEA-ENSTA ParisTech, Palaiseau, France

When loaded in mode I+III, a planar crack generically segments into an array of "daughter cracks" shaped as tilted facets which further coalesce during propagation.

A linear stability analysis has predicted that the coplanar crack propagation is unstable above a critical threshold $(K_{III}/K_I)_c$ (Leblond et al., JMPS, 2011). We aim here to go beyond this first order linear stability analysis, (i) to investigate whether the instability is subcritical, which should explain the discrepancy with the experiments where the segmentation is generally observed far below the predicted threshold and (ii) to study the non-wavy, hence non-linear, shape of the facets.

The non-linear stability analysis is performed using phase-field simulations. The predictions are compared with fatigue experiments (Lazarus et al., IJF, 2008) performed on plexiglas beams (Chen et al., PRL, 2015). We present also some additional fracture experiments performed either under cyclic or monotonic increasing loading.

MM 25.3 Tue 12:15 TC 006

Fracture properties of silica nanoparticle and clay gels — •Gustavo Gimenes and Elisabeth Bouchaud — PSL Research University, ESPCI Paris, UMR Gulliver, MMN, 6 rue Jean Calvin, 75005 Paris Cedex 05, France

Colloids at low volume fractions can gelate into amorphous solids by their aggregation into a space-filling network. Rheological and mechanical tests over those colloidal gels have shown interesting results such as yield localization and delayed yielding. However, direct observation of their fracture behavior at mesoscopic and microscopic scales is hindered by difficulties in imposing a controlled load on a soft material and by the combination of large deformations and viscoelastic processes.

We use two new experimental setups fabricated with microfluidic technology to study the fracture of aqueous colloidal systems made with silica nanoparticles and synthetic hectorite clay Laponite RD (with diameters around 25 nm). A wide range of behaviors was observed as a function of the ionic strength, particle volume fraction and gel times for both materials, from a linear elastic solid which breaks to a viscoelastic liquid flowing under load. During fracture, the measurement of the displacement fields in the vicinity of the crack tip by Digital Image Correlation and of the crack opening displacement enable the determination of the stress intensity factors and the energy release rates. The comparison of both methods allows us to estimate the size of the non-linear zone, which tends to increase for decreasing ionic strengths. We also evaluate the characteristic time by considering the influence of the crack speed.

MM 25.4 Tue 12:30 TC 006

A mesoscopic study of plastic damage of amorphous materials — •Cesare Cejas[1], Gustavo Gimenes[1], Patrick Tabeling[1], and Elisabeth Bouchaud[1,2] — [1]Microfluidics, MEMS, Nanostructures Laboratory, CNRS Gulliver UMR 7083, Institut Pierres Gilles de Gennes (IPGG), ESPCI Paris, PSL Research University, 6 rue Jean Calvin 75005 Paris, France — [2]CEA-Saclay, IRAMIS, SPEC, F-91191, Gif-sur-Yvette, France

Fracture mechanisms in amorphous systems are still not fully understood. Because of their disordered nature, these materials break involving dissipative processes such as secondary cracking ahead of the main crack tip and local structural rearrangements. The aim of our work is to make and fracture amorphous systems composed of big enough "atoms", so that the above mentioned mechanisms can be observed optically.

Our amorphous materials being soft gels, we use microfluidics both to fabricate concentrated emulsions they are made from, and to investigate their controlled fracture. We synthesize soft emulsion gels based on a difunctional acrylic monomer through photopolymerization in order to get an "atom" size of $\sim 50\mu$m. We vary the rheological properties of these emulsions by regulating conditions for polymerization. Using conventional optical microscopy, we hydraulically fracture these soft gels at controlled low rates and examine both micro-cracking and plastic events, i.e. the local irreversible displacements around the crack tip.

MM 25.5 Tue 12:45 TC 006

Precursors of fracture and failure in hierarchical materials — •Paolo Moretti, Bastien Dietemann, and Michael Zaiser — Friedrich-Alexander-Universität Erlangen-Nürnberg

Hierarchical materials are characterized by repeated microstructural features, which appear at different length scales in a self-similar fashion. Biological materials provide important examples of this type of hierarchical arrangement: connective tissue exhibits a hierarchical fiber organization which at different length scales comprises molecules, microfibrils, fibers, and fiber bundles. We study precursors of failure in hierarchical network models of of hierarchical materials where fibrous assemblies are held together by multi-level (hierarchical) cross-links. Our large-scale simulation study shows that when such structures are loaded towards failure, precursory avalanche activity displays generic scale invariance: irrespective of load, precursor events (avalanches) exhibit broad, power-law distributions of sizes without apparent cut-offs. We argue that this behavior can be traced back to the hierarchical microstrcuture, whose construction parameters can be harnessed in order to tune precursor activity and failure. This complex scenario results in super-rough crack morphologies, with large deflections that are reminiscent of crack shapes as encountered in biological materials.

MM 25.6 Tue 13:00 TC 006

Fracture of solid bodies under high pressure torsion — •Roman Kulagin[1], Yan Beygelzimer[2,3], Andrej Mazilkin[1,4], Emma Tröster[1], Yuri Estrin[5,6], and Horst Hahn[1] — [1]Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — [2]Donetsk Institute for Physics and Engineering named after A.A. Galkin, Kyiv, Ukraine — [3]Laboratory of Excellence for Design of Metal Alloys for Light Structures (DAMAS), Metz, France — [4]Institute of Solid State Physics, Chernogolovka, Russia — [5]Department of Materials Science and Engineering, Monash University, Clayton, Australia — [6]Department of Mechanical Engineering, University of Western Australia, Nedlands, Australia

The widely known method of High Pressure Torsion (HPT) was first proposed and described by P. Bridgman in his motivating article [P.W. Bridgman, Phys. Rev. 1935, 48, 825]. The future Nobel Prize winner was inspired by a tremendous multitude of phenomena in Nature associated with shear under high pressure. In his work, P. Bridgman suggested that HPT results in discontinuities in the deforming material, which are immediately healed under high pressure. Our experimental results will show that in the materials which are deformed by the HPT method, fracture and healing processes occur concurrently. To describe the underlying processes, we will present a model of fracture of a structurally inhomogeneous body. It will be shown that, as a result of the fracture and healing processes, intensive deformation-induced mixing of the constituents of the material takes place.

MM 26: Microstructure and Phase Transformations

Nucleation and Wetting

Time: Tuesday 11:45–13:00 Location: TC 010

MM 26.1 Tue 11:45 TC 010

Study on Temperature Rise in Pulsed Laser Atom Probe via Laser-Induced Interface Reactions in Al-Li alloy — •Muna Khushaim[1,2], Ryota Gemma[3], and Talaat Al-Kassab[2] — [1]Department of Physics, Faculty of science, Taibah University, PO Box 344, Medina, Kingdom of Saudi Arabia — [2]Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — [3]Department of Material Science, Tokai University, Kanagawa 259-1292 - Japan

The influence of tuning the laser pulse energy during the analyses on the resulting microstructure in a specimen utilizing an ultra-fast laser assisted atom probe was demonstrated. The decomposition parameters, such as the size, number density, volume fraction, and composition of δ' precipitates, were carefully monitored after each analysis. A simple model was employed to estimate the corresponding specimen temperature for each value of the laser energy. The results indicated that the corresponding temperatures for the laser pulse energy in the range of 10 to 80 pJ are located inside the miscibility gap of the binary Al-Li phase diagram and fall into the metastable equilibrium field. In addition, the corresponding temperature for a laser pulse energy of 100 pJ was in fairly good agreement with reported range of δ' solvus temperature, suggesting a result of reversion upon heating due to laser pulsing. This study proposed one simple method to estimate real specimen temperatures via laser-induced interface reactions during a laser-APT analysis.

MM 26.2 Tue 12:00 TC 010

Surface preparation by laser treatment for liquid phase epitaxy — •David Uebel, Roman Bansen, Christian Ehlers, Thomas Teubner, and Torsten Boeck — Leibniz-Institut für Kristallzüchtung

Bulk-based silicon solar cells consume much more raw silicon than electrically necessary. Therefore we grow crystalline silicon on glass just to the necessary thickness in a two-step process. First, amorphous silicon is applied by PVD to form a seed layer. Afterwards, a polycrystalline layer is deposited from a tin solution, supersaturated with silicon. To improve the growth on the seed, it is treated by a pulsed UV-laser directly before growth. Areal scanning heats up the surface and disruptive silicon oxides react with the chamber atmosphere. We will present a detailed model of the interaction process.

MM 26.3 Tue 12:15 TC 010

Study of the nucleation behavior and solid-liquid interfacial energy of pure metals — •Manoel da Silva Pinto, Martin Peterlechner, and Gerhard Wilde — Institute of Material Physics, Münster, Germany

We examine the liquid-solid transformation of selected pure metals and Germanium. The solid-liquid interfacial energy is of special interest due to its importance in the solidification process and other metallurgical phenomena. Various models suggest a correlation of this energy with bulk properties, e.g. the heat of fusion, which presents a more easily accessible quantity. Yet, so far experimental data of sufficient accuracy that allow for quantitative comparison with the model predictions are missing. In this work, data sets of the undercooling of Gold, Nickel, Copper, Cobalt and Germanium were acquired through calorimetric measurements. For statistical significance, datasets in the range of 100 to 1000 crystallization events were recorded for each material. The statistical analyses of these data yield a quantitative description of nucleation kinetics. The data also yield the solid-liquid interface energy and allows comparing the experimental results with theoretical predictions.

MM 26.4 Tue 12:30 TC 010

Reactive wetting behavior of SnPb micro-solder on Cu and Ni capillary tracks — •Samuel Griffiths, Patcharawee Jantimapornkij, and Guido Schmitz — Institute of Materials Science, Stuttgart, Germany

Micro-solder technologies are ubiquitous in modern electronics industries. And although these industries have pushed practical advancements in solder technologies, little is understood about the flow kinetics and thermodynamic theory which predicts solder flow behavior. This work quantifies and analyzes the capillary flow behavior of eutectic Sn-Pb micro-solder on microstructured linear Cu and Ni conductive tracks for multiple track widths. Solder-flow experiments have been conducted at 350°C in a reducing flux environment. We aim to quantitatively link parameters such as the equilibrium solder-flow distance, wetting/contour angles, and conductive track width. It is shown that, the relationship between the equilibrium solder-flow distance and track width behaves inversely for the Cu and Ni conductive tracks. Additionally, traditional contact angle control measurements are used to draw comparisons with the equilibrium angles of the solder fronts, which are the dimensionally unrestricted wetting angles of the solder-flow experiments. Electron microscopic imaging and chemical analysis as well as theoretical modelling based on surface energy minimization are applied to support our conclusions.

MM 26.5 Tue 12:45 TC 010

Melting and solidification of embedded particles at high heating and cooling rates — •Mark Stringe, Christian Simon, Harald Rösner, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, D-48149 Münster

During solidification of metallic particles embedded in a surrounding matrix, nucleation events take place at different sites and thus can depend on the morphology of the interface between particle and matrix. Moreover, the melting behavior of these particles is also different compared to bulk samples due to possible size, shape and pressure effects. In the present work, metallic particles were embedded in a higher melting matrix by the melt spinning technique. The microstructure was analyzed via x-ray diffraction and transmission electron microscopy. The metallic particles are of different sizes ranging from nanometer sized particles in the matrix grain interiors to micron sized particles at the grain boundaries. Using differential scanning calorimetry (DSC) the melting and solidification behavior was examined. Fast scanning calorimetry based on sensor chips for sample dimensions in the range of 100 microns allows measurements with heating and cooling rates which are by four orders higher than for conventional DSC. This method delivers new insight into the kinetics upon melting and solidification of these particles suggesting different kinetics of the transformations.

MM 27: Poster Session I

Time: Tuesday 18:30–19:45 Location: Poster E

MM 27.1 Tue 18:30 Poster E

Quantitative mapping of transient fields in plasmonic devices employing a novel STEM technique — •Johannes Schultz[1], Jonas Krehl[1], Axel Lubk[1], Darius Pohl[2], Giulio Guzzinati[3], Jo Verbeeck[3], and Tobias König[4] — [1]IFF, IFW Dresden, 01069 Dresden, Germany — [2]IMW, IFW Dresden, 01069 Dresden, Germany — [3]EMAT, University of Antwerp, 2020 Antwerp, Belgium — [4]IPF Dresden, 01069 Dresden, Germany

Surface plasmon polaritons (SPP) are self-sustaining resonances occurring in metallic nanoparticles. They are associated with strongly enhanced, localized electrical fields, which may be coupled to external optical excitations. SPPs can be used for the sub-wavelength control of electromagnetic fields. Based on this, novel electronic devices can be realized, for instance on-chip light spectrometers, plasmonic rectennas for the harvesting of light or LEDs and photovoltaics with a higher efficiency. SPPs can currently be mapped and hence characterized with nanometer resolution by measuring the energy-loss of a sharp electron beam in a TEM, which roughly corresponds to the z-component of the transient field. In order to record also the other components of the induced electric field, we developed a novel technique. We measure the deflection angles of inelastically scattered electrons. There, we take advantage of the fact that the measured deflection angle is proportional to the induced field components. By measuring the complete transient electric field, we comprehensively study the properties of the SPPs including associated dielectric susceptibilities and the field enhancement effect.

MM 27.2 Tue 18:30 Poster E

Contacts Between Cu and Sn Nanowires — •Zezhao Chen, Ziyi Wang, Samuel Griffiths, and Guido Schmitz — Institute of Materials Science Chair of Materials Physics, Heisenbergstr. 3, 70569 Stuttgart, Germany

Due to the commercial push for the size reduction of electronics and components therein, nanowires play an important role in the electronics industry. In this work, Cu-Sn nanowires have been studied, which are of scientific interest as solder-able nanostructures. The nanowires have been produced via electrodeposition using polycarbonate membranes as templates. First, Cu nanowires (50 nm in diameter) are partially grown from a CuSO4 solution and subsequently Sn is electrodeposited onto the Cu using a SnSO4 solution, resulting in segmented Cu-Sn nanowires. Furthermore, heat treatments at temperatures ranging from 220 °C - 400 °C are performed to investigate the formation of intermetallic phases within the dimensionally restricting nanowires. TEM, SEM, and EDX data has been evaluated to identify reaction products and growth mechanism.

MM 27.3 Tue 18:30 Poster E

Synthesis of Heterostructured Cu-Ni Nanowires — •Ziyi Wang, Tim Lehmann, Samuel Griffiths, Efi Hadjixenophontos, and Guido Schmitz — Institute of Materials Science Chair of Materials Physics, Heisenbergstr. 3, 70569 Stuttgart, Germany

In recent years, nanowires have been widely applied in electronic devices such as transistors and batteries due to their outstanding electrical conductivity and miniscule size. This work involves the research of phase stability of Cu-Ni nanowires, in order to determine whether heterostructured nanowires can form by annealing from the single phase solid solution. The whole work is separated into three steps. First, binary nanowires are prepared by electrodeposition using a porous membrane as a template. Second, different heat treatments are conducted at temperatures ranging from 130°C - 600°C in order to induce phase separation. Finally, SEM, TEM as well as EDX are utilized to analyze the nanowires. For a better understanding, Atom Probe Tomography (APT) is suggested for a 3D reconstruction of the nanowires.

MM 27.4 Tue 18:30 Poster E

Nucleation and Growth of Goldnanoparticles — •Felix Bourier, Tobias Redder, Christian Strelow, and Alf Mews — Universität Hamburg, Hamburg, Deutschland

Although inorganic nanocrystals are already used for large-scale technical and biomedical applications such as, biomarkers and drug delivery systems, their wet chemical production is still based on mainly empirical protocols. An understanding of nanocrystal formation exceeding the far too simplified classical models of nucleation and growth is still lacking.

Tracking the reduction of a gold precursor in toluene followed by the formation of nanoclusters, which then grow into particles should give better insights into the underlying mechanisms. This is achieved by combining experimental and simulated data with the use of a numerical aproached based on a set of rate equations.

MM 27.5 Tue 18:30 Poster E

Micro-mechanical behavior investigation of nanoporous gold: searching for the size of the structural unit — •Yijuan Wu[1], Jürgen Markmann[1,2], and Erica T Lilleodden[1,2] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht — [2]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg, Hamburg

Microcompression testing of nanoporous gold (NPG) was carried out in order to investigate the effect of the ratio of deformation length-scale to microstructural length-scale. By varying both the micropillar diameter and the NPG ligament diameter, a critical ratio was found above which the test structure can be considered a representative volume of material resulting in reproducible stress-strain behavior and uniform deformation. This critical ratio was found to be independent of microstructural length-scale, suggesting self-similarity between the different samples. Below this critical ratio, stochastic behavior is observed along with non-uniform deformation and failure, suggesting incomplete load-bearing units.

MM 27.6 Tue 18:30 Poster E

Towards 2D Topological Insulator Devices — •Katharina Polyudov[1], Kristina Vaklinova[1], Marko Burghard[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Spintronics requires the efficient generation, manipulation and detection of spin currents. Graphene has been demonstrated to be a high performance spin transport material, however due to its low spin orbit coupling (SOC), generation and control of the spin polarization by electrical means is difficult. Promising spin generators are the topological insulators (TIs), whose helical surface or edge states feature spin-momentum locking. One intriguing strategy is to locally decorate graphene by a 3D TI in order to create spin generator regions that could be smoothly integrated with laterally adjacent, bare graphene regions as spin transport channels. Along these lines, it is relevant that theory predicts that the interface-induced spin-orbit coupling (SOC) imparted by the 3D TI is able to increase the band gap of the 2D TI graphene. Here, we report the gate-dependent, low temperature charge transport properties of vertical heterostructures composed of graphene and a thin layer of Bi2Te2Se as 3D TI. By using different contact configurations, we explore the extent to which the presence of the Bi2Te2Se top layer modulates the magnetotransport properties of graphene, and furthermore whether signatures of charge transport through helical 1D edge channels within the graphene can be detected.

MM 27.7 Tue 18:30 Poster E

Transparent CdS@TiO2 Nanotextile Photoanode with Boosted Photoelectrocatalytic Efficiency and Stability — •Long Liu, Huaping Zhao, Rui Xu, Shipu Xu, Chenglin Zhang, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Photoelectrocatalytic (PEC) splitting of water into hydrogen and oxygen by direct use of sunlight is an ideal and renewable method for the hydrogen production, which could integrate the solar energy collection and water electrolysis into a single photoelectrode. In this context, we report the exploration of transparent CdS@TiO2 nanotextile photoanode with boosted photoelectrocatalytic (PEC) efficiency and stability, by controllable coating of amorphous TiO2 ultrathin layer via atomic layer deposition (ALD) technique. with precise controlled thicknesses and compositions at an angstrom scale. It is found that the coated pinhole-free TiO2 layers with fixed thicknesses at 0.5-10 nm are effective to stabilize the CdS textile electrode with improved PEC efficiencies, which could not only reliably suppress the active photocorrosion, but also create a tunneling barrier for photogenerated holes, suggesting their promising application for efficient evolution of H2. It is verified that the introduced TiO2 nanoshells could limit the charge recombination, facilitate the charge separation, reduce the charge transfer resistance, and enhance the wettability of electrode, resulting in their significantly enhanced PEC performance.

MM 27.8 Tue 18:30 Poster E

Hydrogen interacting with titanium dioxide: ab initio study — •Mohsen Sotoudeh[1], Marian Bongers[2], Vladimir Roddatis[2], Jakub Čížek[3], Carsten Nowak[2], Martin Wenderoth[4], Peter Blöchl[1,2], and Astrid Pundt[2] — [1]Institute for Theoretical Physics, Clausthal University of Technology, Leibnizstr. 10, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Department of Low-temperature Physics, Charles University in Prague, V Holešovičkách 2, 18000 Praha 8, Czech Republic — [4]IV. Physikalischen Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Electronic and structural properties of hydrogen doped rutile titanium dioxide has been investigated using first-principles calculations. We use density functional calculations with a band gap correction. We rationalize the various defects through the atomic and electronic structure as well as the thermodynamics. The goal is to explain the changes of electron energy loss spectroscopy (EELS) data obtained close to the Pd/rutile interface in different hydrogen environments. The calculations show that increasing the hydrogen partial pressure affects the interface concentration of oxygen vacancies and also the hydrogen content. A change of the electronic structure was observed depending on the defect types, their charge states, and their concentrations.

The work has been supported by the DFG through SFB 1073, projects C03 and C06 as well via the Heisenberg grant PU131/9-2.

MM 27.9 Tue 18:30 Poster E

HYDROGEN SORPTION KINETICS IN MgH2 AND TiH2 THIN FILMS — •Efi Hadjixenophontos[1], Lukas Michalek[1], Andreas Weigel[1], Michael Hirscher[2], and Guido Schmitz[1] — [1]Institut für Materialwissenschaft, (IMW) University of Stuttgart, Stuttgart, GERMANY — [2]Max Planck Institute for Intelligent Systems, Stuttgart, Germany, Stuttgart, Germany

Among metal hydride materials, Mg and its alloys show a great performance for the H-fuel based economy, however they still lack of performance. Transition metals eg.Ti seem to improve such systems.Here, we study separately the 2 systems:Ti-TiH2 and Mg-MgH2 in thin films (50-800nm) which enable us to monitor the hydride growth and determine the diff.coeff.The two metals show a different hydrogenation behaviour.The linear growth, due to the oxide passivation layer, in Ti, and the H diff. coeff. inside the oxide are quantified, as well as a reliable lower bound to the H diffusion coeff. in Ti is derived.The pressure dependence of H absorption is also quantitatively modelled.Micrographs support the fast diffusivity of H into Ti known from literature, since TiH2 is first formed closer to the substrate.In Mg, micrographs show MgH2 formed underneath the surface and a layer-like growth towards the substrate is observed.Surprisingly, a transition between linear (200°C) and parabolic growth regime (300°C) is observed.Resistivity measurements at the same conditions, are investigated to support this transition.Diff. coeff. and surface transport coeff. are determined by XRD,FIB and TEM.

MM 27.10 Tue 18:30 Poster E

Hydride formation in Mg-thin films — •Felix Maischner, Anshu Tyagi, and Astrid Pundt — Universität Göttingen, IMP

Magnesium is an interesting hydrogen storage material because of its high reversible hydrogen capacity in MgH$_2$ of up to 7,6 wt% and its high volumetric capacity of 110 kg/m^3 [1]. But a closed MgH$_2$ layer formed at the sample surface can block hydrogen uptake. Recently, it was shown that controlling the loading pressure allows efficient hydriding of Mg at 293 K [2]. This was interpreted by the related MgH$_2$ nuclei density. Further, the addition of grain boundaries improves the hydriding kinetics of Mg materials [3].

To study the nucleation and growth process in Mg thin films on a local scale, we perform STM measurements in an UHV-system between hydrogen loading steps. This surface sensitive method allows monitoring the hydride growth and morphology in the film via local height changes [4], as MgH$_2$ precipitates locally expand the lattice by about 30% in vertical film direction with respect to the α-phase Mg film [5]. 50 nm Mg films were prepared by cathode-beam sputtering on Si-substrates, covered with 10 nm Pd. The adhesion between the film and the substrate and its impact on the hydride morphology will be considered.

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MM 27.11 Tue 18:30 Poster E

Hydrogen Diffusion in α-Magnesium: Further Investigations into the Influence of Grain Boundaries — •Felix Jung[1], Magnus Hamm[1], Jakub Čížek[2], and Astrid Pundt[1] — [1]Institute of Materials Physics, Georg-August-Universität Göttingen, Germany — [2]Department of Low-Temperature Physics, Charles University, Prague, Czech Republic

In this work we measure the room temperature diffusion coefficient of hydrogen in the α-magnesium-hydrogen system by using gas volumetry. To explore the dependency of the diffusion coefficient on the volume fraction of grain boundaries, the sample grain size is varied. Grain boundary (D_{GB}) diffusion conventionally differs from bulk diffusion (D_{V}). For substitutional solvents in metals, D_{GB} is several orders of magnitude higher than D_{V}, for interstitial solvents it can be either lower or higher, depending on the solvent concentration [1, 2, 3]. Bulk magnesium samples subjected to various degrees of severe plastic deformation are characterized using optical and electron microscopy. Purity and microstructure of the samples are investigated by EDX and EBSD measurements. The grain size distribution is examined by an automated analysis of backscatter SEM images. Details of this method are presented. Financial support provided by the Deutsche Forschungsgemeinschaft via the projects PU131/9-2 and PU131/10-1 is gratefully acknowledged.

[1] Kaur and Gust, Ziegler Press Stuttgart (1989)

[2] Mütschele et al., Scr. Metall. 21, 135-140 and 1101-1104 (1987)

[3] Uchida et al., Acta Mater. 85, 279-289 (2015)

MM 27.12 Tue 18:30 Poster E

Dehydrogenation of the hydrogen storage material sodium borohydride — •Maik Szafarska[1,2], Georgia Sourkouni - Argirusi[1,2], and Wolfgang Maus - Friedrichs[1,2] — [1]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal - Zellerfeld, Germany — [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal - Zellerfeld, Germany

In the last decade, sodium borohydride (NaBH4) has attracted attention in energy storage research, caused by its high hydrogen density of 10.6 wt.% and relatively low cost, making it a potentially better hydrogen (and energy) storage unit compared to compressed hydrogen gas tanks and liquid hydrogen. Therefore it would be an improvement for fuel cell economy and energy storage. To accomplish this, NaBH4 has to be stabilized against decomposition through reaction with water in humid atmospheres and the dehydrogenation process must be understood properly, especially regarding NaBH4 decomposition during dehydrogenation. To investigate the dehydrogenation process and the desorbed components of the material, Thermogravimetric- and Multi Gas-Analysis were performed. The experimental results show correlations between particle size of the material and the desorption rate of hydrogen. In addition, a semi permeable membrane was used to successfully stabilize the NaBH4 against decomposition and analyzed for its influence on the hydrogen desorption process.

MM 27.13 Tue 18:30 Poster E

Hydrogen induced defects in the palladium/rutile titanium dioxide model system — •Marian David Bongers[1], Mohsen Sotoudeh[3], Vladimir Roddatis[1], Carsten Nowak[1], Martin Wenderoth[2], Peter Blöchl[3], and Astrid Pundt[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]IV. Physikalischen Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Institute for Theoretical Physics, Clausthal University of Technology, Leibnizstr. 10, 38678 Clausthal-Zellerfeld, Germany

The Pd/TiO$_2$ system is used in a range of applications where in particular the interaction with H is of interest. An insight into the basic interaction of H with the Pd/TiO$_2$ model system can yield to a fundamental understanding of the property-microstructure relations. We use in-situ environmental transmission electron microscopy (ETEM) and electron energy loss spectroscopy (EELS) on cross-sectional Pd/TiO$_2$ lamella focusing on the interface vicinity. The EELS studies show a small change of the Ti L edge signal in the 2 nm close vicinity of the interface, for H gas pressures of about 10 Pa. These changes are attributed to a shift in the density of states by about 1 eV, in the presence of H. This is supported by projector augmented wave code simulations using the local hybrid density functional PBE0r [1]. We suggest substitutional H to be the dominant H induced defect in bulk and nearby the interface. This work is supported by the Deutsche Forschungsgemeinschaft via SFB1073, project C06 and C03 as well via the Heisenberg grant PU131/9-2. [1] M. Sotoudeh, M. Bongers, et al., submitted

MM 27.14 Tue 18:30 Poster E

Investigations on degradation effects in SOFC fuel cells — •Hanna-Friederike Poggemann[1,2], René Gustus[2], Georgia Sourkouni[2], Christos Argirusis[3], and Wolfgang Maus-Friedrichs[1,2] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [3]School of Chemical Engineering, National Technical University of Athens, 9 Heroon Polytechniou St. Zographos Athens

Fuel cells are an important alternative to conventional processes of power generation. A fuel cell produces electrical power and heat directly from chemical energy. This avoids losses that can occur in conventional thermal and mechanical conversion processes during power generation. Nevertheless, the application of SOFCs for power generation is strongly limited by the life span and the robustness of the cells. In this regard, we investigated the degradation of SOFC fuel cells as a function of runtime and thermal as well as electrochemical strain. We used microscope and spectroscopic methods like Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray analysis (EDX) to investigate the microstructure and chemical composition of the anode and the cathode to get insight into changes in the elemental distribution and porosity of the fuel cells. In this context, we also examined the growth of the grains in the anode of the SOFC. Finally, we used Focused Ion Beam (FIB) tomography to gain further insight into the inner structure of the anode material.

MM 27.15 Tue 18:30 Poster E

Role of native oxide layer in silicon anodes for Li/S batteries — •Luca Silvi, Arne Ronneburg, Sebastian Risse, and Matthias Ballauff — EM-ISFM, Helmholtz-Zentrum Berlin, Berlin, Germany

Lithium/sulfur (Li/S) and Lithium/air systems are possible candidates for future electrochemical energy storage, due to higher gravimetric density compared to conventional Li-ion batteries. In these systems, a lithiated silicon (Si) electrode often replaces the Li metal anode, used as a Li ions reservoir. Detailed studies on lithiation and delithiation of Si anodes are of fundamental importance in understanding capacity fading effects. Silicon crystals are used with the native silicon dioxide (SiO2) layer: upon lithiation and delithiation, Li ions interact first with the SiO2, and subsequently intercalate in the Si crystal forming a Li/Si alloy. Due to the negative scattering length density of Li, neutron reflectometry is a powerful technique for investigating lithiation and delithiation of Si anodes. Two different Li/Si cells were prepared, one with and one without native oxide layer (removed using HF etching) on the Si anode. Both were measured at the reflectometer V6 at the BER II neutron source, to shade some light on the role of the SiO2 native layer formation and its (ir-)reversibility using both electrochemical (CV, EIS, charge/discharge) and in situ/operando neutron reflectometry measurements.

MM 27.16 Tue 18:30 Poster E

Microcalorimetric study of aluminum depositon/dissolution in BMIMCl/aluminium chloride ionic liquid — •junjie xu and rolf schuster — Institute of Physical Chemistry, Karlsruhe Institute of Technology, Fritz-Haber-Weg 2 76131 Karlsruhe

Ionic liquid systems, such as a mixture of 1-Butyl-3-methylimidazolium chloride (BMIMCl) and aluminium chloride, are promising electrolytes for aluminum batteries. In order to improve the performance of aluminum batteries, knowledge of thermodynamic properties of the electrochemical processes is required. In this study, we measured the Peltier heat of the aluminum deposition/dissolution reaction (about 10 kJ/mol at a molar ratio of BMIMCl to aluminium chloride of 1:1.7) with microcalorimetry. The positive Peltier heat corresponds to warming of the electrodes during the aluminum dissolution reaction. Consequences for the aluminum dissolution process in batteries will be discussed.

MM 27.17 Tue 18:30 Poster E

Computational thermodynamics: Meaningful phase diagrams without experimental input? — •Sebastian Schwalbe[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Central Michigan University, Department of Physics, USA

Ab-initio thermodynamic data sets, especially isobaric heat capacities, calculated within our new MD approach for lithium silicides [1,2] are presented. Further, a theoretical phase diagram is discussed, where the melting points are determined using a method based on the evaluation of diffusion behaviour. The key property, the so called diffusion coefficients, and the melting points themselves are compared with experimental data.

[1] Schwalbe et al., CMS, vol. 134, p. 48-57 (2017)
[2] Taubert et al., IJMR, vol. 108, no. 11, p. 942-958 (2017)

MM 27.18 Tue 18:30 Poster E

Examination of the partial electronic conductivity of mixed ionic and electronic conducting secondary particles — •Janis K. Eckhardt[1], Markus S. Friedrich[1], Simon Burkhardt[1,2], Limei Chen[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Gießen, Germany

Lithium ion batteries are widely used as power source in portable electrical applications. In particular with regard to optimization of existing applications or development of new technologies, it is necessary to understand the fundamentals of ionic and electronic transport inside the active cathode material. Most scientists are examining cathode materials by using composite electrodes which also contain additives influencing their electrochemical properties. To avoid such influences it is desirable to investigate the electrochemical properties of the pure active material. By using a specially designed electrochemical cell we performed electrochemical impedance spectroscopy and cyclic voltammetry measurements on single $\mathrm{Li(Ni_{1/3}Co_{1/3}Mn_{1/3})O_2}$ (NCM-111) secondary particles to gather information about their partial electronic conductivity. A cell arrangement that was suppressing the ionic current as a response to an external voltage signal was realized by making use of ion blocking metal electrodes. The results imply a correlation between the total resistance and diameter of the secondary particle, which was used to estimate the electronic partial conductivity.

MM 27.19 Tue 18:30 Poster E

Hydrothermal Synthesis and Functionalization of $\mathbf{LiFe_xMn_{1-x}PO_4}$ for Li-Ion Batteries — •Rouven Zeus[1], Elisa Thauer[1], and Rüdiger Klingeler[1,2] — [1]Kirchhoff Institut für Physik, Universität Heidelberg — [2]Centre for Advanced Materials, Universität Heidelberg

Hierarchically structured $\mathrm{LiFe}_x\mathrm{Mn}_{1-x}\mathrm{PO}_4$ with various doping levels $0 \leq x \leq 1$ has been synthesised hydrothermally. The material contains nanosized primary particles which are functionalised by carbon and agglomerate to microstructures. The effect of various precursors, organic additives and different synthesis conditions on the particle morphology and the hierarchical structuring is investigated. Electrochemical studies are applied in order to assess the feasibility of the resulting materials for energy storage in lithium-ion batteries.

MM 27.20 Tue 18:30 Poster E

TiO2 inverse opals as high-performance sodium-ion battery anodes — •Yang Xu, Min Zhou, Chenglin Zhang, Liying Liang, and Yong Lei — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Study of sodium-ion batteries (SIBs) has been rapidly increasing due to the growing demand of renewable energy. Electrochemical behaves of Na-ions are expected to be different from those of Li-ions because of the larger size of Na-ion, given a same host material. We employed TiO2 inverse opals as a model material to demonstrate the role of the orderliness of atomic arrangement in determining the SIB performance. We revealed that the disordering at the surface benefits to increase the contribution of surface process, while the disordering in the bulk results in improved ion diffusion but degraded electron transport. We therefore achieved high rate capability of the TiO2 inverse opals by enhancing surface ion availability that is enabled by the enhanced solvent wettability, regardless of the type of electrolytes and the concentration of Na-ion in the electrolytes. Our work offers a possibility to realize high SIB performance by adjusting the surface kinetics of the electrodes through controlling the orderliness of the atomic arrangement. This possibility could be transplanted to other energy storage systems.

[1] M. Zhou, Y. Xu, Y. Lei, et al., Adv. Energy Mater. 2016, 1600448. [2] M. Zhou, Y. Xu, Y. Lei, et al., Nano Energy 2017, 31, 514.

MM 27.21 Tue 18:30 Poster E

Concept to describe grain boundary properties depending on misorientation and inclination — •Volker Mohles and Adrian A. Schratt — Interdisciplinary Centre for Advanced Materials Simulation ICAMS, Ruhr-Universität Bochum, Bochum, Germany

In order to characterize the geometry of a grain boundary (GB) in three dimensions, essentially five independent parameters are needed, for instance three angles for the grain misorientation and two for the GB inclination. In order to enable mesoscopic simulations of GB motion with the ability to cover virtually all GBs, a functional description of the GB energy must be chosen, ideally based on a database of pre-calculated energy values. While the orientations of all grains in a mesoscopic GB simulation can be chosen in a discrete manner (using fixed points in a database), it is desirable to have a continuous description of the energy dependence with respect to the GB plane orientation in order to allow unrestricted GB motion. This description must account for the specific symmetries and cusps imposed by the GB plane orientation in relation to the crystal orientations of both pertaining grains. For such a five parameter description, a concept is introduced and discussed with respect to the expected ability to utilize (interpolate) existing or newly simulated data points (e.g. energy values from molecular dynamics simulations), which are discrete in nature, in macroscopic continuous models.

MM 27.22 Tue 18:30 Poster E

Mechanical properties of deformed and undeformed model glass former — •Mehrdad Golkia[1], Gaurav Shrivastav[2], and Jürgen Horbach[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Institut für Theoretische Physik, Sekr. EW 71, Technische Universität Berlin, Germany

The mechanical properties of glasses depend strongly on the history of their production. New glass states can be obtained by melting a glass via an external shear field, followed by a stress relaxation after switching off the shear. Since the imposed shear stress cannot completely relax to zero below the glass transition temperature, one eventually obtains a deformed glass with residual stresses [1],[2]. Here, we compare the elastic properties of deformed glasses to those of undeformed ones, using molecular dynamics computer simulations of a Kob-Andersen Lennard-Jones mixture [3]. The elastic constants of deformed and undeformed glass samples are obtained from the analysis of stress fluctuations. While the bulk modulus and the Poisson ratio are not affected by the shear deformation, slight differences can be seen in the shear modulus as well as Young's modulus. We also compare deformed and undeformed glasses in terms of the vibrational density of states and the boson peak.

References: [1] M. Ballauff *et al.*, Phys. Rev. Lett. **110**, 215701 (2013) [2] I. Binkowski, G. P. Shrivastav, J. Horbach, S. V. Divinski, and G. Wilde, Acta Mater. **109**, 330 (2016) [3] W. Kob and H. C. Andersen, Phys. Rev. Lett. **73**, 1376 (1994)

MM 27.23 Tue 18:30 Poster E

Interatomic interaction governed structural and dynamical evolution in La-based glasses and melts — •Zheng Wang and Konrad Samwer — I. Physikalisches Institut, Georg-August-Universität Göttingen,37077 Göttingen, Germany

Through systematic investigations on structural and dynamical properties of binary La-TM glass-forming alloys, the features of liquid states and the performances in the glasses are connected and found to be governed by the interatomic interactions. A relative loose packing in La-Cu systems from an observed positive excess volume could be the result of a combination of steep repulsion and anharmonic attraction of the potential. Based on the experimental determined potential features, properties of deformation units in glasses could be predicted from the dynamics of the melts, which also relate with the distinct relaxation behaviors. Our findings not only provide deeper insights into the glass-forming system property changes induced by interatomic interaction variations, but also shed light on designing desired metallic glasses from the characteristics of the melts.

MM 27.24 Tue 18:30 Poster E

Structural Study of the Metal Induced Crystallization of Silicon — •Max Stöber[2], Charaf Cherkouk[1], Slawomir Prucnal[2], Marcel Neubert[2], Claudia Funke[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg - Institut für experimentelle Physik — [2]Helmholtzzentrum Dresden Rossendorf - Institut für Ionenstrahlphysik und Materialforschung

Metal induced crystallisation (MIC) is a process of great interest for the design of powerful nanostructured materials in a sustainable way - using comparetively low energy and no wet chemistry. In this study the process was thermally activated using Si thin layers on Ni, Al and Cu substrates. Raman spectre reveal the diameter distribution of nanostructures and the changes in the phase structure. Furthermore, micro/nanostructures and dendrite growth resulting by layer intermixing were investigated using scanning electron microscopy (SEM). Depth profiling and chemical composition were performed by focused ion beam (FIB) and energy dispersive X-ray spectroscopy (EDX) technique.

MM 27.25 Tue 18:30 Poster E

Kinetic analysis of crystallization reaction within Co-Sn alloy — •Muna Khushaim[1,2], Fatimah Alahmary[2], Nessrin Kattan[1], and Ahmad Al-Joraid[1] — [1]Department of Physics, Faculty of science, Taibah University, PO Box 344, Medina, Kingdom of Saudi Arabia — [2]Division of Physical Sciences and Engineering, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

Co-Sn alloy is an important system for Sn- based anode materials of lithium ions batteries due to the different interesting intermetallic compounds nucleate and grow during crystallization reaction. Co -Sn alloys are applied in specific high-tech applications and hence study the kinetics of the crystallization reaction of this system and the dependency of the activation energy for crystallization on the temperature might provide a method to control the reaction and the synthesized products.In this study, Co: Sn alloy with ratio of approximately 1:3 were prepared by using metal flux method. The alloy was heated under a non-isothermal condition by using differential scanning calorimetry (DSC) at different heating rates. Microstructure characterizations of the samples have been done by using x-ray diffraction (XRD) and scanning electron microscopy (SEM). After observing the exothermic change during the DCS scanning, different kinetic methods were applied in order to determine the variation of the activation energy of crystallization with temperature. The effecting of the heating rate on the reaction model will be also presented.

MM 27.26 Tue 18:30 Poster E

Grain boundary morphologies in nanocrystalline $Pd_{90}Au_{10}$ go fractal: a simulation study of the growth kinetics — •Raphael Zeller[1], Christian Braun[2], Mingyan Wang[1], Rainer Birringer[2], and Carl E. Krill III[1] — [1]Institute of Micro and Nanomaterials, Ulm University, Germany — [2]Experimental Physics, Saarland University, Germany

Although abnormal grain growth has been investigated for more than 70 years, our understanding of its underlying physics is still quite tenuous. For nanocrystalline materials, the situation is particularly unsatisfactory, as their dominant mode of coarsening appears to be abnormal. In samples of nanocrystalline $Pd_{90}Au_{10}$ produced by inert gas condensation, abnormal growth is marked by rapidly growing grains sending "tentacles" out into the surrounding matrix, quickly encircling nearby grains and then consuming them. The perimeters of the resulting grains—revealed in metallographic sections—resemble those of fractal objects, and the grain interiors contain a significant number of small-angle boundaries. Modifying a phase field-based model for grain growth, we assess the extent to which these observations are consistent with a growth process based on grain rotation. We find that fractality can be viewed as a consequence of regrouping contiguous matrix grains into larger, simply connected regions. The residual boundary roughness reflects the length scale of the initial grain size.

MM 27.27 Tue 18:30 Poster E

Deviation of Ti-Al-N composition during APT analysis of Ti0.4Al0.6N — •Tim Lehmann[1], Patrick Stender[1], Guido Schmitz[1], and Wolfgang Engelhart[2] — [1]Universität Stuttgart, Institut für Materialwissenschaft, Lehrstuhl für Materialphysik, Heisenbergstr. 3, 70569 Stuttgart — [2]Walter AG, Derendinger Str. 53, 72072 Tübingen

Atom Probe Tomography (APT) is a powerful technique that allows for a three dimensional chemical analysis of needle-shaped specimens. In order to study decomposition processes in TixAl1-xN-thin films, samples of different composition were produced by HiPIMS. Recent measurements on decomposed Ti0.4Al0.6N-thin films have shown deviations from the expected stoichiometry in the Ti- and Al-rich domains. For a better understanding, pure TiN and AlN powder particles are analyzed as calibration samples by APT. The observed nitrogen contents are compared to the compositions measured by gas extraction and ICP-OES. The obtained correction allows for a better analysis of the measured compositions by APT. The powder particles are transferred to W-supports and post-processed via annual milling using a Focused Ion beam (FIB). Ti0.4Al0.6N-films are heat treated in Ar-atmosphere followed by subsequent post processing via FIB-lift-outs and annular milling.

MM 27.28 Tue 18:30 Poster E

Vacancy concentrations in quenched aluminium alloy AA7150 measured by a new fast scanning calorimetry and interrupted quenching method — •Bin Yang and Christoph Schick — Institute of Physic, University of Rostock

Differential fast scanning calorimetry (DFSC) has been combined with a novel differential reheating method (DRM). Interrupted quenching at different temperatures followed by overcritical cooling enables both time and temperature-dependent investigations of vacancy concentrations in aluminium alloys during cooling from solution annealing at cooling rates between 300 K/s and 100,000 K/s. Furthermore, the effect of vacancy on precipitation is investigated. The method can potentially be transferred to similar systems or related solid-state phase transformation systems also beyond the particular system analysed in the present study.

MM 27.29 Tue 18:30 Poster E

Miniaturisation of reactively wetting SnPb micro-solder on Cu and Ni capillary tracks — •Samuel Griffiths, Patcharawee Jantimapornkij, and Guido Schmitz — Institute of Materials Science, Stuttgart, Germany

Micro-solder technologies are ubiquitous in modern electronics industries. And although these industries have pushed practical advancements in solder technologies, little is understood about the flow kinetics and thermodynamic theory which predicts solder flow behavior. Quantification and analyses of the capillary flow behavior of eutectic Sn-Pb micro-solder on microstructured linear Ni and Cu conductive tracks is presented for multiple track widths. Solder-flow experiments have been conducted at 350°C in a reducing flux environment, resulting in reactive wetting. Parameters such as the equilibrium solder-flow distance, wetting/contour angles, and conductive track width are quantitatively linked. It is shown that, the relationship between the equilibrium solder-flow distance and track width behaves inversely for the Ni and Cu conductive tracks. Additionally, traditional contact angle control measurements are used to draw comparisons with the equilibrium angles of the solder fronts, which are the only dimensionally unrestricted wetting angles of the solder-flow experiments. Electron microscopic imaging and chemical analysis as well as theoretical modelling based on surface energy minimization are applied to support our conclusions.

MM 27.30 Tue 18:30 Poster E

Impact of UV light on the mechanical properties of collagen fibrils probed by Raman spectroscopy and Atomic Force Microscopy — •Marcus Schulze, Annika Stocker, Melanie Rogge, and Robert Stark — Physics of Surfaces, Materialwissenschaften, TU Darmstadt, Alarich-Weiss-Str. 16, 64287 Darmstadt

Collagen plays a decisive role in the development of substrates for tissue engineering. The controlled adjustment of its mechanical properties is essential and a potential strategy to achieve this is through physical treatment, such as UV light irradiation.

The focus of this study is to record the influence of heat and UV light on single collagen fibrils in situ. To that end, atomic force microscopy (AFM) was used for the simultaneous mapping of topography and modulus of type I collagen fibrils from rat tail tendon. The fibrils were probed in varied liquid environments (deionized water and phosphate buffered saline (PBS)) under UV light of varied wavelengths and temperatures of up to 45°C. Furthermore, structural changes in hydrated collagen films due to UV irradiation were investigated by means of Raman spectroscopy.

Our results showed that (UV/thermal) treatment performed in deionized water lowered the modulus of the collagen fibril. However, experiments performed in PBS-based solutions in combination with UV-B and UV-C light or thermal treatment of up to 45 °C showed an increase of the modulus within the first 30 to 40 minutes.

MM 27.31 Tue 18:30 Poster E

Subsurface Imaging of magnetic nanoparticles and measurement of nanomechanical properties of polymers and biological materials by bimodal atomic force microscopy. — •Lukas Stühn and Christian Dietz — Technische Universität Darmstadt, Darmstadt, Deutschland

We aim to observe the intrusion process of nanoparticles into human cells by bimodal frequency-modulated atomic force microscopy. To this end, a magnetic tip of an atomic force microscope is used to simultaneously detect the local mechanical properties of human HUVEC-cells and the subsurface locations of superparamagnetic ferritin nanoparticles.

We show that the mechanical characterization of biologic and polymeric matter is possible by the use of low-noise small cantilevers and photothermal excitation of the cantilever. To detect magnetic properties in a liquid environment, we increased the cantilever's oscillation amplitude several times using a backside coating of colloidal graphite. By embedding ferritin nanoparticles into a polymer-film, we studied the depth limits of the subsurface detection. High-resolution measurements of ferritin nanoparticles in liquids of different pH-values provided a first indication of the stability and organization of the protein shell. Moreover, we present images of human HUVEC-cells acquired by dynamic force microscopy.

MM 27.32 Tue 18:30 Poster E

Mechanical properties of 3D printed polymer-metal hybrid materials using FDM technology — Susanna Fafenrot, Nils Grimmelsmann, Martin Wortmann, and •Andrea Ehrmann — Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, 33619 Bielefeld, Germany

Fused deposition modeling (FDM) belongs to the 3D printing technologies. In FDM printing, a polymer is molten in the printer nozzle and placed line by line on the printing bed or the previous layer, respectively. Besides pure polymers, hybrid materials combining polymers with functional materials are also commercially available.

In a recent project, the mechanical properties of objects printed with metal-polymer blends were compared to pure poly(lactic acid) (PLA) printed elements [1]. Tensile and bending tests revealed that hybrid materials had significantly reduced mechanical properties. Unexpectedly, the tensile strengths of the 3D-printed objects were similar to those of the original filaments, indicating sufficient printing quality.

Our investigations show that while FDM printing allows for producing objects with mechanical properties similar to the original materials, metal-polymer blends cannot be used for the rapid manufacturing of objects necessitating mechanical strength.

[1] S. Fafenrot, N. Grimmelsmann, M. Wortmann and A. Ehrmann: Three-Dimensional (3D) Printing of Polymer-Metal Hybrid Materials by Fused Deposition Modeling, Materials 10, 1199 (2017)

MM 27.33 Tue 18:30 Poster E

Functional Principles of Nanostructured Particles as an Industrial Lubrication Oil Additive — •Alexander Beel, Katja Tönsing, and Dario Anselmetti — Experimental Biophysics & Applied Nanoscience, Bielefeld University, Germany

In contrast to conventional solid-state lubrication, the additivation with nanostructured particles not only facilitates the production of stable dispersions but also assures that particles will intrude quickly into the surface contact zone and create a protective layer.

In this contribution, we show by testing a dispersion including base oil, an additive package, and TiO_2-nanostructured particles in disc-disc triboexperiments that TiO_2-nanostructured particles yield a substantial friction reduction in specific material combinations. In order to clarify the mechanism of nanostructured particles as a lubricating agent, we discuss different approaches from literature, e.g. the ball-bearing effect, a surface polishing, the structural lubricity, rheological behavior, and a protective layer.

The friction reduction was observed in experiments where the lowest surface roughness was exhibited after the test procedure (polishing). As a consequence a titanium (dioxide) layer was built up on the disc surface which was detected with element-specific energy dispersive X-Ray analysis (EDX). By performing an experiment with used discs from a former TiO_2-dispersion experiment, we could conclude that the surface polishing and the titanium layer play an essential role for superior friction performance where a ball-bearing effect could be excluded

(Beel et al., 2017, Materials Today: Proceedings).

MM 27.34 Tue 18:30 Poster E

Mechanical Control of Atomic-Scale Transistors — •Florian Wertz[1], Torben Staiger[1,2], Fangqing Xie[1], Marcel Heinze[1], Philipp Schmieder[1], Christian Lutzweiler[1], and Thomas Schimmel[1,2] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein- Leopoldshafen, Germany

The atomic-scale transistors are devices that allow to open and close an electrical circuit by the controlled and reversible repositioning of just one or a few metal atoms. By means of a small electrochemical voltage in the millivolt range applied to a gate electrode, a few silver atoms are reversibly moved in and out of an atomic-scale junction, in this way reversibly closing and opening an electrical quantum point contact (QPC). The atomic-scale transistor is realized in an electrochemical cell at room temperature.

In the experiments presented here we integrated a three-point bending configuration within the cell to combine the electrochemical control (EC) with a mechanically controllable break junction (MCBJ) technique. With this EC-MCBJ technique we can perform mechanically controllable bistable quantum conductance switching of an atomic-scale transistor in an electrochemical environment. The device can be controlled both mechanically and electrochemically, and the operating modes can be combined, which expands the possibilities for controlling QPCs. Both operating modes of the QPC allow control with atomic-scale precision.

MM 28: Invited talk De Vita

Time: Wednesday 9:30–10:00 Location: TC 006

Invited Talk MM 28.1 Wed 9:30 TC 006

Accurate and fast machine learning n-body force fields — Aldo Glielmo[1], Claudio Zeni[1], James Kermode[2], and •Alessandro De Vita[1,3] — [1]King's College London, Strand, London WC2R 2LS, UK — [2]Warwick Centre for Predictive Modelling, University of Warwick, Coventry CV4 7AL, UK — [3]Department of Engineering and Architecture, University of Trieste, I-34127, Trieste, Italy

Modelling phenomena that couple complex local chemistry with higher scales, such as stress corrosion, embrittlement or friction is beyond the reach of first-principles MD techniques. Recent Machine Learning (ML) approaches might achieve the necessary accuracy [1] and, coupled with "on the fly" learning [2] and flexible use of large QM databases, offer a way to tackle the validation problem. However, ML-based MD simulations are not, as yet, mainstream. Key outstanding issues are how to construct ML-based schemes that are (i) verifiably more accurate than the available parametrised force fields (FFs) while being (ii) as efficient for incorporating prior knowledge on the target systems and (iii) as fast for predicting MD forces. I will review these problems, and discuss how they might be solved by Gaussian Process regression techniques using n-body covariant force kernels whose predicted forces can be suitably "remapped" to give new, fully efficient n-body non-parametric machine-learning force fields ("M-FFs")[3-4]. [1] F.Bianchini et al., Mod. Sim. Mat. Sci. Eng. 24, 045012 (2016) [2] Z.Li et al, Phys. Rev. Lett., 114, 096405 (2015) [3] A.Glielmo et al., Phys. Rev. B 95, 214302 (2017) [4] A.Glielmo et al., in prep.

MM 29: Nanomaterials

Synthesis and Characterization

Time: Wednesday 10:15–11:15 Location: H 0106

MM 29.1 Wed 10:15 H 0106

Solution-based synthesis of copper nanowires and automated diameter analysis — •Josef Mock[1], Marco Bobinger[1], Markus Becherer[1], and Paolo Lugli[2] — [1]Technical University of Munich, Institute for Nanoelectronics, Munich, Germany — [2]Free University of Bozen-Bolzano, Faculty of Science and Technology, Bozen, Italy

The demand for applications that require transparent conducting electrodes (TCEs) is rapidly growing and therefore, a low cost alternative to indium tin oxide (ITO), the prevailing TCE material, is needed. In this contribution, we present an environmentally friendly synthesis for CuNWs in aqueous solution at mild process temperatures. The synthesis employs Copper(II) chloride dihydrate as the copper-containing precursor, L-Ascorbic acid as the mild reducing agent and Oleylamine as the capping agent that directs the uniaxial wire growth. The optimum process temperature is found at 81 °C, which produces nanowires with a mean diameter of 100 nm and a mean length of 40 μm, respectively. With the aid of DiameterJ, the diameters of the CuNWs were analyzed in an automated and reproducible way from SEM-images. DiameterJ is a plugin developed for ImageJ and consists of two main components: the i) the segmentation part and ii) the analyzing part. The segmentation part of DiameterJ transforms the SEM image to a binary image, which is used for the analyzing part. As a result from the analyzing part, DiameterJ extracts two different diameters, the so called super pixel diameter and a fiber diameter histogram. Further, both diameters show good agreement to the manual analysis for the same SEM-images.

MM 29.2 Wed 10:30 H 0106

3D X-ray Diffraction Microscopy (3DXRD) using high resolution X-ray nanodiffraction — •Hergen Stieglitz, Christina Krywka, and Martin Müller — Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany

The existing technology called 3DXRD, is a well-established technique to map the grain structure of polycrystalline systems (e.g. metals). This technology is based on reconstruction algorithms which trace the positions of multiple Bragg-Peaks as a function of the rotation angle during the rotation of the sample. Due to a given beamsize and the software-based limit only a few grains can be tracked, resulting in a minimum mappable grainsize.

The planned experiment shall utilize a nano-focused synchrotron beam (e.g. Nanofocus Endstation of P03, PETRA III) to examine very fine-grained systems. The small beamsize allows detecting grains below the size limit of standard 3DXRD. With respect to the small beamsize of about 100 nm cross section, the precise positioning of the sample becomes more important to secure a constant scanned volume (the so called gauge volume). Otherwise some grains may be outside the gauge volume in some scans therefore they cannot be traced and produce mistakes while reconstructing.

To meet this challenge a stable and wobble-free rotary stage is planned to ensure a constant gauge volume. We are planning to use an interferomenter-based feedback loop to compensate the runout of the sample with a XY-stage. A further step is the adjustment of the existing software for the needs of a nano-focused beam.

MM 29.3 Wed 10:45 H 0106

Cryo-Atom probe tomography of soft matter and biological materials — •Jonas Ott, Patrick Stender, and Guido Schmitz — Institut für Materialwissenschaft, Lehrstuhl für Materialphysik, Stuttgart, Deutschland

Atom probe tomography (APT) is a well-established technique of chemical analysis with sub-nanometer resolution for metals, semiconductors and ceramics. Initially limited to metals (atom probe analysis available since 1968), the extension by pulsed laser enabled regular APT investigations of non-conductive materials since 2004. Still organic materials, soft matter or even liquids have not become a reasonable part of APT investigations, which is mainly due to the difficult sample preparation and unsuitable mechanical properties of the produced tips. Regarding biological materials such as cells and proteins in nanobiology or porous soft matter for catalysis, the expansion of APT technique to organic materials would offer exciting new opportunities. In our studies, we successfully created a new instrument by combining a dual beam FIB and a miniaturized atom probe chamber which allows the fast direct cryo-transfer and innovative measurement protocols. With this instrument, preparation of the required needle even of frozen liquids becomes possible, avoiding complex lift-out and gluing processes becomes. Measurements of natural honey and supersaturated glucose solution are presented and discussed.

MM 29.4 Wed 11:00 H 0106

A novel 3D test pattern for full-field transmission x-ray microscopy * nanoporous gold — •Emanuel Larsson[1], Malte Storm[2], Fabian Wilde[1], Markus Ziehmer[1], Kaixiong Hu[1], Doga Gursoy[3], Francesco de Carlo[3], Erica Lilleodden[1,4], Martin Müller[1], and Imke Greving[1] — [1]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, 21502 Geesthacht, Germany — [2]Diamond Light Source Ltd, Didcot, UK — [3]Advanced Photon Source, Argonne National Laboratory, Argonne, 60439, USA — [4]Institute of Advanced Ceramics, Technische Universität Hamburg, 21073 Hamburg, Germany

Nanoporous gold (NPG) is the structure resultant from dealloying of an Ag-rich AgAu alloy (Mameka et al., 2016).

The high absorbing capabilities of NPG together with the possibility to tailor the ligament diameters (from 20 nm up to 1 μ m) with respect to the achievable resolution of a given synchrotron or lab-based Full-field Transmission X-ray Microscopy (XTM) setup makes NPG an optimal 3D test pattern for XTM.

Reconstructed slices of NPG were analyzed with both qualitative and quantitative image parameters, e.g. Contrast-to-Noise Ratio, Percentage Volume, Ligament Thickness, Specific Surface Area, Sphericity etc. using the Pore3d software package (Brun et al., 2010). These parameters can then be used to compare the efficiencies in-between different XTM-setups.

MM 30: Interfaces

Structure and Properties

Time: Wednesday 10:15–11:30 Location: H 0107

MM 30.1 Wed 10:15 H 0107

Tailoring the thickness of intermetallic interfacial nanolayers by temperature control of FSW in Al-Cu lap joints — •Roland Marstatt[1], Markus Krutzlinger[2], Johannes Luderschmid[1], Michael F. Zäh[2], and Ferdinand Haider[1] — [1]Chair for Experimental Physics 1, University of Augsburg, D-86159 Augsburg — [2]Institute for Machine Tools and Industrial Management (iwb), Technical University of Munich, D-85748 Garching

The Friction Stir Welding (FSW) process is suitable to join dissimilar materials. The solidus temperature is not exceeded during FSW. Hence, joints between dissimilar metals can be produced with minimal intermetallic phase formation. The intermetallic phases can cause embrittlement and also lower the electrical and thermal conductivity across the interface. However, nano-scale intermetallic layers between joining partners have been reported in literature repeatedly, and these play a key role in material bonding. The layer thickness is related to welding temperature via an Arrhenius law. However, the correlation of the process parameters and the interface structure is still a subject of ongoing research. In this study, the potential of temperature control during FSW in order to improve the joint quality has been analyzed. The influence on and control over intermetallic layer thickness was investigated by welding dissimilar lap joints of aluminium and copper at different temperatures. The temperature was controlled by varying the rotational speed using a PI-controller. The results expand the existing knowledge and prove the applicability of temperature control during FSW of dissimilar metals. Supported by the DFG as part of SPP1640.

MM 30.2 Wed 10:30 H 0107

Direct observation of novel structures and transitions in [111] tilt grain boundaries — •Thorsten Meiners[1], Timofey Frolov[2], Christian H. Liebscher[1], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf — [2]Lawrence Livermore National Laboratory

It is well known that grain boundaries (GBs) have a significant influence on the materials macroscopic mechanical properties. Recently, thermodynamic models and atomistic calculations have predicted the possibility of GB phase transitions, which can alter the GB properties. In our study, we investigate the structure of symmetric and asymmetric [111] tilt GBs in copper by aberration-corrected scanning transmission electron microscopy (STEM) and molecular dynamics simulations (MD). The structural units of two symmetric Σ 19b tilt boundaries (46.83° [111]/{253} and 46.83° [111]/{178}) agree well with that obtained by the molecular static simulations. The symmetric 46.83° [111]/{178}) GB shows a regular pattern consisting of two structural units. In case of a asymmetric 46.83° [111]/{1-10}{9-2-7} tilt boundary we observe the same structural units, but now irregularly interrupted by a defect. These different structural units are also in agreement with MD simulations. At a special location, a sharp transition of the structural units with a stronger disorder at the asymmetric GB is observed. The coexistence of both structural motives provides first experimental evidence for the coexistence of two different GB phases. The differences in atomic ordering of the irregular structural units and transitions between structural motives will be discussed in detail.

MM 30.3 Wed 10:45 H 0107

A simple descriptor for energetics at fcc-bcc metal interfaces — •Linda Angela Zotti[1,2], Stefano Sanvito[2], and David D O' Regan[2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [2]School of Physics, AMBER and CRANN Institute, Trinity College, Dublin 2, Ireland

We developed a new and user-friendly method to calculate interface energies which avoids problems deriving from numerical differences between bulk and slab calculations (such as the number of k points along the direction perpendicular to the interface). We applied it to 36 bcc-fcc metal systems in the (100) orientation and found a clear dependence of the interface energy on the difference between the work functions of the two metals on the one hand, and the total number of d electrons on the other. Mechanical deformation was observed more in the fcc crystal than in the bcc counterpart. For each bcc metal, the interface energy was found to follow the position of its d- band, whereas the same was not observed for the fcc.

MM 30.4 Wed 11:00 H 0107

structural prediction of low-energy interface reconstructions of Σ 5 grain boundaries — •lin sun — Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena, Germany

We performed *ab initio* global structural predictions with the minima hopping method of interface reconstructions in three different silicon grain boundaries, Σ5(012), Σ5(031) and Σ5(521). We calculated interface energies and electronic density of states. Compared with locally optimized structures, our new structures have lower total energies and significantly smaller interface energies. We observed some recurrent geometrical features of the lowest energy interfaces: Si atoms prefer to form spiral structures rather than simiple rings. Concerning the electronic properties, defect energy levels in the band gap of locally-optimized interfaces can disappear after interface reconstruction. Our investigation suggests that global structural prediction is extremly important to predict the effect on transport and optical properties of grain boundaries in semiconductors.

MM 30.5 Wed 11:15 H 0107

Ab-initio based study of topological segregation of C impurities at Si grain boundaries — •Masud Alam, Liverios Lymperakis, Christain Liebscher, and Jörg Neugebauer — Max-Planck Institute for Iron Research,Max-Planck Str.1 , 40237 Duesseldorf, Germany

Interfaces significantly influence the properties of multi-crystalline Si.

More specifically, they introduce states in the fundamental band gap thereby allowing preferential impurities segregation and/or the formation of stable or metastable equilibrium interface phases. In the present work we investigate the segregation of C impurities at flat and faceted Si Grain Boundaries (GBs). In a first step we employ density functional theory (DFT) calculations to parametrize Si, C and Si-C modified embedded atom method (MEAM) interatomic potentials. Careful benchmarks show that the potentials provide an accurate description of the atomic geometry and energetics of intrinsic Si GBs (Wulff diagram) as well as of the C segregation at the aforementioned interfaces. Based on the new potential, we identify the preferential carbon segregation at faceted GBs. Using this insight we are able to interpret recent experimental findings on the topological segregation of impurities at facet junctions. More specifically, the presence of the energetically favorable non symmetric Σ3 112 GB results in strong anisotropy of the strain field and hence in strong selectivity of C impurities at the GB junctions.

MM 31: Topical session (Symposium MM): Fundamentals of Fracture

Atomistic Aspects of Fracture II

Time: Wednesday 10:15–11:30 Location: TC 006

Topical Talk MM 31.1 Wed 10:15 TC 006

Multiscale QM/MM Modelling of Materials Chemomechanics — •James Kermode — Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry, UK

Fracture is the dominant failure process underlying many materials reliability issues. At the same time, it remains one of the most challenging multi-scale modelling problems, requiring both an accurate description of the chemical processes occurring in the near tip region and the inclusion of a much larger region in the model systems. These requirements can be met simultaneously by combining a quantum mechanical description of the crack tip with a classical atomistic model that captures the long-range elastic behaviour of the surrounding crystal matrix, using a QM/MM (quantum mechanics/molecular mechanics) approach such as the 'Learn on the Fly* (LOTF) scheme [1]. I will review recent applications of this scheme to slow crack growth [2] and chemically activated fracture [3], and discuss a recent extension to the approach that uses the principle of virtual work with a modified nudged elastic band (NEB) algorithm to compute energy barriers for activated processes within the QM/MM framework [5]. The new method has been applied to compute lattice trapping barriers to brittle fracture in silicon as well and dislocation migration barriers in molybdenum and tungsten.

[1] G. Csányi et al., Phys. Rev. Lett. 93, 175503 (2004); [2] J. R. Kermode et al., Phys. Rev. Lett. 115, 135501 (2015); [3] A. Gleizer et al., Phys. Rev. Lett. 112, 115501 (2014); [5] T. Swinburne and J.R. Kermode, Phys. Rev. B 96, 144102 (2017)

MM 31.2 Wed 10:45 TC 006

The Brittle to Ductile Transition and the core structures of dislocations in silicon — •Jacques Rabier — Institut Pprime, DPMM, UPR 3346 CNRS-Université de Poitiers-ENSMA, BP30179, F-86962 Chasseneuil Futuroscope Cedex, France

It is now admitted that perfect shuffle dislocations control the plasticity of silicon in the high stress low temperature brittle domain and dissociated glide dislocations in the high temperature low stress domain [1]. The BDT appears then relevant to the transition between these two domains of plasticity. Unlike dissociated glide dislocations, core computations of perfect dislocations show that various core configurations can exist for a given dislocation. Some of these cores are sessile and differently from metals, these sessile dislocations cannot be mobilized under stress promoting the nucleation of crack [2]. Concurrently TEM experiments have shown that perfect dislocations nucleated in the brittle domain possess very efficient pinning points the density of which increases with temperature [2], [3]. Those pinning points appear to be intrinsic and relevant to some parts of sessile perfect dislocation cores. This induces a shut off of the perfect dislocations sources and a severe discontinuity in the apparent mobility of available dislocations close to the BDT, the consequences of which will be discussed.

[1] J Rabier, P Cordier, T Tondellier, J L Demenet, H Garem , Journal of Physics: Condensed Matter 12, 10059 (2000) [2] J. Rabier, L. Pizzagalli, J. L. Demenet, Elsevier B. V., 16, 47 (2010) [3] T. Okuno, H. Saka,, Journal of Materials Science, 48, 115 (2013)

MM 31.3 Wed 11:00 TC 006

Influence of large strains on the properties of dislocation cores in silicon: is a dislocation can initiate a crack? — •Laurent Pizzagalli, Julien Godet, and Sandrine Brochard — Institut Pprime, CNRS UPR 3346, Université de Poitiers, Poitiers, France

It is now well established that a usually brittle material like silicon can be plastically deformed at room temperature, if one considers low dimensional systems such as thin films, nanowires, nanopillars, or nanocubes. In these latter, due to the lack of bulk sources, the onset of plasticity usually occurs through the nucleation of dislocation from surfaces, and at large strains typically greater than 5%. The influence of these large strains on the properties of dislocation cores is usually overlooked and is currently unknown. We have investigated the properties of silicon 60° dislocation in these conditions, by performing atomistic calculations using several interatomic potentials, a tight-binding approach, and density functional theory. We found that the stability of the dislocation core is highly dependent on the imposed strain. In particular, it is revealed that a dislocation core could initiate a crack opening in conditions of bi-axial tension. Alternatively, we found that the formation of a localized disordered zone is favored in the case of bi-axial compression. These points constitute a possible explanation of the observed brittle-ductile transition as a function of size in nano-objects. Besides, this work also suggests that empirical interatomic potentials are not appropriate to describe dislocations in such conditions.

MM 31.4 Wed 11:15 TC 006

New theory for crack-tip dislocation emission and twinning in fcc metals — •Predrag Andric and William A. Curtin — Ecole Polytechnique Fédérale de Lausanne, Switzerland

Dislocation emission from a crack tip is a necessary precursor to crack blunting and toughening. Intrinsically ductile fcc metals under Mode I loading first emit a partial dislocation followed either by a trailing partial ("ductile" behavior) or a twinning partial ("quasi-brittle" behavior). The critical stress intensity factor K_{Ie} at which these processes occur is usually estimated by the Rice and Tadmor/Hai theories. Atomistic simulations show these models to be reasonable but not highly accurate, for predicting K_{Ie}. Analysis of the energy changes during nucleation reveals that the first and trailing partial emission are always accompanied by creation of a surface step, while twinning partial emission is not. Here, we present a new analysis in which first and trailing emission are controlled by a crack-tip instability due to the necessity of step formation. The absence of the step during twinning motivates another new model that accounts for the fact that twin nucleation does not occur directly at the crack tip. Both theories are quantitatively validated against molecular statics simulations across a wide set of fcc metals described with EAM potentials and excellent agreement is obtained. A twinning mode is also reported wherein the crack first advances by cleavage and then emits the twinning partial at the new crack tip.

MM 32: Microstructure and Phase Transformations

Precipitates and Grain Growth

Time: Wednesday 10:15–11:15 Location: TC 010

MM 32.1 Wed 10:15 TC 010

Multi Scale Modelling of the Size Evolution of Precipitate Clusters — •Tobias Stegmüller and Ferdinand Haider — Universität Augsburg, Institut für Physik, 86135 Augsburg

Precipitation processes in modern aluminium alloys are due to their significance for mechanical properties of great technical interest. The choice of an appropriate heat treatment, which evolves the distribution of precipitates in space, is the key that influences material parameters like strength, hardness and corrosion resistance.

The size distribution of precipitates during heat treatments is an important function for the characterisation of the temper state. In this work we will present a multi scale approach covering DFT, Cluster Expansion Monte Carlo simulations and the so-called Cluster Dynamics which directly calculates the evolution of the precipitate size distribution. The model was applied to the formation of Guinier-Preston zones in Al-Cu alloys and the results will be presented.

MM 32.2 Wed 10:30 TC 010

Investigating the size advantage of potentially abnormal grains — •Dana Zöllner[1] and Paulo R. Rios[2] — [1]B CUBE Center for Molecular Bioengineering, TU Dresden, Arnoldstr. 18, 01307 Dresden, GERMANY — [2]Escola de Engenharia Industrial Metalurgica, Universidade Federal Fluminense, Av. dos Trabalhadores, 420 Volta Redonda, RJ, 27255-125, BRASIL

The well-investigated process of curvature driven grain growth progresses by the motion of grain boundaries to the center of their curvature. In polycrystalline grain boundary networks this leads over time to a decrease in the total interfacial area and therewith also to a decreasing interfacial free energy. As a result, the grain microstructure evolves such that it has a unimodal size distribution. In contrast, abnormal grain growth proceeds in such a way that certain grains show an exaggerated growth, which leads to changes in the average growth law as well as to a bimodal size distribution. In the present work, Monte Carlo computer simulations of grain growth are employed to determine how grains showing a very large size advantage behave within a matrix of finer grains that can grow without restrictions. We demonstrate that true abnormal grain growth does not develop from those large grains. In fact, the large grains tend to decrease their size advantage over time and may eventually be *captured* by the grain size distribution of the matrix. However, another phenomenon may happen: the persistence of the size advantage of these grains may lead to pseudo-abnormal grain growth.

MM 32.3 Wed 10:45 TC 010

Evolution of the Prismatic Ultrastructure in Molluscan Shells via Hierarchical Grain Boundary Motion — •Dana Zöllner and Igor Zlotnikov — B CUBE Center for Molecular Bioengineering, TU Dresden, Arnoldstr. 18, 01307 Dresden, GERMANY

Biomineralization of complex composite architectures comprising the shells of molluscs proceeds via self-assembly in accordance with thermodynamic boundary conditions set by an organic macromolecular framework that is regulated by the organism. Hence, the formation of these ultrastructures can be reproduced using the analytical backbone of various physical theories that are commonly employed to express the growth of manmade materials. In this work, we develop an analytical framework for a quantitative study of the process of shell morphogenesis. The method is based on Monte Carlo simulations of grain boundary motion that, classically, were developed to study coarsening of polycrystalline metals. By employing this approach, we fully reconstruct the growth process of the two-level hierarchical prismatic morphology found in the shell of the mollusc Pinctada nigra. Spatial data on the latter was obtained using synchrotron-based microtomography imaging at beamline (ID19) at ESRF. The proposed framework is a fundamentally novel approach to study the structural regulation during biomineralization. It has the capacity to evaluate physical parameters, set by the organism, that are responsible for mineralized tissue morphogenesis in time and in space. Besides providing key insights into the fields of biomineralization, these parameters are pivotal to the fields of biomimicry, bio-inspiration and bottom-up materials synthesis.

MM 32.4 Wed 11:00 TC 010

Abnormal coarsening of nanoscale microstructures goes fractal — •Christian Braun[1], Raphael Zeller[2], Carl Krill[2], and Rainer Birringer[1] — [1]Experimental Physics, Saarland University, Germany — [2]Institute of Micro and Nanomaterials, Ulm University, Germany

Despite the supposed rarity implicit in its name, abnormal grain growth (AGG) appears to be a rather common mode of coarsening in nanocrystalline materials, regardless of composition or synthesis route. In inert-gas-condensed nanocrystalline Pd90Au10, thermally induced coarsening fulfills the criteria for AGG, but with an unusual twist: here, the subpopulation of abnormally growing grains sends offshoots in many directions into the surrounding matrix. The resulting irregular growth fronts manifest a fractal-like morphology characterized by a box-counting fractal dimension of 1.2 instead of the smooth interfaces observed in conventional samples. To gain insight into the nonstandard mechanisms and driving forces initiating and accordingly acting during this mode of coarsening in nanocrystalline PdAu-alloys, it is required to answer amongst others the following questions: Are there further differences in the coarsened morphology compared to conventional samples prepared by melting and solidification? What about correlations between fractality and local characteristics in microstructure? Can the fractal dimension be influenced by a variation of gold concentration, heating rate and dwell time? In this talk we will present our recent results to narrow down potential mechanisms responsible for fractal grain boundary migration in nanocrystalline metals.

MM 33: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 10:30–13:00 Location: HL 001

Invited Talk MM 33.1 Wed 10:30 HL 001

Correlating electrons via adiabatic connection approach: a general formalism, approximations, and applications — •Katarzyna Pernal — Institute of Physics, Lodz University of Technology, Poland

Electronic systems are usually described by assuming a model Hamiltonian, which only partially recovers electron correlation effects. To assure a quantitative description one faces a problem of recovering the missing part of the correlation. Over years different methods have been developed, most of them originating from the perturbation theory.

In my talk I will present another, fairly general, approach based on the adiabatic connection formalism. The idea itself is not novel although it has not been considered as a way of adding electron correlation for multireference models. Until recently it has not been realized that by combining the adiabatic connection (AC) with the extended random phase approximation one obtains a general tool capable of accounting for dynamical electron correlation for a broad class of multireference wavefunctions, applicable even to systems including strongly correlated electrons. It will be shown that the AC-based approximation yields excellent results when applied to multireference models, exceeding in accuracy second-order perturbation-theory-based methods.

MM 33.2 Wed 11:00 HL 001

Density functional theory of electron transfer beyond the Born-Oppenheimer approximation: case study of LiF — •Chen Li[1], Ryan Requist[1], and Eberhard. K. U. Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

We demonstrate that beyond Born-Oppenheimer (BO) effects can be accurately and seamlessly incorporated within a density functional framework. In alkali halides like LiF, there is an abrupt change in the ground state electronic distribution due to an electron transfer at a critical bond length $R = R_c$. We find that nonadiabatic electron-nuclear coupling produces a sizable elongation of the critical R_c by 0.5 Bohr, an effect which is very accurately captured by a simple and rigorously-derived nuclear mass-dependent correction to the exchange-correlation potential in density functional theory. Since this nonadiabatic term depends on gradients of the nuclear wave function and conditional electronic density, $\nabla_R \chi(R)$ and $\nabla_R n(r, R)$, it couples the Kohn-Sham equations at neighboring R points. Motivated by an observed localization of nonadiabatic effects in nuclear configuration space, we propose an approximation that reduces the search for nonadiabatic density functionals to the search for a single function. This work is a step towards bringing density functional theory beyond the limitations of the BO approximation.

MM 33.3 Wed 11:15 HL 001

Ground-State Quantum-Electrodynamical Density-Functional Theory — •Michael Ruggenthaler — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

In this talk I present a density-functional reformulation of correlated matter-photon problems subject to general external electromagnetic fields and charge currents [1]. I first show that for static minimally-coupled matter-photon systems an external electromagnetic field is equivalent to an external charge current. I employ this to show that scalar external potentials and transversal external charge currents are in a one-to-one correspondence to the expectation values of the charge density and the vector-potential of the correlated matter-photon ground state. This allows to establish a Maxwell-Kohn-Sham approach, where in conjunction with the usual single-particle Kohn-Sham equations a classical Maxwell equation has to be solved in order to capture the correlation induced by the transversal photon field. In the magnetic mean-field limit this reduces to a current-density-functional theory that does not suffer from non-uniqueness problems and if furthermore the magnetic field is zero recovers standard density-functional theory.

[1] "Ground-State Quantum-Electrodynamical Density-Functional Theory", M. Ruggenthaler, arXiv:1509.01417 (2017).

MM 33.4 Wed 11:30 HL 001

Design of auxiliary systems for observables: the dynamic structure factor and the electron addition and removal spectra — Marco Vanzini, Martin Panholzer, Lucia Reining, and •Matteo Gatti — LSI, CNRS, Ecole Polytechnique, Palaiseau, France

Density functional theory tells us that the external potential, and therefore all observables, are functionals of the ground state density. The exact functionals, however, are not known, and one has to find approximations. To obtain the density, Kohn and Sham have proposed the idea to use an "auxiliary system". Much research effort goes into finding better and better Kohn Sham potentials for the density and the total ground state energy. In order to access also observables other than the density, we have proposed to generalize the Kohn-Sham idea of an auxiliary system [1], and to design a "connector" that allows us to profit from calculations done in a model system [2,3]. We have recently shown that this is a successful strategy for the dynamic structure factor [2] and for the one-body spectral function of simple metals, semiconductors and insulators [3]. [1] M. Gatti, V. Olevano, L. Reining, and I. V. Tokatly, Phys. Rev. Lett. 99, 057401 (2007) [2] M. Panholzer, M. Gatti, and L. Reining, arXiv:1708.02992 [3] M. Vanzini, L. Reining, and M. Gatti, arXiv:1708.02450

MM 33.5 Wed 11:45 HL 001

Exact exchange energy of the ferromagnetic electron gas with dipolar interactions — •Camilla Pellegrini, Tristan Mueller, Kay Dewhurst, Sangeeta Sharma, and Eberhard K. U. Gross — Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We propose a density functional treatment of the magnetic dipole-dipole interaction as a spin-spin correction to the Coulomb force in the Breit-Pauli Hamiltonian. Within this microscopic approach, the Hartree-like term for the dipolar coupling corresponds to the classical magnetostatic energy currently implemented in micromagnetic calculations. In addition, we have derived quantum corrections by evaluating analytically the exact exchange energy (Fock term) for the homogeneous electron gas, within the linear response to a noncollinear magnetic field. We expect our functional to open the path towards a full ab initio description of inhomogeneous magnetic structures at the nanoscale, with applications to domain-wall operated spintronic devices.

MM 33.6 Wed 12:00 HL 001

Precise total-energy calculations at a significantly reduced cost — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In density-functional calculations, the total-energy functional is stationary with respect to the density, the Kohn-Sham orbitals and the Kohn-Sham effective potential. This means that approximations for these quantities only lead to total-energy errors of second order provided that the total-energy functional is evaluated accurately without further uncontrolled approximations.

Unfortunately, usually the Kohn-Sham orbitals and thus the kinetic part of the total energy are evaluated by using a projection of the potential into a finite subspace of basis functions. This approximation damages the stationarity of the total energy as a functional of the potential.

A technique will be discussed which can relieve this deficiency so that a considerably smaller subspace of basis functions can be used for a precise evaluation of the kinetic part of the total energy. The advantage will be illustrated for the particular example of angular projection potentials as they are used in the full-potential Korringa-Kohn-Rostoker Green function method.

MM 33.7 Wed 12:15 HL 001

Approach to Orbital-free DFT with Englert-Schwinger model — •Jouko Lehtomäki and Olga Lopez-Acevedo — COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland

We briefly present the Englert and Schwinger (ES) model in comparison with other approaches to orbital-free DFT. Essential failure of many kinetic energy density functionals is that they can not describe the most tightly bound core electrons in a satisfactory manner. Englert-Schwinger model allows treating these problematic electrons with more accurate single-particle wavefunctions while still obtaining the self-consistent orbital-free solution to the electronic problem.

Specifically, we detail how the ES model compares to the more known Thomas-Fermi-Dirac-Weizsäcker model self-consistently in atoms. We look at the total energy and few geometric properties. We show qualitative improvement in Pauli potential, which shows unphysical singularities near nucleus when the most tightly bound electrons are not treated correctly. We present how augmentation of the model with Kohn-Sham orbitals allows us to explore all-electron solution to the OFDFT problem and how this paves way for an orbital-free DFT method which does not need pseudopotentials.

MM 33.8 Wed 12:30 HL 001

The Kerker Preconditioner for FLAPW Methods with Charge Density Mixing — •Miriam Hinzen, Edoardo Di Napoli, Daniel Wortmann, and Stefan Blügel — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In metallic systems of larger size the self-consistent field convergence of electronic structure calculations is often slowed down substantially due to charge sloshing: close to the Fermi level, little change in energy can cause large fluctuations in charge density. Mathematically speaking, the problem is ill-conditioned. For plane-wave methods the Kerker preconditioner effectively solved this problem, but for many other electronic structure methods, in particular all-electron methods as the

FLAPW or KKR methods, a real-space formulation would be needed. We developed a formulation of the Kerker preconditioner for FLAPW methods with charge density mixing, implemented in `FLEUR` [1]. Numerical experiments show an enormous reduction of the number of iterations needed for convergence; even more importantly, the SCF convergence has become independent of the system size.
[1] www.flapw.de

MM 33.9 Wed 12:45 HL 001

Effect of spin on the generalized Pauli constraints in Reduced Density Matrix Functional Theory — •Nicole Helbig[1], Iris Theophilou[2], and Nektarios N. Lathiotakis[3] — [1]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece

Reduced Density Matrix Functional Theory is a method that relies on the 1-1 correspondence between the many-body ground-state wave function and the first order reduced density matrix (1RDM) and uses the latter as its fundamental variable. Enforcing the generalized Pauli constraints during the energy minimization ensures that the 1RDM corresponds to a fermionic pure state. We demonstrate that these constraints are modified for open-shell systems if the spin degrees of freedom are taken into account. From the generalized Pauli constraints we also derive properties of the exact occupation numbers and natural orbitals which ensure that the 1RDM corresponds to an eigenstate of the total spin.

MM 34: Nanomaterials

Grain Boundaries and Interfaces

Time: Wednesday 11:45–12:45 Location: H 0106

MM 34.1 Wed 11:45 H 0106

Equilibrium nanoparticle shapes for any size from atomistic simulations — •Magnus Rahm and Paul Erhart — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

In the pursuit of complete control over morphology in nanoparticle synthesis, knowledge of the thermodynamic equilibrium shapes is a key ingredient. While the classical Wulff construction provides a solution in the continuum limit, the small particle regime has been studied using global minimum energy search method reaching particle diameters of roughly 1 or 2 nm. The experimentally important intermediate size regime, however, has largely remained elusive. Here, we present an algorithm, based on atomistic simulations in a constrained thermodynamic ensemble, that efficiently predicts equilibrium shapes for any number of atoms in the range from a few tens to 10,000, corresponding to diameters between approximately 1 and 7 nm. We apply the algorithm to Cu, Ag, Au and Pd and reveal an energy landscape that is more intricate than previously suggested. In particular, we demonstrate that, as a result, the transition from icosahedral particles to decahedral and further into FCC particles occurs very gradually. One must thus expect more than one shape in thermodynamic equilibrium and not only for for kinetic reasons.

MM 34.2 Wed 12:00 H 0106

A Live Broadcast From Within Deforming Nanocrystalline PdAu Aggregates — •Michael Johannes Deckarm[1], Andreas Leibner[1], Marta Majkut[2], Vadim Dyadkin[2], and Rainer Birringer[1] — [1]Saarland University, D-66123 Saarbrücken — [2]ESRF, F-38043 Grenoble Cedex 9

Scaling the grain size of PdAu down to the low end of the nano scale (≈ 10nm) entails a dramatic change in mechanical properties. In a recent study, Grewer et al. [1] examined the deformation of nanocrystalline PdAu in an in-situ experiment using a combination of optical strain and synchrotron-based X-ray diffraction measurement. The central result was a quantitative estimate of the contributions of various processes to the deformation. In continuation of this work, we explored the effects of different strain rates and stress states, respectively, by a series of experiments at beamline ID11 at the ESRF. Scattering data with high temporal resolution spanning the entire deformation provide us with a broadcast of the evolving stress state. Specifically, we discuss a whole powder pattern modelling approach to extract structural information from our scattering data [2], to then reconstruct average stress and strain states of differently oriented grains as well as the signature of the elastic anisotropy of PdAu crystallites and its relation to the stresses or strains arising from the compatibility constraints in nanocrystalline PdAu aggregate.

[1] M. Grewer et al., Mechanics of Materials, 114, 2017, 254-267 [2] Scardi, P; Leoni, M., Acta crystallographica. Section A, Foundations of crystallography., 57., 2001, 604-613.

MM 34.3 Wed 12:15 H 0106

Evaluation of tension-compression asymmetry in nanocrystalline PdAu using a Drucker-Prager type constitutive model — •Andreas Leibner[1], Michael Deckarm[1], Hasan Raza Syed[2], Benjamin Klusemann[2], and Rainer Birringer[1] — [1]Experimentalphysik, Universität des Saarlandes — [2]Institut für Produkt- und Prozessinnovation, Leuphana Universität Lüneburg

There is ample evidence that the deformation behavior in nanocrystalline materials differs significantly from their coarse grained counterpart [1]. NC PdAu alloys at the low end of the nanoscale (≈ 10nm), where plasticity is predominantly mediated by grain boundaries [2], exhibit a distinct tension*compression asymmetry, which is unusual for fcc metals.

We performed deformation experiments utilizing a specific geometry. Tuning this geometry allows one to tailor the state of stress, in terms of compression to shear ratio, in the gauge section of the specimen. In order to evaluate the general deformation behavior of NC PdAu we employed FEM simulations and used a customized Drucker-Prager type constitutive material model.

In particular, we studied four different specimen geometries and varied the strain rate over five orders of magnitude down to 10^{-5}. As a result, we find an intriguing variation of deformation and failure behavior. Nevertheless, we tried to explore whether or not a single material law is capable of capturing the stress strain evolutions.

[1] E.N. Hahn and M.A. Meyers, Mat. Sci. Eng. A, 646 (2015) 101-134 [2] M. Grewer et al., Mechanics of Materials, 114 (2017) 254-267

MM 34.4 Wed 12:30 H 0106

Influence of local grain boundary structure on electronic transport in polycrystalline graphene — •Delwin Perera, Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Graphene is a promising material for microelectronics and sensor technology due to its high charge carrier mobility, high strength and optical transparency. Recently, it was found that nanocrystalline graphene is piezoresistive which makes it suitable for strain sensing [1]. Theoretical studies attribute this piezoresistivity to grain boundaries, which can induce transport gaps. The size of the transport gap is believed to depend only on the misorientation of adjacent grains [2].

Here, we investigate the effect of the local grain boundary structure on the electron transport properties of graphene. We use density functional theory together with the non-equilibrium Green's functions formalism to calculate transmission functions and current-voltage curves within the ballistic approximation [3]. Our results show that the size of the transport gap is indeed not affected by local structural changes. However, the details of the transmission function are sensitive to the local grain boundary structure. Therefore, the current-voltage characteristics depend not only on the misorientation.

[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)
[2] Kumar *et al.*, Nano Lett. **12**, 1362 (2012)
[3] Brandbyge *et al.*, Phys. Rev. B **65**, 165401 (2002)

MM 35: Interfaces

Segragation

Time: Wednesday 11:45–13:00 Location: H 0107

MM 35.1 Wed 11:45 H 0107

Strain-controlled electrocatalysis on gold thin film — •Xinyan Wu[1], Matthias Graf[2,3], and Jörg Weissmüller[1,3] — [1]Institute for Materials Physics and Technology, Hamburg University of Technology, Hamburg — [2]Institute for Electronic and Optical Materials, Hamburg University of Technology, Hamburg — [3]Insitute for Materials Technology, Helmholtz-Zentrum Geesthacht, Geesthacht

It is well known that the elastic deformation of a surface in its tangent plane modifies adsorption enthalpies. The observation is particularly relevant in heterogeneous catalysis, where strain - for instance in pseudomorphic active layers - is recognized as a means of tuning the reactivity and selectivity. Yet, quantifiable experimental observations of the impact of strain for catalysis are exceedingly rare. In other words, the field lacks a quantitative experimental database. Here, we use Dynamic Electro-Chemo-Mechanical Analysis (DECMA) in order to investigate the impact of strain on the electrocatalytic methanol oxidation on planar gold surfaces as a model reaction. Our approach works with a cyclic elastic strain applied to the surface and it detects modulations in the surface state and in the reaction current by means of a lock-in technique. In this way, DECMA affords quantifying the coupling between mechanics and reactivity as a function of the overpotential. In this way, the coupling strength can be explored separately for each reaction step.

MM 35.2 Wed 12:00 H 0107

Vacancy behaviour at FePt/MgO interface — •Petr Sestak[1,2], Miroslav Cerny[1,2], and Mojmir Sob[1,2,3] — [1]Institute of Physics of Mater., Academy of Sci. of CZ — [2]Central European Institute of Technology, Brno, CZ — [3]Faculty of Science, Masaryk University, Brno, CZ

Interfaces between two phases represent important parts of material structure. They have a significant effect on mechanical and magnetic properties. In particular, they can attract material defects like vacancies or dislocations. Moreover, vacancies located at interfaces can also serve as a place where impurities segregate. In our study we present ab initio simulations of formation of vacancies at the FePt/MgO interface. We analyze vacancy formation energy as a function of distance from the interface, the effect of vacancies on magnetic and mechanic properties and interaction between vacancies close to the interface.

MM 35.3 Wed 12:15 H 0107

Atom probe tomography of grain boundary segregation in the FeCr system — •Helena Solodenko, Patrick Stender, Sebastian Eich, and Guido Schmitz — Institute for Materials Physics, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Nanocrystalline materials have unique properties. This is due to the small grain size and high amount of interfaces, like grain boundaries (GB) or even triple junctions (TJ). Unfortunately, nanocrystalline materials are not thermally stable. The high amount of interfaces usually leads to a high interfacial excess energy, which is reduced by grain growth. A chance to overcome this problem is segregation of solutes to GBs, which can lower the interfacial energy and thus the driving force for grain growth. Density functional theory and experimental data suggest that the iron-chromium (Fe-Cr) system is expected to show exceptional thermodynamic behavior, which was also recently predicted by atomistic simulations based on a thermodynamically accurate embedded-atom potential. The key prediction is a distinctive negative GB energy for very specific compositions close to the phase boundary on the chromium-rich side, thus inhibiting grain growth. In this work, the segregation behaviour of Fe-Cr is investigated by atom probe tomography (APT). Nanocrystalline APT samples of a Cr(Fe) alloy with predefined compositions are produced by ion beam sputtering and focused ion beam. Reconstructed samples show strong segregation of the minority component Fe to Cr grain boundaries. The segregation isotherm is investigated at different compositions and compared with available atomistic studies.

MM 35.4 Wed 12:30 H 0107

Understanding chemical trends of solute-GB segregation by high-throughput analytics — •Liam Huber, Blazej Grabowski, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH

Microstructure evolution is critically influenced by solute interaction with grain boundaries (GBs). Depending on the mobility and driving force of solutes to segregate at GBs, even small additions of alloying elements may have a dramatic effect on microstructure evolution. We present high-throughput calculations of solute segregation to aluminium grain boundaries using a variety of available classical potentials. Using a cluster geometry unrestricted by periodic boundary conditions, we sample both high-symmetry boundaries commonly found in literature, as well as low-symmetry boundaries which are ubiquitous in real materials. We extract simplified descriptors based on the local structure and build models for predicting segregation energies on a per-site basis. To test the predictive capability of these models we apply data science techniques. We show that despite their relative simplicity these models deepen our physical understanding and provide novel insights into the nano-scale effects which influence solute-GB interaction. Based on this insight we discuss how to calculate model parameters a priori, leading to fit-free segregation predictions.

MM 35.5 Wed 12:45 H 0107

Mesoscopic simulations of grain boundary motion: influences on the Zener drag — •Volker Mohles — Interdisciplinary Centre for Advanced Materials Simulation ICAMS, Ruhr-Universität Bochum, Bochum, Germany

A new three-dimensional vertex model of grain boundary motion has been developed in which, for now, a single grain boundary is pushed through an array of particles in order to derive the Zener drag, i.e. the effective pinning force of these particles on grain boundaries. The spherical particles have a realistic size distribution and spatial arrangement. Like the grain boundary itself, the particle interfaces are described by a network of triangular facets, with the distinction that the nodes connecting the particle facets can only move tangentially along the surface of the prescribed particle shape. The model also accounts for the energy of the triple lines connecting the particles with the grain boundary. The simulations allow to derive the Zener drag as a function of the grain boundary energy, for now assumed to be independent of the grain boundary inclination, the triple line energy (constant), the mean particle size, and their volume fraction. The effects of varying size distribution and spatial arrangement are also tested. The results are compared to established formulations for the Zener drag.

MM 36: Topical Session (Symposium MM): Fundamentals of Fracture

Atomistic Aspects of Fracture III

Time: Wednesday 11:45–13:00 Location: TC 006

MM 36.1 Wed 11:45 TC 006

Cohesive stress heterogeneities and the transition from intrinsic ductility to brittleness — •Döme Tanguy — University Lyon 1, Villeurbanne, France

The influence of nanoscale cavities on the fracture of the $\Sigma 33\{554\}[110]$ symmetrical tilt grain boundary is studied by atomistic simulations. The crack crystallography is chosen such that dislocation emission is easy. A transition from a ductile behavior of the tip to a brittle one is obtained for a dense (coverage beyond 15% and inter-cavity spacing smaller than 4 nm) distribution of small cavities (sizes in between 1 and 2 nm). Nevertheless, the character of the crack is highly sensitive to the initial position of the tip and a mixture of ductile and brittle responses is found. A heterogeneous cohesive zone model, with parameters extracted from the simulations and enriched with a criterion for plasticity, can explain the simulations and reproduce the transition. Outside this range of small sizes and dense packing, dislocation half loops appear. They constitute, together with regions of low coverage/small cavities, efficient obstacles to brittle cracking. Furthermore, the generic character of the conclusions is evaluated by using the {554} single crystal to determine to which extent the results depend on the details of the core structure vs. the cavity distribution. Paper accepted in Phys. Rev. B.

MM 36.2 Wed 12:00 TC 006

Temperature Dependent Fracture Toughness of Defected Graphene — •Samaneh Nasiri, Debagyan Kalita, and Michael Zaiser — Friedrich-Alexander Universität Erlangen-Nürnberg, Department of Materials Science, Institute for Materials Simulation WW8 and Cluster of Excellence EAM/FUMIN Dr.-Mack-Strasse 77, 90762 Fürth, Germany

It is well known that sp* bonded carbon nanoparticles, in particular Graphene and Carbon Nanotubes, possess excellent mechanical properties in terms of in-plane elastic modulus and rupture strength. It is therefore an obvious question whether these properties can be influenced by defects. The present work investigates crack nucleation and crack propagation in defected graphene sheets over a wide range of temperatures. We consider the fracture behavior of graphene containing localized defects (vacancies) and/or extended defects (cracks) using atomistic (molecular dynamics) simulation. Fracture strength is shown to obey a Bazant-type size effect law where the internal length (process zone size) is of the order of the atomic spacing. The fracture toughness is also calculated in terms of the critical stress intensity factor for various temperatures from zero to as high as 3200 K. Results indicate a transition towards a different failure behavior and crack propagation pattern at temperatures above 2000K which may be interpreted in terms of a sub-nanometer scale brittle-to-ductile transition.

Keywords: graphene, fracture, temperature, crack, toughness, brittle-ductile transition

MM 36.3 Wed 12:15 TC 006

T-stress and the brittle-ductile behavior of edge cracks in 3D iron crystals — Anna Machová, •Radek Kolman, Alena Uhnáková, and Petr Hora — Institute of Thermomechanics, v.v.i., CAS, Dolejskova 5, 18200 Prague 8, Czech Republic

According to continuum treatment, the sign of T-stress in SEN specimens loaded uni-axially in mode I depends on boundary conditions and sample geometry. Since the sign of the T-stress can change theoretically brittle vs. ductile behavior of cracks, we verified recently the continuum predictions via molecular dynamic simulations (MD) in 3D bcc iron atomistic samples of SEN type. Crack orientation is (-110)[110] (crack plane/crack front), the axis of potential crack extension corresponds to [001] direction.

Under boundary conditions corresponding to constant stress at the borders the T-stress sign is negative for a short edge. For a relatively long crack it is positive. At higher level of linear loading, dislocation emission on <111>{112} slip systems was detected at the short crack with negative T-stress, while cleavage or brittle fracture was detected at the long crack with positive T-stress under relatively slow loading rates.

Behavior of relatively long cracks has been studied under constant displacement conditions, where negative T-stress is predicted. MD stress calculations confirm the change of the T-stress sign with the change of boundary conditions. Under higher loading, dislocation emission on <111>{112} slip systems and crack blunting were detected.

Acknowledgements to GACR 17-12925S.

MM 36.4 Wed 12:30 TC 006

Modelling Chemomechanical Materials Failure Processes in SiC and Diamond — •Punit Patel and James Kermode — University of Warwick, United Kingdom

Atomistic simulations of crack propagation are key to understanding the fracture behaviour of materials. Cracks involve strong coupling across the scales, with bond breaking on the quantum scale driven by long range stress fields. Current QM methods are limited to simulation sizes too small to accurately describe fracture dynamics and improved QM/MM methods are able to adequately capture elastic effects [1]. However these methods are still heavily limited temporally and to coarse grain into the continuum scale while maintaining the overall fracture dynamics an expanded multiscale approach is required.

Applications in covalently bonded single crystals to complex alloys are underway. Screened classical potentials [2] predict a brittle response in both silicon carbide (SiC) and diamond, giving confidence in their applicability. DFT SiC surface energy calculations produced predictions in good agreement with experiment [3]. Extension of the multiscale approach for fracture includes a novel approach in correcting for finite domain boundary conditions in order to compute energy barriers for crack extension bridging DFT and long time scale MD.

[1] N. Bernstein et al., Rep. Prog. Phys. 72, 026501 (2009).
[2] L. Pastewka et al., Phys. Rev. B. 87, 205410 (2013).
[3] G. Sernicola et al., Nat. Commun. 8, 108 (2017)

MM 36.5 Wed 12:45 TC 006

Atomistic-based fracture criteria for continuum models — Johannes Möller[1,3], Hamad ul-Hassan[2], Erik Bitzek[1], Alexander Hartmaier[2], and •Rebecca Janisch[2] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg — [2]ICAMS, Ruhr-Universität Bochum — [3]Fraunhofer Institut für Werkstoffmechanik, Freiburg

Continuum mechanics provides an efficient way to model fracture at the engineering scale, based on stresses, stress intensity factors, and energy release rates. Additionally, material-specific information and failure criteria are required to describe fracture at this scale. At the atomic scale, in contrast, the breaking of atomic bonds is caused by critical forces acting on individual atoms. Here, we present a systematic, mesh-independent approach that directly connects the interatomic forces to stress-based failure criteria for finite element implementations of continuum models. We base our approach on a detailed analysis of the forces acting between the atoms in front of a crack tip, as well as between two semi-infinite half-crystals, the latter being the common approach, e.g., for ab-initio density functional theory calculations of cohesive properties. The analysis shows, that the interatomic forces at a crack tip can be directly related to the restoring tractions between the two planar surfaces. This allows for an unambiguous scaling of the critical stresses and displacements, from GPa / Å on the atomic level, to the order of hundreds of MPa and nm on the mesoscale. The implementation in a finite element scheme will be demonstrated.

MM 37: Microstructure and Phase Transformations

Transformation investigations by diffraction and imaging (TEM, XRD)

Time: Wednesday 11:45–13:00 Location: TC 010

MM 37.1 Wed 11:45 TC 010

X-Ray Studies of Large Crystals with Small Holes: The Case of Virtual Nanoporous Gold — •Bao-Nam Dinh Ngô[1], Matthias Graf[2], Jörg Weissmüller[1,2], and Jürgen Markmann[1,2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (NPG) made by dealloying is a polycrystalline material with 10 – 100 μm sized crystallites that are interpenetrated by a network of 10 – 100 nm sized pores. X-ray powder diffraction by such structures has not been systematically studied so far. We explore the issue by theory, experiment, and virtual diffraction, with an eye on establishing a method for nondestructive microstructure characterization of NPG. Virtual diffraction studied a computer-generated NPG sample with crystal size 61 nm and ligament size 4 nm. The diffraction pattern of the truncated (porous) periodic crystal lattice in its unrelaxed state agrees well with our theory: A narrow central component of the Bragg reflections reflects the long-range lattice coherency while a broad foot reflects the loss of atomic neighbors due to nanopores. Thermal relaxation using molecular dynamics leads to a complete loss of the narrow component. This can be attributed to crystal lattice distortion (microstrain) due to surface stress. The virtual diffraction is in excellent agreement with experimental diffraction data.

MM 37.2 Wed 12:00 TC 010

Effect of Ca substitution on structural, dielectric and optical properties of Ba5NdTi3Nb7O30 ceramic — Vipin Kumar[1], Satender Nath Pandey[2], and •Sardool Singh Ghumman[1] — [1]Physics department, Sant Longowal Institute of Engineering & Technology, Deemed University, Longowal, District Sangrur Punjab 148 106 India — [2]Physics Department, Motilal Nehru National Institute of Technology, Allahabad 211 004 India

The polycrystalline samples of pure Ba5NdTi3Nb7O30 and Ca substituted Ba4CaNdTi3Nb7O30, in the tetragonal tungsten bronze (TTB) family, are prepared by solid state reaction method. Formation of single phase of the complex compound of orthorhombic type has been verified by X-ray diffraction analysis in both the cases. Surface morphology and uniform growth of grains are examined by scanning electron microscopy. The dielectric properties as a function of frequency and temperature demonstrate dielectric anomaly of ferroelectric to paraelectric phase transition with raised Curie temperature at 107 oC in comparison to 100 oC of calcium free compound. Optical absorption spectrum with FTIR indicates red shift in M-O absorption bond which signifies the distortion in the lattice. The enhanced dielectric stability over a considerable range of temperature calls for the calcium doped material for use in devices on low frequency and high temperature operation.

MM 37.3 Wed 12:15 TC 010

Atomic scale structural transitions at stacking faults in C14 Fe2Nb Laves Phase — •Christian Liebscher[1], Michaela Šlapáková[1,2], Sharvan Kumar[3], and Frank Stein[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]Charles University, Department of Physics of Materials, 12116 Prague, Czech Republic — [3]Brown University, School of Engineering, Providence, RI 02912, USA

Laves phases belong to the group of tetrahedrally closed-packed phases (TCP) and are commonly observed to exist in many material systems. The complex crystal structure of the C14 Fe2Nb Laves phase can be described by a layered arrangement of small (Fe) and large (Nb) atoms forming interpenetrating single and triple layers. By combining aberration-corrected scanning transmission electron microscopy (STEM) with atomic scale chemical spectroscopy, we unravel composition-induced atomic scale structural transitions at stacking faults in a Nb-rich Fe2Nb Laves phase. The fault density is observed to significantly increase with the presence of excess Nb atoms. Two basic variants, confined and highly extended faults are present. In the case of basal faults extending over several micrometers, nanometer-thin layers of the Fe7Nb6-phase are observed to form by the intercalation of multiple three-layer stacks of Nb atoms into the host Laves structure. At confined basal stacking faults, the formation of a fragmentary Fe7Nb6-phase is established, where a complete Fe kagomé layer is absent. This complexion is stablized by the imposed elastic and compositional constraints at the stacking fault.

MM 37.4 Wed 12:30 TC 010

Oxide texture as cause and effect in the corrosion of zirconium fuel cladding - an atomistic simulation and electron microscopy study — •Maria S Yankova, Felicity Baxter, Alistair Garner, Philipp Frankel, and Christopher P Race — School of Materials, University of Manchester, UK

Oxidation of the Zr alloy fuel cladding in light water reactors is one of the key degradation mechanisms, limiting the amount of fuel burned. The structural and electronic properties of monoclinic and tetragonal zirconia grain boundaries strongly affect the transport of species through the oxide layer. Hence, changes in oxide texture and phase fractions under irradiation can significantly alter the oxidation kinetics. We are exploiting a combination of density functional theory (DFT) simulation, scanning precession electron diffraction in the transmission electron microscope (TEM) and novel Python-based texture analysis to obtain an improved mechanistic understanding of the oxide microstructure. We have performed DFT calculations of the stiffness of key lattice planes in bulk zirconia to explore the effect of transformational stresses on the growth of grain orientations strongly represented in our experimental texture maps. We have revealed a correlation between the metal-oxide interface and a preferred texture orientation previously hidden by conventional texture analysis. We have investigated the effect of irradiation-induced defects and alloying elements on the structural and electronic properties of representative oxide grain boundaries using DFT and have identified the dominant point defects that control the oxide growth in an electrochemical environment.

MM 37.5 Wed 12:45 TC 010

Dynamics of sub-nm Pt clusters on carbon-based materials: Computation meets STEM measurements — Marta Bon, Trond Henninen, Daniele Passerone, and •Rolf Erni — Empa Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Crystallization, condensation and precipitation from a solution are three different phase transitions which are commonly described by the classical nucleation theory (CNT). CNT is generally in agreement with experiments, however does not define what fundamentally constitutes a pre-nucleation state or how a nucleus is formed at all. State-of-the-art scanning transmission electron microscopy (STEM) allows observing the dynamics of clusters smaller than 2 nm in size at atomic resolution.[1] Being however 2D projections of the 3D geometry of the clusters, STEM images are challenging to interpret directly. Molecular dynamics simulations boosted by enhanced sampling techniques, such as metadynamics,[2] can complement the high-resolution STEM measurements, and shed light on the formation, dynamics, stability, and evolution of tiniest atomic clusters which represent the embryos of solid matter. We show, in particular, the Pt 3D structures deposited on carbon-based materials, explaining how temperature and the interactions between the Pt atoms and the substrate can affect the clustering process.

[1] T. J. Woehl, et al. ACS Nano 6.10 (2012): 8599-8610. [2] A. Barducci, G. Bussi, and M. Parrinello. Phys. Rev. Lett. 100.2 (2008): 020603.

MM 38: Nanomaterials

Energy applications

Time: Wednesday 15:15–16:15 Location: H 0106

MM 38.1 Wed 15:15 H 0106

Structural Features of the Micromesoporous Carbons for Supercapacitors — •Eneli Härk[1], Albrecht Petzold[1], Günter Goerigk[1], Sebastian Risse[1], Nikolay Kardjilov[1], André Hilger[1], Sven Schneider[1], Matthias Ballauff[1], Uwe Keiderling[1], Indrek Tallo[2], and Enn Lust[2] — [1]Soft Matter and Functional Materials, Helmholtz-Zentrum für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Institute of Chemistry, University of Tartu, 14a Ravila Str., 50411, Tartu, Estonia

Depending on the synthesis route and conditions chosen, the carbons have different physico-chemical properties. A number of works led to the conclusions that the electrochemical properties vary widely depending on the hierarchical structure of the micromesoporous carbons. Several simulations have shown that an appropriate combination of three structural features determines at first the properties of the carbon, and consequently performance of the device. Due to the complexity of the morphology of the micromesoporous carbon there is still deficiency due date of the unambiguous correlation between the systematical structural features and electrochemical characteristics. A key structural features of micromesoporous carbons will be the subjects of a presentation. For characterization, the x-ray microcomputed tomography (μCT), small-angle neutron scattering (SANS), and small-angle x-ray scattering (SAXS) techniques were applied. The detailed structural information will be used for further optimization and development of the supercapacitors based on micromesoporous carbon.

MM 38.2 Wed 15:30 H 0106

Absolute Seebeck coefficient of individual silver nanowires — •Maximilian Kockert[1], Danny Kojda[1], Rüdiger Mitdank[1], Johannes Ruhhammer[2], Zhi Wang[2], Michael Kröner[2], Peter Woias[2], Toni Markurt[3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, D-12489 Berlin — [2]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, D-79110 Freiburg — [3]Leibniz-Institute for Crystal Growth, D-12489 Berlin

The Seebeck coefficient S consists of the diffusion part and the phonon drag part. The first part occurs due to thermal diffusion of charge carriers in the material caused by a temperature gradient. The second part is due to the interactions between electrons and phonons. Phonon drag is still today not fully understood. In order to investigate the influence of the phonon-phonon interaction and electron-phonon interaction on S, the absolute S of individual, highly pure and single crystalline silver nanowires is determined. In a comparison between the absolute S of bulk silver and silver nanowires, we demonstrate the influence of micro- and nanostructuring on the temperature-dependent profile of S. We show a reduction of the thermodiffusion part of S of the silver nanowires and a shift of the phonon drag peak towards higher temperatures compared to the bulk material, but without changing the maximum value of S. Here, we present a model for the absolute S, which demonstrates a reduction of the phonon-phonon interaction with respect to the electron-phonon interaction in the silver nanowires compared to bulk silver.

MM 38.3 Wed 15:45 H 0106

Nanoscale engineering for thermoelectrics: an ab initio study — •Phil Hasnip[1], Matt Probert[1], and Mahmoud Hussein[2] — [1]University of York, UK — [2]University of Colorado-Boulder, USA

Thermoelectric materials have the potential to dramatically improve the energy efficiency of many devices by converting waste heat into electricity. An ideal thermoelectric material has high electrical conductivity and low thermal conductivity, requirements which are often in conflict. When the thermal conduction is mediated by phonons, some improvements can be made by introducing point scatters and other defects to reduce the thermal conductivity; however these same defects often scatter electrons too, causing a simultaneous decrease in the electrical conductivity. In this work we use ab initio simulations to show that the thermal conductivity can instead be reduced by introducing phononic resonators on the surface of a material, scattering heat-carrying phonons whilst leaving the electronic properties almost unchanged.

MM 38.4 Wed 16:00 H 0106

Hybrid Materials Made From Nanoporous Metals and Electrically Conductive Polymers for Electrochemical Actuation — •Benedikt Roschning[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

The variation of an applied electrical potential modifies the surface stress of solid metals immersed in electrolyte. This variation of surface stress is transferred to the underlying bulk material, where it causes compensating stresses. The associated strain strain may be exploited for electrochemical actuation. The effect is small in conventional macroscopic bodies, due to their small surface to volume ratio. By contrast, nanoporous metals have a high internal surface area; these materials may be suitable as functional materials like sensors or actuators. Electrically conductive polymers, such as polypyrrole, swell or shrink through the potential-controlled incorporation or removal of anions. They constitute another class of chemo-mechanical actuators. Fast ion exchange is possible within thin polymer layers on planar conductive substrates, but the stiffness of the substrate limits the actuation amplitude. Combining the two mentioned approaches we investigate the actuation with nanoporous gold functionalized by coating the internal surface with polypyrrole. We show that these hybrid materials exhibit significantly enhanced actuation. The presentation also addresses the underlying coupling mechanisms.

MM 39: Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales

Grain Boundaries and Nanoporous Materials

Time: Wednesday 15:15–16:45 Location: H 0107

MM 39.1 Wed 15:15 H 0107

Observation of dislocation interactions with an asymmetric grain boundary in Cu by high frame-rate in-situ TEM — •Nicolas J Peter[1], Vasfi B Özdöl[2], Colin Ophus[2], Chrsitian H Liebscher[1], Christoph Kirchlechner[1], Andrew Minor[2], and Gerhard Dehm[1] — [1]Max-Planck Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]National Center for Electron Microscopy, Berkeley, USA

In-situ TEM nanomechanical testing enables direct visualization of plasticity mechanisms for deformation experiments at small scales. For instance, dislocation source operation and dislocation-dislocation interactions were studied in single crystalline materials to resolve the mechanisms controlling size scaling effects. However, far less studies are focused on unraveling dislocation interactions with interfaces, although understanding these plasticity mechanisms is important for structural materials. In the present study the atomic grain boundary structure of an artificially grown bicrystal was characterized by high-resolution STEM. Nano pillars containing the boundary and from adjacent grains were FIB-machined and tested in-situ inside a TEM equipped with a direct electron detector at a framerate of 400 fps. Fully and partially annealed samples were tested to investigate and reduce the impact of FIB damage that strongly affects the initial dislocation densities. Stable dislocation loop emission and dislocation glide were found to be main plasticity features in the single crystal references. Dislocation absorption, emission and pinning at the grain boundary were observed in the bicrystals and will be discussed in the talk.

MM 39.2 Wed 15:30 H 0107

Grain Boundary Effects in a High Entropy Alloys: Insights from Atomistic Computer Simulations — •Daniel Utt, Alexander Stukowski, and Karsten Albe — FB Materialwissenschaft FG Materialmodellierung, Technische Universität Darmstadt, Deutschland

High entropy alloys (HEAs) contain principle elements in concentrations between 5 and 35 at.%. Here we investigate the equimolar model alloy CuNiCoFe using atomistic simulations. We employs the embedded atom method potential by Zhou et al. (PRB **69**, 2004), which has been used for HEA simulations before, but was not characterized further. We systematically determine thermodynamic properties of all binary subsystems, with a focus on mixing enthalpies of random solid solutions, and confirm its validity. [Koch et al. (JAP **122**, 2017)]. We investigate the grain boundary (GB) segregation behavior in bicrystalline Cu$_x$(NiCoFe)$_{1-x}$ samples using a hybrid Monte Carlo / Molecular Dynamics algorithm. We discover significant Cu segregation at these GBs and show that the McLean model is not capable of describing GB segregation in this psudobinary system. Opposite to that, we find, that there is no segregation to planar defects like stacking and twinning faults. Further, we investigate nanocrystalline samples and discover that the HEA is much more resilient against thermal and stress-driven grain growth than elemental elemental nanocrystalline Cu or Ni. Comparing the grain growth and yield strength of a Cu segregated and truly random nanocrystalline CuNiCoFe HEA sample shows no significant influence of the Cu enrichment.

MM 39.3 Wed 15:45 H 0107

Tensorial elastic properties and thermodynamic stability of $\Sigma5(210)$ grain-boundary interface states in Ni$_3$Al — •Martin Friák[1,2], Monika Všianská[1,3,4], David Holec[5], and Mojmír Šob[3,1,4] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [4]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic — [5]Department of Physical Metallurgy and Materials Testing, Montanuniversitaet Leoben, Leoben, Austria

Grain boundaries (GBs) are among the most important defects in solids and their properties are crucial for many materials properties including their (in)stability. We calculate and analyze (tensorial) anisotropic elastic properties of interface states associated with GBs in Ni$_3$Al. Selecting the $\Sigma5(210)$ GBs as a case study, we address the mechanical stability of the GB interface states by checking elasticity-based Born stability criteria. One of critically important elastic constants, C_{55}, is found three times lower than in the bulk. Having the complete elastic tensor of $\Sigma5(210)$ GB states we combine a Green's-function based homogenization techniques and an approximative approach to the Debye model to compare thermodynamic properties of a perfect Ni$_3$Al bulk and the $\Sigma5(210)$ GB states. A significant reduction of the melting temperature is predicted (see IOP Conf. Series: Mat. Sci. Eng. 219 (2017) 012019 doi:10.1088/1757-899X/219/1/012019).

MM 39.4 Wed 16:00 H 0107

Mechanical properties of nanoporous gold - impact of solid fraction — •Birthe Zandersons[1], Lukas Lührs[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]InstitInstitute of Materials Physics and Technology, Hamburg University of Technologyute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

Nanoporous gold (NPG) is an attractive model system for studies of small scale mechanical behavior. Its centimeter-sized open porous bodies are structured by a monolithic network of struts or "ligaments". The ligament size can be tuned in the range of a few to several hundred nanometer. In the last years several studies find the mechanical behavior of NPG reproducible and highly consistent, except that the results fall in groups of substantially different strength. A widespread theory connects these differences to the variation of solid fraction due to different preparation. Here, we present a systematic investigation of the influence of preparation for the mechanical properties of NPG, using the most common preparation methods. Precursor alloys Au$_x$Ag$_{100-x}$ with $x = 20, 25, 30, 35$ are dealloyed electrochemically in 1 M HClO$_4$ and with free corrosion in concentrated HNO$_3$. Using continous loading and load/ unload compression tests we investigate the stress-strain behaviour, Young's modulus and Poisson's ratio and confirm substential differences depending on the initial alloy composition.

MM 39.5 Wed 16:15 H 0107

Effect of Polypyrrole Coating on the Elasticity of Nanoporous Gold — •Jie Li[1], Nadiia Mameka[1], Jürgen Markmann[1,2], and Jörg Weissmüller[1,2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Dealloying-derived millimeter-size nanoporous gold (np-Au), consisting of interconnected single nanoligaments network with large surface area, exhibits a switchable elastic modulus when its surface is electrically polarized in aqueous electrolyte [1]. Here, we decorate the surface of np-Au by a conductive polymer polypyrrole (PPy) that is also known to exhibit tunable Young's modulus upon charging in electrolytes [2]. While keeping the original porous structure, we have achieved a uniform PPy coating of various thicknesses in bulk np-Au by electropolymerization. The np-Au/PPy composites are then infiltrated by an aqueous electrolyte and subjected to potential variation in dynamic mechanical analyzer (DMA). The in situ DMA experiments reveal that the stiffness variation reaches the same magnitude as in the oxidation/reduction regime on pure gold without polymer coating. The material softens upon negative charging. We discuss possible mechanisms for the stiffness variation. [1] Mameka et al , Acta Mater. 76 (2014) 272. [2] Shoa et al, Synthetic Mater. 160 (2010) 1280.

MM 39.6 Wed 16:30 H 0107

Self-assembled monolayers of alkanethiols strengthen nanoporous metal — •Nadiia Mameka[1], Hartmut Gliemann[2], Jörg Weissmüller[1,3], and Christof Wöll[2] — [1]Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [3]Hamburg University of Technology, Hamburg, Germany

As one of the consequences of the large specific surface area of nanoporous metals, their mechanical behavior is sensitive to the surface chemistry. Studies on nanoporous gold (NPG) modified by a molecular monolayer of OH$^-$ ions exemplify this, finding two-fold increase of strength [1] and 8% increase of stiffness [2].

Here, we employ self-assembled monolayers (SAMs) of alkanethiols to modify NPG surface. Alkanethiol molecules, consisting of a sulfur headgroup that strongly interact with a metal substrate, a hydrocarbon chain and end-group, are known to spontaneously self-organize into well-ordered, dense two-dimensional molecular films. Alkanethiols with various chain lengths and terminal groups were used to prepare SAMs on bulk NPG and compression tests were performed on the SAM-modified and non-modified macroscopic samples. Our experiments reveal the substantial strengthening of the material due to the thiol adsorption that can reach up to 40%. This talk will discuss possible strengthening mechanisms mediated by the metal-sulfur interaction.

[1] Jin, Weissmüller, Science, 332 (2011) 1179. [2] Mameka et al, Acta Materialia, 76 (2014) 272.

MM 40: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data I

Big Data in Materials Science: Managing and exploiting the raw material of the 21st century organized by Claudia Draxl (Humboldt University, Berlin, Germany) and Peter Fratzl (MPI of Colloids and Interfaces, Golm, Germany)

Time: Wednesday 15:15–16:45 Location: TC 006

Topical Talk MM 40.1 Wed 15:15 TC 006

Novel high-entropy carbides discovered by synthesizability descriptors — •Stefano Curtarolo — Duke University, Durham NC, USA — Fritz Haber Institut, Berlin, Germany

High-entropy materials have attracted considerable interest due to their combination of potentially unique properties and promising technological applications. Predicting their formation from previously known parameters remains the major hindrance to the discovery of new systems. In this seminar, we introduce a descriptor - entropy forming ability - for predicting the synthesizability of such systems from first principles calculations. The formalism, based on the energy distribution spectrum of randomized calculations, captures the accessibility of equally-sampled states near the ground state and quantifies configurational disorder potentially leading to high-entropy homogeneous single-phases. The methodology is used to seek for disordered refractory 5-metal carbides | potential systems for ultra-high temperature applications. The descriptor correctly predicts a set of candidates that are experimentally synthesized as novel high-entropy homogeneous phases, validating the ansatz of the model. The method has the potential to accelerate the search and development of high-entropy crystalline systems by rationally combining first principles approaches with experimental synthesis.

MM 40.2 Wed 15:45 TC 006

First-Principles Thermodynamics of ZrO_2 at a Hybrid Level Using a Machine-Learned Potential — •Emre Ahmetcik, Angelo Ziletti, Matthias Scheffler, Christian Carbogno, and Luca M. Ghiringhelli — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

Due to their outstanding electronic and thermal properties, zirconia-based materials are used in a wide range of industrial applications, e.g., as catalyst support, as ionic conductor, and as thermal barrier coating [1]. Computational studies of its thermodynamic properties have hitherto relied on LDA/GGA-type functionals. However, it is well known that the exchange-correlation functional significantly affects the outcome of the calculations for this material [2]. We overcome this limitation by building a machine-learned Gaussian Approximation Potential [3] from a small number of first-principles calculations performed with a hybrid exchange-correlation functional. This allows us to simulate the dynamics of zirconia in supercells containing several hundreds of atoms and for several nanoseconds. By this means, we are able to obtain the phase diagram of ZrO_2 and to understand the mechanism that drive the monoclinic-tetragonal phase-transition.

[1] A. Evans, D. Clarke, and C. Levi, J. Eur. Ceram. Soc. 28, 1405 (2008)
[2] C. Carbogno *et al.*, Phys. Rev. B 90, 1441 (2014)
[3] A. P. Bartok *et al.*, Phys. Rev. Lett. 104, 136403 (2010)

MM 40.3 Wed 16:00 TC 006

First-Principles High-Throughput Study of Thermal Lattice Expansion Coefficients — •Maja-Olivia Lenz, Florian Knoop, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The thermal lattice expansion of bulk solids plays an important role in practical applications. Nonetheless, little of the respective data is tabulated to date ($< 2,000$ entries on Springer Materials) and the existing few first-principles data is in part obtained within arguable approximations [1]. We have used the quasi-harmonic approximation [2] to compute the thermal expansion for more than 1,000 materials from first principles using our recently developed Python framework HIGH-aims. Besides performing the necessary structure relaxations and phonon calculations, this framework also handles automatized convergence of numerical settings and evaluates different exchange-correlation functionals for cross-checking. We discuss the practical challenges of this approach and the trends observed across structural and chemical space. Eventually, we discuss opportunities to apply machine-learning techniques to predict different thermal properties of new, possibly so far unknown materials.

[1] C. Toher *et al.*, *Phys. Rev. B* **90**, 17417 (2014).
[2] S. Biernacki and M. Scheffler, *Phys. Rev. Lett.* **63**, 290 (1989).

MM 40.4 Wed 16:15 TC 006

High Throughput Screening for Novel Non-magnetic Antiperovskites — •Harish K. Singh, Ingo Opahle, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, Otto-Berndt-Straße 3, 64287 Darmstadt, Germany

Analogous to ABO_3 perovskite compounds, antiperovskite materials are one of the most commonly explored materials in recent years, due to many intriguing physical properties, such as superconductivity, solid electrolytes in batteries, thermoelectricity etc. In this work, we focus on nonmagnetic antiperovskite in the $Pm\bar{3}m$ space group with chemical formula M_3XY, where M and X are s-block, d-block (except Cr-Ni), and p-block elements (except noble gas, Po and At), and Y is B, N and C. This results in approximately 9,500 compounds. We carried out high throughput density functional theory calculations to evaluate the stability, including thermodynamical, mechanical, and dynamical stabilities, which are obtained by evaluating the formation energy together with the convex hull, elastic constants, and phonon dispersion, respectively. The distance from the convex hull is evaluated by considering all possible decompositions into binary and ternary compounds from the Materials Project database. Many novel non-magnetic antiperovskites compounds are predicted which satisfy all the above mentioned stability criteria, with interesting electronic properties awaiting for further experimental validation.

MM 40.5 Wed 16:30 TC 006

Finding new superconductors: doped insulators and the construction of computational descriptors — •Antonio Sanna[1], Jose' A. Flores-Livas[2], Henning Glawe[4], Kay Dewhurst[1], Gianni Profeta[3], and E.K.U. Gross[1] — [1]MPI of microstructure physics, Halle — [2]University of Basel — [3]Universita' de L'Aquila — [4]MPI for the structure ad dynamics of matter, Hamburg

Searching for thermodynamically stable new superconductors is computationally quite demanding. But thermodynamic stability is not a necessary requisite for a system to exist and to be of technological and scientific relevance. Simple cases of non thermodynamically stable materials are doped insulators that, at high doping, can become metallic and even superconductors. We show a few interesting cases we have recently investigated: phosphorene and water under pressure.

This type of ab-initio approaches are however computationally expensive and can not easily be applied to the investigation of large databases of materials or within accelerated material design algorithms. In this case a viable strategy could be to try to construct *superconductivity descriptors*, meant to be computationally cheap quantities (on the order of a Kohn-Sham DFT calculation) that, still, are able give a reliable indication of the superconducting coupling in a system. We review some past ideas, present a few new descriptors and validate them towards the actual ab-initio calculation.

MM 41: Liquid and Amorphous Metals

Thermodynamics and Kinetics

Time: Wednesday 15:15–16:45 Location: TC 010

MM 41.1 Wed 15:15 TC 010

Development and Characterization of Sulfur-bearing Bulk Metallic Glasses — •Alexander Kuball, Oliver Gross, Benedikt Bochtler, and Ralf Busch — Saarland University, Saarbrücken, Germany

Bulk metallic glass formation can be observed in many metallic systems by rapid cooling from the equilibrium liquid. However, the best metallic glass formers known so far can be found in systems with high concentrations of expensive and/or toxic elements like zirconium, phosphorous, or beryllium, limiting their commercialization.

Recently, we reported on a completely novel family of sulfur-bearing bulk metallic glasses (BMGs) excluding toxic elements. Bulk glass formation is observed in several multicomponent systems like in Pd-, Zr-, Cu-, Ni- and Ti-based alloys. Among these systems, especially the novel Ti-based alloys are of great interest for many fields of application. They show casting thicknesses for the synthesis of fully amorphous samples of up to 1 mm in combination with record Ti-contents of up to 70 at%, yielding to enormously high specific strength values.

The process of glass formation in these novel systems is discussed in terms of kinetics and thermodynamics. Because of the compositional differences in comparison to the BMG forming liquids known so far, the thermophysical characterization of sulfur-bearing BMGs may lead to an extended understanding of the glass forming ability in metallic systems in general.

MM 41.2 Wed 15:30 TC 010

Effect of Co microalloying on thermodynamic properties of a Pd40Ni40P20 bulk metallic glass — •Rene Hubek[1], Mikhail Seleznev[2], Isabelle Binkowski[1], Martin Peterlechner[1], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Germany — [2]Togliatty State University, Togliatty, Russia

The physical properties of bulk metallic glasses are subject of intensive research especially with respect to their mechanical behavior. Recently, it was shown that the mechanical properties of a Pd40Ni40P20 bulk metallic glass could significantly be enhanced through cobalt microalloying [1]. In this report we are focusing on the low-temperature hear capacity and DSC measurements. The results are discussed in comparison to the reference Pd40Ni40P20 glass [2, 3]. The effect of plastic deformation and post-deformation annealing on the excess heat capacity at low temperatures, known as the *boson peak*, is thoroughly examined. For DSC measurements the relaxation behavior of the fictive temperature and the overshoot enthalpy is investigated.

These data are discussed with respect to the excess free volume distribution in the PdNiP glass and the impact of Co microalloying.

[1] N. Nollmann et al., Scripta Mererialia 111 (2016), 119-122

[2] Y.P. Mitrofanov et al, Acta Materialia 90 (2015) 318-329.

[3] I. Binkowski et al, Acta Materialia 109 (2016) 330-340.

MM 41.3 Wed 15:45 TC 010

On the high glass-forming ability of Pt-Cu-Ni/Co-P-based liquids — •Oiver Gross, Sascha S. Riegler, Moritz Stolpe, Benedikt Bochtler, Alexander Kuball, Ralf Busch, and Isabella Gallino — Chair of Metallic Materials, Saarland University, Campus C6.3, 66123 Saarbrücken, Germany

Continuous and isothermal crystallization diagrams of the Pt42.5Cu27Ni9.5P21 and the Pt60Cu16Co2P22 bulk glass forming compositions are determined using calorimetric experiments. For the Pt42.5Cu27Ni9.5P21 liquid, the formation of the primary crystalline phase can be prevented by rapid cooling in a conventional DSC. In contrast, for similar cooling conditions, the formation of the primary precipitating compound in Pt60Cu16Co2P22 cannot be prevented in a conventional DSC as also observed in in-situ synchrotron X-ray scattering experiments. This is attributed to a critical overheating, above which remaining structures dissolve, resulting in a drastic increase of the degree of undercooling, similar to what is observed in Zr-based BMGs. Using the classical nucleation theory, the combined thermodynamic and kinetic data are used to model the isothermal crystallization data for Pt42.5Cu27Ni9.5P21, yielding an interfacial energy value of 0.11 J/m2 between the primary nucleating crystal and the liquid. This value is three times higher than the value for good Zr-based glass-formers, suggesting that the interfacial energy plays a pivotal role in the exceptionally high glass-forming ability of Pt-P-based systems and compensates for the fragile liquid behavior and the large driving force for crystallization.

MM 41.4 Wed 16:00 TC 010

The role of the Ga addition to the thermodynamics, kinetics, and tarnishing properties of the Au-Pd-Cu-Ag-Si bulk metallic glass forming system — •Nico Neuber[1], Oliver Gross[1], Miriam Eisenbart[2], Ulrich Klotz[2], Isabella Gallino[1], and Ralf Busch[1] — [1]Chair of Metallic Materials, Saarland University, Campus C6.3, 66123 Saarbrücken, Germany — [2]FEM, Research Institute for Precious Metals & Metals Chemistry, Katharinenstrasse 17, 73525 Schwäbisch Gmünd, Germany

In the last decade, the 18-karat gold Au-Ag-Pd-Cu-Si bulk metallic glass (BMG) system has received considerable attention as jewelry material due to its extraordinary premium-white gold color, the absence of allergen constituents such as Ni, Cr, and Co, twice the hardness of cold worked or age hardened conventional white gold alloys, melting temperatures below 700 K, less than 0.5% solidification shrinkage and a good processing ability. However, this system is affected by non-uniform tarnishing that is detrimental to its application. This behaviour is typical for a mixture of elements with very different nobility, where preferential oxidation and partitioning are common processes observed upon reaction with the environment. Based on thermodynamic considerations we have judiciously added Ga to the aforementioned system and developed novel 18-karat premium-white gold BMG compositions with improved tarnishing resistance. We report here upon the strategy applied to develop the novel compositions and the influence of the added Ga on the thermodynamics and kinetics of the system is assessed and possible further solutions are reviewed.

MM 41.5 Wed 16:15 TC 010

Synthesis and characterization of Tb75Fe25 nanoglass — •Shiv Prakash Singh, Herbert Gleiter, and Horst Hahn — Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

Nanoglasses have been developed with the original idea to generate a new kind of amorphous material, by the controlled introduction of defects and alterations of the chemical microstructure. This approach is similar to that used in nanocrystalline materials. In this work, we have synthesized a Tb75Fe25 nanoglass using the inert gas condensation method, by compaction of nanometer sized Tb75Fe25 glassy particles at 3 GPa. The as prepared nanoglass specimen (NG) was subjected to high pressure torsion (HPT) at 6 GPa with three complete rotations. X-ray diffraction pattern for the NG and the nanoglass specimen prepared using HPT (NGT) demonstrate the amorphous nature. Transmission electron microscopy revealed the amorphous structure with a small fraction of a crystalline phase for both NG and NGT. Differential scanning calorimetry demonstrated a lower crystallization temperature for the NGT in comparison to the NG. The NG showed a higher coercivity and lower magnetization than the NGT at 1.8K. The above NG and NGT specimens have then been heat treated at 390 oC for 30 minutes. The coercivity decreased for both heat treated samples compared to NG and NGT due to evolution of iron reach crystalline phase (Fe2Tb).

MM 41.6 Wed 16:30 TC 010

Low temperature excess heat capacity of AlYFe metallic glasses — •Marius Gerlitz, René Hubek, Martin Peterlechner, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster

The deformation behavior of metallic glasses differs from their crystalline counterpart due to the absence of defects like dislocations. Metallic glasses deform at ambient temperatures typically by nanometer sized, localized shear bands. To what extend a change in the structure of the surrounding matrix contributes to the plastic deformation is under current investigation. The vibrational states of atoms depend on their bonding and consequently on their mechanical coupling.

Thus, low temperature specific heat measurements are well suited to understand fundamental characteristics of vibrational modes. The excessive contribution to the specific heat at low temperatures, known as the boson peak, is a distinct feature in glasses and is though as being closely related to the structural states that allow for unit shear events. This work focuses on AlYFe as a representative of marginally glass forming systems. Deformed and relaxed sample states were analyzed by heat capacity measurements, X-ray-diffraction, calorimetric measurements as well as electron microscopy. The results are discussed with respect to the present literature on the boson peak. An enhanced relaxation behavior of metallic glasses is observed in deformed samples. The matrix is stated to be involved in the relaxation process.

MM 42: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 15:00–17:45 Location: HL 001

Invited Talk MM 42.1 Wed 15:00 HL 001

Computational Approach to the Electronic Structure of Strongly Correlated Materials: Towards Theoretical Spectroscopy and Theory Assisted Material Design — •Gabriel Kotliar — Serin Physics Laboratory Rutgers University — Brookhaven National Laboratories

We will introduce a project, to build algorithms and a suite of open source codes, to compute the electronic structure of correlated materials. It involves different methods, to provide different compromises between speed and accuracy, and to treat different types of correlation (static and dynamic). The suite includes methods ranging from vertex corrected GW, rotationally invariant slave bosons and LDA+DMFT, and we will illustrate some of these methods (and their failures) in d and f electron systems.

MM 42.2 Wed 15:30 HL 001

Spectral properties of Sr2IrO4 from first principles — •Cyril Martins[1], Benjamin Lenz[2], and Silke Biermann[2,3] — [1]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The spin-orbit system Sr2IrO4 has raised tremendous interest recently, due to intriguing similarities to the high-Tc superconducting copper oxides.

We study the evolution of the electronic structure of Sr2IrO4 using a combination of ab-initio density functional theory and many-body techniques. The effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions are included on a first-principles level. We calculate the momentum-resolved spectral function and compare to recent photoemission data, finding good agreement with experiment.

MM 42.3 Wed 15:45 HL 001

Role of non-local correlations in doped Sr_2IrO_4 — •Benjamin Lenz[1], Cyril Martins[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

When doping the spin-orbit system Sr_2IrO_4 recent photoemission experiments found pseudogap behavior at low temperatures, which raises the question of its relation to the pseudogap found in high-Tc superconducting copper oxides.

Here, we study the evolution of the electronic structure of Sr_2IrO_4 upon electron- and hole-doping by combining ab-initio density functional theory and two quantum cluster techniques. Our treatment includes the effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions on a first-principles level. We show that short-range antiferromagnetic fluctuations are crucial to account for the electronic properties of the material even in the high-temperature paramagnetic phase. Furthermore, pseudogap features in the momentum-resolved spectral function of the emerging exotic metallic state are analyzed and found to be in good agreement with experiment.

MM 42.4 Wed 16:00 HL 001

Describing the coupled structural and metal-insulator transition in rare-earth nickelates with DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\mathrm{NiO}_3$, display a rich phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT) that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and is related to a charge disproportionation driven by correlation effects, resulting in an insulating state. Here, we employ density functional theory together with dynamical mean field theory (DFT+DMFT) to explore the interplay between lattice distortions and electronic correlation effects in these compounds. By utilizing a symmetry-based distortion mode analysis, we are able to isolate the specific lattice distortion occurring at the phase transition. Calculating total energies within DFT+DMFT then allows us to relax the structures with respect to this distortion. We find, that the resulting distortion amplitudes and its variation across the series are in good agreement with experimental results. Our work highlights the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom.

MM 42.5 Wed 16:15 HL 001

Magnetocrystalline anisotropy of FePt: LDA+DMFT study — •saleem Ayaz Khan[1], Junqing Xu[2], johan Schott[3], Ondřej Šipr[1], and Jan Minár[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany — [3]Uppsala University, Sweden

In our recent work (Phys. Rev B, 94, 144436, 2016) we employed ab initio methods (FLAPW and KKR) to get a reliable value for the magnetocrystalline anisotropy (MCA) energy of FePt. The theoretical MCA energy of FePt (3.0 meV) is significantly larger than the experimental value (1.3 meV), implying that the LDA cannot properly describe the MCA of FePt. Considering that the MCA essentially arises from spin orbit coupling it appears that to obtain reasonable agreement with experiments, it is necessary to include orbital correlations. To account realistically for both the electronic and geometric structure of materials, we use a combined density functional and dynamical mean field theory, LDA+DMFT. Our computation is based on the fluctuation exchange approximation and an analytic continuation method for the self-energy. Our results show that dynamical correlation effects are important for a correct treatment of the 3d-5d hybridization in FePt, which in turn plays a significant role for the magnetocrystalline anisotropy

MM 42.6 Wed 16:30 HL 001

Diagnostics for plasmon satellites and Hubbard bands in transition metal oxides — •Steffen Backes[1], Hong Jiang[2], and Silke Biermann[1] — [1]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau, France — [2]College of Chemistry and Molecular Engineering, Peking University, China

The generally accepted picture of $SrVO_3$ is that of a correlated electron metal where a renormalized quasi-particle peak at the Fermi level coexists with upper and lower Hubbard bands, separated by Coulomb interaction U. Recently, this picture has become blurred with the rise in interest in additional plasmonic satellites. Distinguishing plasmonic features from Hubbard bands is a non-trivial question. In this talk we employ combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") to discuss the processes that give rise to these different satellites and show how to identify their origin in realistic materials. We present an application of this scheme to different transition metal oxides, which we find to exhibit both Hubbard and plasmonic satellites at similar energetic positions.

MM 42.7 Wed 16:45 HL 001

Phase transitions of the 2D Hubbard-Holstein model — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In the 2d Hubbard-Holstein model at zero temperature, a quantum phase transition between Mott and Peierls insulator can be observed. Whether a metallic phase emerges in between remains an open question [1,2]. As the emergence of the Mott phase is a many body effect, a description beyond the mean field level is crucial. At the same time, a method that can cope with two dimensions is needed.

To address this open question, we have extended Density Matrix Embedding Theory (DMET) from the purely electronic case [3,4] to coupled fermion-boson systems. DMET is an embedding theory which benefits from the exponentially decaying correlation in most quantum systems thus allowing a description beyond mean field at low cost.

We show the phase diagram of the 2d Hubbard-Holstein model at zero temperature obtained for different cluster sizes. [1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012) [2] S. Wouters, C. A. Jiménez-Hoyos, G. K.-L. Chan, arXiv:1605.05547 (2016) [3] R. T. Clay and R. P. Hardikar, Phys. Rev. Lett 95, 096401 (2005) [4] J. Bauer, EPL 90 27002 (2010)

MM 42.8 Wed 17:00 HL 001

A quantum embedding theory combining many-body perturbation theory with configuration interaction — •Marc Dvorak and Patrick Rinke — Department of Applied Physics, Aalto University School of Science, 00076-Aalto, Finland

We present a new quantum embedding theory called dynamical configuration interaction (DCI). It captures non-local and static correlation in an orbital active space with configuration interaction (CI) and high-energy, dynamic correlation in the complementary bath space with many-body perturbation theory (MBPT). The formulation is general, but we focus on molecular systems with an *ab-initio* Hamiltonian. The conceptual key to our approach is to replace the exact electronic Hamiltonian in the bath space with one of excitations defined over the correlated ground state. This transformation is naturally suited to the language and methodology of many-body Green's functions. Correlation in the bath is therefore described at the quasiparticle level with Green's functions instead of with the many-body wave function. Our approach avoids computational and conceptual difficulties associated with Green's function embedding and improves upon wave function methods by including dynamical correlation from the bath space. A major advantage to DCI is that it naturally treats ground and excited states on equal quantum mechanical levels. For ground state properties, we present dimer dissociation curves for H_2 and N_2 in excellent agreement with exact results. Excited states of N_2 give excellent agreement with experiment, and we demonstrate the scalability of our method by computing excited states of a free-base porphyrin molecule.

MM 42.9 Wed 17:15 HL 001

Real-Structure Effects and Correlation in Layered Sodium Cobaltates — Sophie Chauvin[1,2], Silke Biermann[1], Lucia Reining[2], and •Claudia Rödl[3] — [1]Centre de Physique Théorique, École polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Na-doped layered cobaltates Na_xCoO_2 feature a rich phase diagram with a plethora of physical phenomena ranging from metal-insulator transitions over magnetism to charge ordering. These instabilities of the electronic structure are mostly attributed to correlation effects within the quasi-2D CoO_2 layers. Here, we focus on $Na_{2/3}CoO_2$, a doping for which the system is metallic and exhibits an experimentally established charge disproportionation on the Co atoms.

We study the electronic properties of the CoO_2 layers and investigate the impact of the intercalated Na atoms on the electronic structure in the ordered layered superstructure. The problem is tackled from an *ab-initio* point of view using density-functional theory (DFT) and many-body perturbation theory (MBPT). Moreover, we study the static charge-density response of the material to understand instabilities in the system. Our approach complements recent model calculations from extended dynamical mean-field theory (EDMFT). The calculated results are compared to experimental spectroscopic data.

MM 42.10 Wed 17:30 HL 001

Slave rotor approach to impurity models with correlated dp orbitals — •Jakob Steinbauer and Silke Biermann — École Polytechnique, Palaiseau, France

We propose a slave rotor method for the solution of many-orbital quantum impurity problems, which maps the original problem onto one with reduced degeneracy. This is particularly useful for the dynamical mean field theory treatment of transition metal oxides where the interactions between ligand states with d-electrons are all too often simply neglected. We derive a general formalism relying on an optimized effective model obtained from the variational principle of Feynman and Peierls and test the method in the atomic limit.

MM 43: Nanomaterials

Applications

Time: Wednesday 17:00–18:00 Location: H 0106

MM 43.1 Wed 17:00 H 0106

Exploiting Electrocapillary Coupling at Metal Surfaces for Active Strain Sensing with Nanoporous Gold — •Charlotte Stenner[1], Li-Hua Shao[2], Nadiia Mameka[3], and Jörg Weissmüller[1,3] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institute of Solid Mechanics Beihang University, China — [3]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Germany

We inspect a hybrid material consisting of two separate phases, nanoporous gold (NPG) and electrolyte. The metal acts as an electrode, which is polarized against the electrolyte. NPG has a large surface-to-volume ratio therefore the properties of the hybrid material are particularly determined by the metal-electrolyte interface. Our experiments show that space charge and potential couple to mechanical deformation of the hybrid material, so that external loading induces either an electric current or a potential variation. The generated electric signals are strain-dependent, robust, and strong. We introduce a theoretical strain-sensing actuation relation to connect both effects measured on the NPG-based hybrid material. The theoretical relation leads to excellent agreement with the experimental results. [1]

[1] C. Stenner, L.-H. Shao, N. Mameka, and J. Weissmüller, Adv. Funct. Mater. 26 (2016) 5174

MM 43.2 Wed 17:15 H 0106

Ideal Dimers of Gold Nanospheres for Precision Plasmonics: Experiment and Theory — •Jun Hee Yoon, Florian Selbach, Ludmilla Langolf, and Sebastian Schlücker — Department of Chemistry, University of Duisburg-Essen, Universitätsstraße 5, 45141 Essen, Germany

A dimer of two noble metal nanoparticles is the simplest system in which electronic coupling between the particles via plasmon hybridization occurs. Theoretical predictions are typically based on ideal dimers comprising two perfectly spherical particles. Here, we present the synthesis and characterization of single ideal dimers of spherical gold nanoparticles with control over both gap distance and gap morphology. Electron microscopic and optical microspectroscopic experiments at the single-particle level show an excellent structural uniformity and an unprecedented homogeneity of their optical scattering spectra. In contrast, non-ideal dimers, i.e., dimers of non-spherical/nanocrystalline particles, with the same gap distance exhibit highly non-uniform properties. Interestingly, non-ideal dimers generate blue-shifted longitudinal plasmon peaks compared with the ideal dimers. We therefore performed FDTD calculations on non-ideal dimers with different gap morphologies using icosahedral particles. The calculations clearly demonstrate that plasmonic coupling in non-ideal dimers strongly depends on the gap morphology, i.e., the orientation of the crystal facets of the particles in the gap.

MM 43.3 Wed 17:30 H 0106

Hotspot-mediated non-dissipative and ultrafast plasmon passage — Eva-Maria Roller[1], Lucas V. Besteiro[2], Claudia Pupp[1], Larousse Khosravi Khorashad[2], Alexander O. Govorov[2], and •Tim Liedl[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Ohio University, Athens, Ohio, USA.

Charge oscillations between two spatially separated entities via a virtual middle state are examples of electron-based population transfer but their realization requires precise control over nanoscale assembly of heterogeneous plasmonic particles. We here show the assembly and optical analysis of a triple particle system consisting of a chain of two Au nanoparticles with an inter-spaced Ag island [1]. We observe strong plasmonic coupling between the spatially separated Au particles mediated by the connecting Ag particle with almost no dissipation of energy. This is a result of the too high excitation energy of the Ag island compared to that of the Au particle leading to only quasi-occupation of the transfer channel. We describe this effect both with exact classical electrodynamic modeling and qualitative quantum-mechanical calculations. We identify the formation of strong hot spots between all particles as the main mechanism for the loss-less coupling between the remote partners. The observed spectra are consistent with a description of coherent ultra-fast energy transfer and could thus prove useful for applications such as quantum gate operations but also for classical charge and information transfer processes [2].

[1] Roller et al. Nat. Phys. 13 (2017) 761

[2] Maier, S. A. et al. Nat. Mater. 2 (2003) 229

MM 43.4 Wed 17:45 H 0106

Fabrication, Encapsulation and Characterization of Transparent Heaters Based on Solution-Processed Copper Nanowires — •Christian Bogner[1], Marco Bobinger[1], Josef Mock[1], Paolo Lugli[2], and Markus Becherer[1] — [1]TU München, Lehrstuhl für Nanoelektronik — [2]Freie Universität Bozen

Solution processed copper nanowires (CuNWs) possess significant economic advantages over indium tin oxide (ITO). However, the biggest issue, for copper nanowires (CuNWs) is the degradation of the copper due to ambient gases. In this work, encapsulation methods for transparent conducting electrodes based on solution processed copper nanowires applied as thin film heaters have been studied. The protective effect of the encapsulation layer has been investigated at temperatures ranging from approximately 80°C to 150°C. A model description allows to factor out side effects influencing the measurement.

With PMMA a 10 times longer life time of a protected heater in comparison to a pristine copper nanowire heater has been achieved. Furthermore, it has been pointed out that the protective effect of PMMA is significantly reduced above the glass transition temperature of PMMA at 105°C.

Next to the temperature induced degradation it has also been shown in this work that copper nanowire thin films are severely affected by UV-light. This work provides an additional step for establishing efficient encapsulations on CuNWs in order to utilize the promising material properties for transparent conducting electrodes.

MM 44: Topical Session (Symposium EPS and MM): Mechanical Properties at Small Scales

Metallic Glass

Time: Wednesday 17:00–18:15 Location: H 0107

Topical Talk MM 44.1 Wed 17:00 H 0107

Atomistic plasticity mechanisms in metallic glass thin films : new insights from advanced transmission electron microscopy — •Hosni Idrissi[1], Matteo Ghidelli[1,3,4,5], Sebastien Gravier[4], Jean-Jacques Blandin[4], Jean-Pierre Raskin[3], Dominique Schryvers[2], and Thomas Pardoen[1] — [1]Institute of Mechanics, Materials and Civil Engineering. Université Catholique de Louvain. Louvain-la-Neuve. Belgium — [2]Electron Microscopy for Materials Science (EMAT). University of Antwerp. Antwerp. Belgium — [3]Institute of Information and Communication Technologies, Electronics and Applied Mathematics. Université Catholique de Louvain. Louvain-la-Neuve. Belgium — [4]Science and Engineering of Materials and Processes, SIMaP. Université de Grenoble. Grenoble. France — [5]Micro- and Nanostructured Materials Laboratory, Department of Energy, Politecnico di Milano. Milano. Italy

Although intensive research on the deformation and fracture mechanisms has been performed on metallic glasses (MGs), the fundamental mechanisms governing the mechanical behaviour as well as the recently observed mechanical size effects in this class of materials are still not fully understood. In the present study, quantitative nanobeam electron diffraction and aberration corrected TEM techniques have been used to investigate the elementary plasticity mechanisms activated in amorphous ZrNi freestanding thin film MGs exhibiting exceptional mechanical properties uncharacteristic of metallic glasses with a yield strength close to the theoretical value (3 GPa), as well as highly enhanced ductility (up to 15%!).

MM 44.2 Wed 17:30 H 0107

Deformation and failure mechanisms of metallic glass nanostructures — •Mehdi Jafary-Zadeh[1], W. Gu[2], R. Liontas[2], S.W. Lee[2], J Greer[2], and Y.W. Zhang[1] — [1]Institute of High Performance Computing (IHPC), A*STAR, Singapore 138632 — [2]Department of Materials Science and Engineering, California Institute of Technology (Caltech), USA

Metallic glasses (MGs) are at the cutting-edge of materials research in advanced applications such as nano-electro-mechanical systems (NEMS). The overall mechanical response of MGs is a combination of their intrinsic properties, e.g. chemical composition, atomistic structure, etc., and extrinsic factors, e.g. sample size, structural flaws, and structural hierarchy. Here, we report our recent works on fabrication and in situ fracture testing of nanosize MG structures with geometries ranging from simple nanopillars to complex nanolattices, i.e. metamaterials [1-3]. We also employ large-scale molecular dynamics (MD) simulations to reveal insights into the underlying atomistic mechanisms of the rich spectrum of deformation modes. We demonstrate the importance of processing and post-processing conditions in achieving MGs with certain intrinsic features such as atomic-level structure. We show that an extrinsic flaw (notch) can shift the failure mode from shear banding to cavitation and crack propagation [2]. We further present that in hollow-tube nanolattices, the shell thicknesses leads to a unique transition in deformation mode [3].

[1] Acta Materialia 118, 270-285 (2016) [2] Nano Letters 14, 5858 (2014) [3] Nano Letters 15, 5673 (2015).

MM 44.3 Wed 17:45 H 0107

Interface mediated creep behavior of Cu-Zr metallic glass composites — •Constanze Kalcher, Tobias Brink, and Karsten Albe — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Otto-Berndt-Str. 3, D-64287 Darmstadt, Germany

Metallic glasses are known for their high yield strength and resilience, but their most severe shortcoming remains the brittle failure mechanism due to strain localization. A more homogeneous deformation behavior at room temperature can be enforced by including crystalline secondary phases. Their role in the deformation behavior under creep conditions, however, has not been fully assessed. In this molecular dynamics study, we show that the properties of the glass-crystal interfaces in such composites directly influence the creep behavior. To that end we model a $Cu_{64}Zr_{36}$ metallic glass with different phase fractions of the reinforcing Cu_2Zr Laves phase and manipulate the glass-crystal interfaces by disturbing the atomic structure in the immediate neighborhood of the crystallites. The different samples are then probed under the same creep conditions. In analogy to Borisov's model for grain boundary diffusion, we observe that the creep rates of the metallic glass composites scale exponentially with the excess energy of the disturbed interfaces.

MM 44.4 Wed 18:00 H 0107

Viscoelastic stress relaxation of amorphous TiAl thin film under tension measured by selected area electron diffraction — •Christian Ebner[1], Rohit Sarkar[2], Jagannathan Rajagopalan[2], and Christian Rentenberger[1] — [1]University of Vienna, Physics of Nanostructured Materials, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Arizona State University, Department of Materials Science and Engineering, School for Engineering of Matter Transport and Energy, Tempe 85287, USA

Amorphous samples loaded by an external stress show a time-dependent viscoelastic strain response. To study this behaviour on small scaled samples, in-situ tensile tests are performed on amorphous TiAl in a Philips CM200 transmission electron microscope. Selected area electron diffraction (SAED) is used as a method to extract the local atomic-level elastic strain, since elliptic distortions of the radial intensity maxima positions are introduced in the SAED patterns by tensile straining [1]. By precisely measuring these distortions, the 2-dimensional strain tensor is calculated with respect to a reference pattern. This allows to quantify the principal strain e_1 (parallel) and e_2 (perpendicular to the loading direction) as a function of the external stress σ. The viscoelastic response to stress jumps is measured by the time dependent changes in principal strain Δe_1.

[1] Ebner et al. (2016) Ultramicroscopy, 165, 51-58.

C. E. and C. R. acknowledge financial support by the Austrian Science Fund FWF: [I1309]. R. S. and J. R. acknowledge funding from the NSF grants CMMI 1400505 and DMR 1454109.

MM 45: Topical Session (Symposium MM): Fundamentals of Fracture

Combining Experiments and Simulations, Multiscale Aspects of Fracture

Time: Wednesday 17:00–18:30 Location: TC 006

Topical Talk MM 45.1 Wed 17:00 TC 006

Fracture tougness of tungsten alloys — •Reinhard Pippan[1], Vladica Nicolic[1], Manuel Pfeifenberger[1], Daniel Scheiber[2], Lorenz Romaner[2], and Daniel Firneis[1] — [1]Erich Schmid Institut of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, 8700 and Department Materials Physics, Montanuniversität Leoben, Franz-Josef-Strasse 18 8700 Leoben, Austria — [2]Material Center Leoben Forschung GmbH, Roseggerstrasse 12, 8700 Leoben, Austria

We have performed in the last few years theoretical as well as experimental studies to investigate fracture relevant phenomena of tungsten. A summary of the result will be presented in this paper. The theoretical studies are based on density function theory analyses of dislocation mobility and the effect of impurities on decohesion energy. The experimental studies are mainly focused on the variation of the fracture toughness as a function of: temperature, in the temperature interval between the temperature of liquid nitrogen and 800°C; the effect of processing conditions, degree of deformation and effect of recovery and recrystallization etc.; the influence of alloying elements; the orientation dependence of fracture toughness, special attention was devoted to the effect of texture, grain size and grain shape, in order to improve the understanding of the brittle fracture process of tungsten alloys. In addition micro mechanical experiments have been performed to study in more detail the cleavage crack propagation process. .

MM 45.2 Wed 17:30 TC 006

Combined experimental and theoretical study of Fe_2AlTi/Fe-Al superalloys — •Martin Friák[1,2], Ivana Miháliková[1,2], Anton Slávik[1,2], Vojtěch Homola[2], Vilma Buršíková[2], Naděžda Pizúrová[1], Petr Dymáček[1], Ferdinand Dobeš[1], David Holec[3], Yvonna Jirásková[1], and Mojmír Šob[4,1,5] — [1]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czech Republic — [2]Faculty of Science, Masaryk University, Brno, Czech Republic — [3]Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben, Leoben, Austria — [4]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czech Republic — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic

Fe-Al-based superalloys containing sub-micron Fe_2AlTi cuboids coherently embedded into a disordered Fe-Al solid solution are intensively studied as materials for high-temperature applications. We focused on the $Fe_{71}Al_{22}Ti_7$ alloy composition for which the transmission electron microscopy (TEM) revealed the superalloy nano-structure and the energy-dispersive X-ray (EDX) technique detected the composition of individual phases. Subsequent quantum-mechanical calculations predicted these two phases to be elastically very different. The differences in the elastic response were detected also experimentally by room-temperature quasistatic nano-/micro-indentation and nano-scale dynamic mechanical analysis (nanoDMA). Regarding high-temperature macro-scale measurements, small-punch testing was performed and the data were analyzed using a rheological model.

MM 45.3 Wed 17:45 TC 006

Extraction of Information about Fracture at High Imposed Strain Rates from Ballistic Indentation Experiments — •Max Burley[1], Bill Clyne[1], Jimmy Campbell[1], and James Dean[2] — [1]University of Cambridge, UK — [2]Double Precision Consultancy, Cambridge, UK

Ballistic indentation experiments have been carried out, using high-speed photography to monitor projectile motion and stylus profilometry to record residual indent shapes. In addition, X-ray computed tomography has been used to capture the 3-D architecture of crack patterns in impacted samples. This experimental work has been coupled with iterative FE modeling of projectile penetration and rebound. Cermet spheres of 5 mm diameter were incident on cylindrical samples of pure Mg, with velocities in the range 50-200 m s-1. The strain rates operative during these experiments were ˜104 - 106 s-1. In addition, quasi-static uniaxial compression tests were carried out, at several temperatures, to obtain the values of parameters characterizing the plastic deformation and its sensitivity to temperature. The Johnson-Cook formulation was then employed and ABAQUS software used for iterative simulation of the impact event. A Nelder-Mead convergence algorithm was then used to obtain best-fit values for the coefficient of friction and the J-C strain rate sensitivity parameter. Correlation was then established between the crack pattern and the stress field during the period of crack growth. It is concluded that the cracks are likely to have propagated largely under mode II conditions, with critical strain energy release rates that were considerably lower than those under quasi-static loading.

MM 45.4 Wed 18:00 TC 006

Towards physically-based fatigue design in ductile poly-crystalline metals — •Christian Robertson[1] and Christophe Déprés[2] — [1]DEN-Service de Recherches Métallurgiques Appliquées, CEA, Université Paris-Saclay, Gif-sur-Yvette, France — [2]Laboratoire SYMME Université de Savoie74940 Annecy-le-Vieux, France

Actual components withstand in-service conditions involving many aggravating factors, including: multi-axial loading, variable amplitude and mean stress. These factors and the inherent data scattering due the microstructural material heterogeneities are usually addressed by adopting important (if not overly conservative) safety margins. In other words, none of the standard fatigue design approaches are truly predictive, missing out cyclic plasticity mechanisms involved during crack propagation, in actual poly-crystalline metals.

The fatigue response of ductile poly-crystalline metals involves dislocation motion and multiplication, at the scale of individual grains (1-100 *m, typically). Two-dimensional dislocation dynamics (DD) studies adapted to crack propagation have been conducted earlier and were able to capture several fatigue lifetime controlling mechanisms. Our goal in this paper is to further investigate fatigue crack propagation using DD simulations, including 3D boundary conditions adapted to face-centred cubic grains, in presence of both short (stage-I) and long (stage-II) cracks. The results are analysed quantitatively, with a view to develop advanced fatigue design criteria and concepts, accounting for typical complex loading conditions and material microstructural heterogeneities.

MM 45.5 Wed 18:15 TC 006

A multi-physics approach to investigate the effect of hydrogen on short fatigue crack growth — •Volker Schippl[1], Sven Brück[1], Hans-Jürgen Christ[1], and Claus-Peter Fritzen[2] — [1]Institut für Werkstofftechnik, Universität Siegen, 57068 Siegen, Germany — [2]Institut für Mechanik und Regelungstechnik - Mechatronik, Universität Siegen, 57068 Siegen, Germany

Hydrogen leads to a macroscopic embrittlement and under cyclic loading to increasing crack growth rate and a shorter fatigue life of mechanically loaded components. To address this problem, a better understanding of the hydrogen damaging mechanism is needed.

As the short crack propagation could dominate the whole fatigue life, a two-dimensional model is presented to simulate short crack propagation to get a better understanding of the fundamental mechanisms leading to failure. The model includes intergranular and transgranular crack growth and considers the plastic deformation along shear bands. The hydrogen concentration in the microstructure is calculated and the amount of the local hydrogen at the crack tip changes the crack growth mechanism. This multi-physics problem is addressed by using a sequential staggered BEM & FEM approach. At first, stresses and displacements are calculated by using a boundary element method. Based on the calculated hydrostatic stress field, the redistribution of hydrogen is determined using a finite element method. With this approach, it could be found that hydrogen leads to an increasing part of the irreversible plastic deformation at the crack tip which results in increasing crack growth rates and thus to shorter lifetime.

MM 46: Liquid and Amorphous Metals

Relaxation and Rejuvenation

Time: Wednesday 17:00–18:30 Location: TC 010

MM 46.1 Wed 17:00 TC 010

Analysis of a severely deformed $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass — •Afrouz Hassanpour, Sergiy Divinski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, Westfälische Welhilms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

For practical usage of bulk metallic glasses (BMG) it is crucial to enhance material properties, such as tensile and compression ductility and fracture toughness. In the present work, $Pd_{40}Ni_{40}P_{20}$ bulk metallic glass was analyzed to study its behavior under conditions of severe deformation via high-pressure torsion (HPT). Amorphous samples were produced by copper mold casting in a melt spinner under argon atmosphere. X-ray diffraction, differential scanning calorimetry (DSC), and Transmission Electron Microscopy (TEM) were performed. The degree of deformation was systematically varied by applying different numbers of rotation with HPT from 0 (just compression) to 10 turns. HPT causes significant changes of the thermo-mechanical properties. It turned out, that unlike after deformation by cold-rolling, HPT deformation at room temperature induced a nanocrystallization transformation in the deeply undercooled liquid above the glass transition. Also structural relaxation by annealing and its impact on the nanocrystallization at higher temperatures was experimentally investigated for as-cast and HPT-processed states. The results are discussed in conjunction with dedicated TEM investigations for annealed and as-deformed amorphous samples.

MM 46.2 Wed 17:15 TC 010

Rejuvenation behavior and specific heat capacity of Pd40Ni40P20 bulk metallic glass influenced by severe plastic deformation — •Hongbo Zhou, Niklas Nollmann, René Hubek, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

The effects of severe plastic deformation (high pressure torsion, HPT) on rejuvenation behavior and specific heat capacity have been investigated. The results of differential scanning calorimetry (DSC) illustrate that the as-cast metallic glasses could be rejuvenated effectively during the HPT. The deformed state glasses possess much more structural relaxation enthalpy in contrast with the as-cast state, and an enhanced rejuvenation could be achieved with increasing deformation. Besides, it is assumed that atomic re-arrangements take place as a consequence of HPT because the deformed state glasses have an apparently different crystallization behavior compared to the as-cast state. The results of low-temperature specific heat capacity measurements using a physical properties measurement system (PPMS) reveal that the heights of boson peak increase with a similar trend as function of strain. Moreover, the effects of rejuvenation on the mechanical properties will be discussed.

MM 46.3 Wed 17:30 TC 010

Elastostatic Reversibility: Structural Changes in Thermoplastically Formed Metallic Glass — •Baran Sarac[1], Christoph Gammer[1], Liang Deng[2], Eunmi Park[2], Yoshihiko Yokoyama[3], Mihai Stoica[4], and Jürgen Eckert[1] — [1]Erich Schmid Institute, Leoben, Austria — [2]IFW Dresden, Dresden, Germany — [3]Tohoku University, Sendai, Japan — [4]ETH Zurich, Zürich, Switzerland

Albeit high processing capabilities of BMGs, thermoplastic forming (TPF) can severely degrade their mechanical and physical properties. Present work places an importance on elastostatic loading (ESL) which not only fully recovers the lowered room temperature plasticity originated from TPF or post-cryostatic conditions, but also activates a rejuvenation mechanism by yielding an extended resistance against strain softening. The drop in the supercooled liquid region and crystallization enthalpy measured by differential scanning calorimeter are found to be temporary, and can be reversed to its initial condition. Individual nanobeam diffraction patterns taken by the fluctuation electron microscopy are acquired with a probe size of 1.2 nm. Normalized variance of a series of nanodiffraction patterns of the post-ESL sample reveals height decrease in the first broad peak of normalized intensity variance, suggesting the modifications in the medium-range order which in turn dramatically restores mechanical and thermal properties. The combination of TPF and post-ESL treatment in BMGs can open a new avenue for ultra-high mechanical and thermal performance micro- and nanomechanical devices for biosensors, MOSFETs, and robotics.

MM 46.4 Wed 17:45 TC 010

Cryogenic Cycling of Bulk Metallic Glasses — •Jonas Lübke, Niklas Nollmann, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, WWU Münster, Germany

Metallic glasses show interesting properties, such as high strength, toughness and corrosion resistance. However, a severe lack of ductility makes the material unsuitable for many applications. In the past, much effort was made on reducing this disadvantage using micro-alloying or crystalline precipitates with some notable success. A different approach is provided by the concept of free volume in metallic glasses, where the increment of such may lead to enhanced ductility. This so called rejuvenation was already achieved by severe plastic deformation and shot-peening. However, Ketov et al. [1] claim to achieve this rejuvenation by using the heterogeneous thermal expansion coefficient of metallic glasses to induce internal strain by thermal cycling, which could lead to increased free volume. To avoid structural relaxation, these cycles have to be at cryogenic temperatures. By this, the ductility of the metallic glass is said to be improved in a different and simple way which would make the material suitable for new applications.

The effects of different amounts of cryogenic cycles on the well-known metallic glass $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ (VIT1) and its free-volume, by analysing thermal- and mechanical properties, are presented and discussed.

[1] S. V. Ketov et al. Rejuvenation of metallic glasses by non-affine thermal strain. Nature 524, 2015

MM 46.5 Wed 18:00 TC 010

Abnormal structural relaxation spectrum observed by dynamic mechanical analysis in an Au-based bulk metallic glass — •Maximilian Frey, Nico Neuber, Isabella Gallino, and Ralf Busch — Chair of Metallic Materials, Saarland University, C6.3, 66123

Saarbrücken, Germany

The structural relaxation time spectrum of a recently developed gold-based metallic glass former is investigated via isochronal temperature scans performed with a dynamic mechanical analyzer. The α-relaxation event for each applied measurement frequency manifests as a maximum in the loss modulus curve. The respective frequency-temperature data points are pictured in an Arrhenius plot and used to evaluate the temperature dependence of the structural relaxation time in the framework of Angell's fragility concept. At low measurement frequencies, the supercooled liquid exhibits a strong temperature dependence, which is in agreement with recent results obtained by calorimetric and thermomechanical studies. For intermediate frequencies, the single maximum peaks of the loss modulus curves perform an unusual splitting in several distinguishable peaks. By further increasing the measuring frequencies, the normal single peak appearance is restored, but with a distinctly more fragile temperature behavior. Calorimetric and thermomechanical studies are performed and compared to the dynamic mechanical data set. Taking recent literature findings for similar alloys into account, the results can be most likely interpreted as the fingerprint of a strong-to-fragile transition event.

MM 46.6 Wed 18:15 TC 010

The Stokes-Einstein relation of a simple liquid metal and its relationship to changes in the microscopic dynamics with increasing temperature: the experimental viewpoint — •Franz Demmel — ISIS Facility, Didcot, UK

For liquid rubidium the Stokes-Einstein-relation is well fulfilled near the melting point with an effective hydrodynamic diameter, which agrees with a value from structural investigations. A wealth of thermodynamic and microscopic data exist for a wide range of temperatures for liquid rubidium and hence it represents a good test bed. With increasing temperature the SE-relation shows a departure from the expected temperature behaviour. That temperature range coincides with an observed change in the microscopic relaxation dynamics on nearest neighbor distances [1]. The derived average relaxation time for density fluctuations on this microscopic length scale shows a non-Arrhenius behaviour. Combining the experimental macroscopic self-diffusion coefficient with the average relaxation time, a violation of the SE-relation at the same temperature range can be demonstrated. Simulations and experimental results from other metals and alloys demonstrate a similar behavior and point to a possible universal change in the dynamics of liquid metals [2]. [1] F. Demmel et al, Phys. Rev. B 73, 104207 (2006) [2] F. Demmel et al, J.Phys.: Condens. Matter 27 455102 (2015); A. Jaiswal et al, Phys. Rev. Lett. 91 205701 (2016); X.J. Han and H.R. Schober, Phys Rev B 83 224201 (2011)

MM 47: Poster Session II

Time: Wednesday 18:30–19:45 Location: Poster C

MM 47.1 Wed 18:30 Poster C

The impact of magnetism on properties of defects in Fe-Co alloys — •Van Truong Tran and Chu Chun Fu — SRMP, CEA Saclay, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France

Fe-Co alloys have been demonstrated as an intriguing magnetic material with the highest magnetization saturation compared to all known magnetic alloys. They are widely employed for magnetic devices.[1]

The magnetic properties of binary Fe-Co alloys have been investigated extensively by numerous experimental and theoretical studies. However, several properties of structural properties in this alloys are still poorly understood and need to be unfolded.

Our study in an attempt to explore the interplay between magnetic properties and vacancies present in Fe-Co systems in the framework of density functional theory (DFT). In particular, formation energies and migration barriers for the vacancy and the Co solute as functions of local chemical and magnetic environments.

The obtained DFT results will also be used as input data for parameterizing an effective interaction model (EIM). In combination with Atomistic Monte Carlo simulations, we aim to investigate the defect properties as functions of temperature. In particular, the impact of magnetic excitation and transition will be elucidated.

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MM 47.2 Wed 18:30 Poster C

Towards an ab initio phase diagram of Fe-Nb: Importance of Magnon-Phonon coupling — •Ali Zendegani, Fritz Körmann, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Ferritic steels containing Fe-Nb TCP phases form a promising materials class for high-temperature applications. To tailor this high-temperature strength, e.g., via heat treatments, a precise knowledge of the thermodynamic stability of the TCP, i.e. the hexagonal and Laves (C14, C36) phases, and the cubic Laves (C15) phase, is essential.

Combining density functional theory (DFT) and thermodynamic concepts, we evaluate the ground state energy as well as finite temperature entropy contributions of these structures. All relevant magnetic configurations, ranging from non-magnetic simulations over selected ferro/ferri-magnetic ones to fully paramagnetic are considered. In particular, the spin-space averaging (SSA) method is utilized to average forces over many magnetic configurations characterizing the disordered magnetic states. Only with these methods, paramagnetic phonons, which are of central importance for temperature dependent phase stabilities, can be calculated. We demonstrate that in contrast to non-magnetic (non-spin-polarized) calculations, not only quantitative changes are obtained, but even dynamical instabilities, e.g. in C36, will disappear. Only when employing the paramagnetic state explicitly, we obtain agreement with experiment. The results provide direct insight into the mechanisms that stabilize these phases.

MM 47.3 Wed 18:30 Poster C

Metal-organic frameworks (MOFs): mechanical properties, electronic structure and molecular magnetism — •Sebastian Schwalbe[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Central Michigan University, Department of Physics, USA

Density functional theory is applied to determine the electronic structure of metal-organic frameworks (MOFs) based on special model systems [1]. Within this contribution the authors discuss the possibility to tune the electronic structure by adjusting the local magnetism represented by single molecule magnets (SMMs) and their local transition metal centers within three-dimensional MOFs [2]. Further, it is discussed that model systems can be used to calculate the magnetic shielding within MOFs [3]. Finally, the authors want to emphasize that the understanding of several mechanical properties (pore sizes, void volume, accessible volume, pore-size distribution and elastic properties) is essential for experimentalists and the interpretation of measured values.

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MM 47.4 Wed 18:30 Poster C

Anomalous Nernst effect in Ir22Mn78/Co20Fe60B20/MgO layers with perpendicular magnetic anisotropy — Sa Tu[1,2], •Junfeng Hu[1], Guoqiang Yu[3,4], Haiming Yu[1], Chuanpu Liu[1], Florian Heimbach[1], Xiangrong Wang[5], Jianyu Zhang[1], Youguang Zhang[1], Amir Hamzic[6], Kang L. Wang[3], Weisheng Zhao[1], and Jean-Philippe Ansermet[2] — [1]Fert Beijing Institute, School of Electronic and Information Engineering, BDBC, Beihang University, Xueyuan Road 37, Beijing 100191, China — [2]Institute of Physics, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne CH-1015, Switzerland — [3]Department of Electrical Engineering, University of California, Los Angeles, California 90095, USA — [4]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — [5]Physics Department, Hong Kong University Science & Technology, Kowloon, Hong Kong, People's Republic of China — [6]Department of Physics, Faculty of Science, University of Zagreb, Zagreb HR-10001, Croatia

The anomalous Nernst effect in a perpendicularly magnetized Ir22Mn78/Co20Fe60B20/MgO thin film is measured using well-defined in-plane temperature gradients. The anomalous Nernst coefficient reaches 1.8 uV/K at room temperature, which is almost 50 times larger than that of a Ta/Co20Fe60B20/MgO thin film with perpendicular magnetic anisotropy. The anomalous Nernst and anomalous Hall results in different sample structures revealing that the large Nernst coefficient of the Ir22Mn78/Co20Fe60B20/MgO thin film is related to the interface between CoFeB and IrMn.

MM 47.5 Wed 18:30 Poster C

Magnetic short range order in Fe1-xCrx alloys

— Isabelle Mirebeau[1], •Veronique Pierron-Bohnes[2], and Georges Parette[1] — [1]Laboratoire Léon Brillouin, CEA-CNRS, Université Paris-Saclay, CEA-Saclay, F-91191 Gif-sur-Yvette, France — [2]Université de Strasbourg, CNRS, UMR7540 Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess BP 43, 67034 Strasbourg Cedex 2 France

The FeCr alloys encounter recently a renewed interest as they eliminate irradiation damages spontaneously. This could be due to a unique inversion of atomic short range order (SRO) at xc=0.11 [1]: they tend to order below xc and to cluster above xc.

In FeCr, a coupling of the ordering and magnetic local orders can also be suspected. We have studied Fe1-xCrx solid solutions (for 0.03<x<0.15), by magnetic neutron diffuse scattering, using both polarized and unpolarized neutrons. The alloys were annealed to ensure equilibrium SRO states. At low Cr content, the Cr moments orient anti-parallel to the Fe moments and perturb the neighboring Fe moments, decreasing their magnitude in the first two nearest neighbor shells and increasing it in the 4-5 neighbor shell.

These results are compared with previous ab initio predictions concerning the amplitude and sign of the local moments and perturbations.

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MM 47.6 Wed 18:30 Poster C

3D Discrete Dislocation Dynamics simulations of crack-tip plasticity

— •Elena Jover Carrasco and Marc C. Fivel — Science and engineering of materials and processes, SIMAP, Univ. Grenoble Alpes / CNRS, BP46, 38402, Saint-Martin d'Hères, France

3D Discrete Dislocation Dynamics (DDD) simulations are conducted in order to better understand the relationship between dislocation activity and crack advances. The final objective is to understand the crack tip processes at a microscopic scale during initiation, propagation and arrest as well as to study the interactions of cracks and microstructure elements such as dislocations and grain boundaries.

The numerical tool used here is the 3D DDD code TRIDIS coupled to the Finite Element code CAST3M used to enforce the boundary conditions, including the presence of the crack. Dislocations can interact with the cracks in two major ways; they can reduce the stress on the crack tips due to the screening phenomena or they can increase the stress as they organize themselves in particular microstructures. The DDD along with the finite element allow to take into account the dislocations contribution on the stress at the crack tip and to observe the behavior of the dislocations near the free surfaces of the crack.

MM 47.7 Wed 18:30 Poster C

Nucleation in Ni-Al alloys: An atomistic study

— •Yanyan Liang, Grisell Díaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany

Ni-Al alloys are a basic component of high-temperature superalloys, the ordered L1_2 phase in Ni$_3$Al is of particular interest. Nucleation is a crucial step in solidification, but atomistic insight still remains elusive due to the extended time scale and complexity of the nucleation process in binary alloys. We investigate the nucleation in Ni$_3$Al on the atomic scale. We employ transition path sampling and generate an ensemble of molecular dynamics trajectories to extract thermodynamic and kinetic properties, such as nucleation rates and free energies. A strong competition between fcc, hcp and bcc in the growing nucleus predetermines the final dominant polymorphs in the crystallization. In particular, we find that the composition of the growing nucleus remains constant while there is a decreased short-range chemical order in the nuclei. The size of the growing nucleus alone is not a complete reaction coordinate for the nucleation process, in contrast to what we observed in elemental metals. A multi-dimensional description is needed to fully characterize the nucleation process in binary alloys.

MM 47.8 Wed 18:30 Poster C

Transition Path Sampling of Seeded Nucleation during Solidification in Nickel

— •Sarath Menon, Grisell Diaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum

Almost all technologically relevant solidification is based on heterogeneous nucleation. While it is known that the presence of impurities enhances nucleation processes and influences the evolution of the microstructure, little is known about the initial stages of nucleation from an atomic scale. This is because nucleation time scales are too long for conventional molecular dynamics methods and therefore a 'rare event'. We employ transition path sampling, an atomistic simulation method, to study the effect of prestructured seeds on nucleation in nickel. We use seeds of varying sizes and crystal structures and quantify their effect on the rate constant and free energy barrier to understand the role of seeds in nucleation mechanism. Even small seeds are capable of inducing spontaneous nucleation. The nucleation rate is controlled by the size and surface geometry of the seed. Moreover, the structure of the seed determines the structure of the solid crystal. The seeds facilitate pre-ordering in the liquid and different seeds may be used to induce the formation of specific polymorphs.

MM 47.9 Wed 18:30 Poster C

First-principles design of biocompatible Ti-xNb ($0 < x < 35$) alloys

— •Julio Gutierrez Moreno[1,2], Dimitris Papageorgiou[2], Giorgios Evangelakis[3], and Christina Lekka[2] — [1]Tyndall National Institute, University College Cork — [2]Departament of Materials Science and Engineering, University of Ioannina — [3]Departament of Physics, University of Ioannina

In this work, we present a systematic ab initio study on the structural, electronic and mechanical properties of Ti-xNb (x<35at%) alloys. This necessity is originated from the lack of biocompatibility and high Young's modulus (E) in the currently used Ti-6Al-4V implants, which may lead to bone atrophy and implant loosening. Our results predict a variety of phases (including ω, α', α' and β) depending on the Nb concentration. The α' and ω are stable for Nb<6.25%at, the β phase is stable at high Nb compositions Nb>18.75at% while the α" phase may form in intermediate concentrations. The α' and ω hexagonal phases become unstable at high Nb content due to the electronic band filling at the Fermi level. In β-Ti-25at%Nb, the depletion of the occupied electronic states at Fermi level results in a stable β-TiNb structure. Our results prove the Eω>Eα'>Eα">Eβ sequence, revealing the importance of the phases coexistence for the E reduction. The Young's modulus surface revealed high anisotropic E values for all Ti-Nb phases, while the Eβ along the [100] direction exhibits E<30GPa. These data could enlighten the electronic origin of the Ti-Nb phase stability and guide the design of novel alloys suitable for biomedical applications.

MM 47.10 Wed 18:30 Poster C

Control of (in)coherent dynamics in phononic superlattices

— •Dennis Meyer, Daniel Metternich, Roland Potthast, and Henning Ulrichs — I. Physikalisches Institut, Georg-August-Universität Göttingen

We present methods to control (in)coherent phonon dynamics in multilayer films by tailoring the elastic band structure or exploiting external manipulation of material properties. On the experimental side we show how a wedge-shaped metallic thin film of tungsten, together with a pump-probe technique can be used as an on-sample spectrometer for probing phonon band gaps. Measurements on samples of insulating multilayers, manganites and block copolymers are accompanied by a theoretical model which is implemented as a finite differences time-domain simulation. Besides applying this method, a link between the phonon spectrum and thermal transport will be drawn by transient thermoreflectance measurements. We acknowledge financial support by the DFG within the CRC 1073 Atomic scale control of energy conversion.

MM 47.11 Wed 18:30 Poster C

Structure and energetics of Y-Ti-O nanoclusters in bcc Fe

— •Muthu Vallinayagam[1], Matthias Posselt[2], and Jürgen Fassbender[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR) — [2]HZDR — [3]HZDR

In this research project the nature of yttria-based oxide nanoclusters in a bcc Fe matrix is be investigated by DFT calculations. The main goal of these studies is the better understanding of the nucleation as well as the structure and composition of the clusters. In the first part of the work three types of structures are considered: (i) clusters consisting of parts of the bixbyite (Y2O3) or pyrochlore (Y2Ti2O7) structure embedded in bcc Fe, (ii) clusters with Y, Ti, and O on substitutional sites, and (iii) clusters with of Y, Ti, on substitutional sites and O on octahedral interstitial sites of the bcc lattice. Simulation cells containing different structures but the same composition of atoms (Fe, Y, Ti, O) are compared. It is found that the energetics of three different structure types, i.e. their total binding energy, is very similar. This modifies the statement of Barnard et al. [1] who only considered the first type of structure and concluded that this is the most favorable. Further, more stable cluster structures are constructed using another model with the nanocluster core similar to the metal monoxide structure. Also the binding energy of monomers like O, Y, Ti, and the vacancy to the cluster are studied. O and the vacancy are strongly attracted by the nanoclusters, while the interaction with metal atoms is weaker. [1] L. Barnard et al. Acta Mater. 60 935 (2012)

MM 47.12 Wed 18:30 Poster C

Structure and energetics of Y-Ti-O nanoclusters in bcc Fe — •Muthu Vallinayagam[1], Matthias Posselt[2], and Jürgen Fassbender[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR) — [2]HZDR — [3]HZDR

In this research project the nature of yttria-based oxide nanoclusters in a bcc Fe matrix is be investigated by DFT calculations. The main goal of these studies is the better understanding of the nucleation as well as the structure and composition of the clusters. In the first part of the work three types of structures are considered: (i) clusters consisting of parts of the bixbyite (Y2O3) or pyrochlore (Y2Ti2O7) structure embedded in bcc Fe, (ii) clusters with Y, Ti, and O on substitutional sites, and (iii) clusters with of Y, Ti, on substitutional sites and O on octahedral interstitial sites of the bcc lattice. Simulation cells containing different structures but the same composition of different atoms (Fe, Y, Ti, O) are compared. It is found that the energetics of three different structure types, i.e. there total binding energy, is very similar. This modifies the statement of Barnard et al. [1] who only considered the first type of structure and concluded that this is most favorable. Further, more stable cluster structures are constructed using another model with the nanocluster core similar to the metal monoxide structure. Also the binding energy of monomers like O, Y, Ti, and the vacancy to the cluster are studied. O and the vacancy are strongly attracted by the nanoclusters, while the interaction with metal atoms is weaker. [1] L. Barnard et al. Acta Mater. 60 935 (2012)

MM 47.13 Wed 18:30 Poster C

Diffusion of oxygen in bcc Fe under the influence of other foreign atoms — •Xiaoshuang Wang[1], Matthias Posselt[2], and Jürgen Fassbender[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR) — [2]HZDR — [3]HZDR

First-principle calculations and kinetic Monte Carlo simulations are applied to investigate the diffusion of oxygen in bcc Fe under the influence of other foreign atoms, such as Al, Si, P, S, Ti,, Cr, Mn, Ni, Y, and Mo. In the first part of this work jumps of oxygen in pure bcc Fe, between first-, second-, and third-neighbor octahedral interstitial sites were investigated by DFT. It is found that a second-neighbor jump consists of two consecutive first-neighbor jumps and that the barrier of the third-neighbor jump is too high to be relevant. In the second part DFT was applied to determine the modified migration barriers, i.e. for the oxygen jump between the first and the second neighbor of a foreign atom, etc. It is found that Si, P, Ni and Mo influence the migration barriers of oxygen only slightly. Al and Cr cause moderate changes, while S, Ti, and Y lead to strong modifications. With the exception of Y the migration paths are first-neighbor jumps between (modified) octahedral sites with (modified) tetrahedral sites as saddle points. Y changes some migration paths considerably. Using the migration barriers calculated by DFT the diffusion coefficient of oxygen was determined by kinetic Monte Carlo simulations considering a dilute iron alloy. In general the foreign atoms cause a reduction of the mobility of oxygen compared to that in pure bcc Fe. The strongest decrease is obtained for the foreign atoms S, Ti, and Y.

MM 47.14 Wed 18:30 Poster C

Temperature dependence of interface energies in WC Co cemented carbides — •Erik Fransson, Martin Gren, and Göran Wahnström — Materials and Surface Theory, Chalmers University of Technology, Gothenburg, Sweden

Cemented carbides is a group of materials consisting of fine carbide phase (WC) particles cemented into a composite by a binder metal (Co). Cemented carbides combine superb hardness with high toughness making them ideal for usage in cutting applications and in wear resistance tools. Interfaces in cemented carbides play an important role in the sintering process of the material and for the resulting mechanical properties. Density Functional Theory has been used to calculate the driving force for spreading and binder phase infiltration of grain boundaries. However since sintering is carried out at 1800K, temperature effects are likely important. In this study we carry out a thorough investigation of temperature effects for interfaces in cemented carbides using an analytic bond order potential. We compute free energies using quasi-harmonic approximation and molecular dynamics simulations. Our calculation captures the vibrational and configurational entropy effects serves as a benchmark for free energy calculations methods for interfaces in general. The obtained temperature effects indicate that the spreading and infiltration parameters in cemented carbides increase with roughly $0.35\mathrm{J/m}^2$. This combined with previous DFT studies yield a picture consistent with recent spreading measurements and the fact that the material consists of a continuous carbide grain network.

MM 47.15 Wed 18:30 Poster C

Test and analysis of nonlocal van der Waals density functionals for solids — •Leila Kalantari, Fabien Tran, and Peter Blaha — Vienna University of Technology, Vienna, Austria

Recently, a scheme for the implementation of nonlocal van der Waals (NL-vdW) functionals into all-electron codes was proposed by Tran *et al.* [Phys. Rev. B **96**, 054103 (2017)]. With this method, benchmark results can be obtained at reasonable computational time since it is based on fast Fourier transformations as proposed by Román-Pérez and Soler [Phys. Rev. Lett. **103**, 096102 (2009)] after the all-electron density is smoothed. In this work, the results of a comparison of some of the most recently developed NL-vdW functionals will be presented, and the test set consists of simple cubic solids as well as several vdW bounded solids. Among the latter are some rare gases, graphite, h-BN and several transition metal dichalcogenides MX_2, where M represents transition metals and X being either S, Se or Te. We have determined the ground state geometry and interlayer binding energy of the MX_2 compounds. The calculations are done with the WIEN2k code which is based on the linearized augmented plane-wave basis set. The convergence of the results with respect to parameters like the size of the basis set, the number of **k**-points, the cutoff for smoothing the density and the FFT-grid will also be discussed.

MM 47.16 Wed 18:30 Poster C

Molecular Dynamics Simulations of Laser Ablation in Covalent Materials — •Dominic Klein, Alexander Kiselev, and Johannes Roth — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart, Germany

Non-equilibrium phenomena in highly excited covalent systems induced by strong laser radiation fields have received much attention in recent years. Despite of many theoretical and computational investigations these ultra fast processes are still not well understood. Here we use multi-million particle molecular dynamics simulations to study the laser ablation in covalently bonded materials. A combined self-consistent continuum-atomistic model was applied for carrier-lattice interaction and electron-hole recombination processes. In addition, the temporal and spatial dependence of the exited carrier density was taken into account by fitting the inter atomic forces to finite-temperature density functional theory calculations.

Both, spatially homogeneous and Gaussian distributed laser power densities have been carried out. Furthermore, by using single-, double- and triple-pulse femtosecond laser irradiations it is demonstrated how the properties of the pulse sequence lead to drastic changes in bulk properties like the ablation threshold or the absorption length due to the time scale of free carriers relaxation.

MM 47.17 Wed 18:30 Poster C

The AiiDA-FLEUR package and how you can predict XPS spectra with it — •Jens Bröder[1,2], Nicola Helfer[2], Gregor Michalicek[1], Daniel Wortmann[1], Rudi Koslowski[2], Christian Linsmeier[2], and Stefan Blügel[1] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Energie- und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We present some workflows of the AiiDA-FLEUR [1] package, allowing the user to easily perform complex tasks with the all-electron density functional theory (DFT) code `FLEUR` [2] through AiiDA [3] (Automated interactive Infrastructure and database for material science).

The package empowers users with the ability to run `FLEUR` simulations just with python code and connects them to the tools of the python universe (i.e. Jupyter, pymatgen, ase, ...).

Further we focus on certain results of the core level shifts, turn-key solutions for X-ray photoelectron spectroscopy (XPS) results of bulk materials and surfaces for surface science. These *ab initio* results are compared to experimental data (i.e. Beryllium compounds) and we demonstrate how they help with spectra interpretation.

We acknowledge partial support from the EU Centre of Excellence "MaX Materials Design at the Exascale" (Grant No. 676598).

[1] www.github.com/broeder-j/aiida-fleur

[2] www.flapw.de

[3] G. Pizzi, et al. Comp. Mat. Sci. 111, 218-230 (2016)

MM 47.18 Wed 18:30 Poster C

pyiron - an integrated framework for developing, running, and analyzing complex simulation protocols in computational materials science — •Jan Janssen[1], Sudarsan Surendralal[1], Yury Lysogorskiy[2], Tilmann Hickel[1], Ralf Drautz[2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, Germany

Over the past years progress in computational materials science both with respect to predictive power and scalability (e.g. high-throughput computations) has been tremendous. These advances are not only related to the large gain in computer power but often to the development of advanced and computationally highly efficient algorithms and methods. A challenge in this respect is that the resulting simulation protocols are getting ever more complex: They often require the combination of high performance codes implemented in low-level programming languages with incompatible input/output formats, the implementation of flexible interfaces to adjust the order of the steps in the simulation protocol dynamically and the distribution of tasks on highly heterogeneous computing platforms. To foster the development of these novel techniques and their dissemination and use in our department we started several years ago with the development of a framework that allows to automatize routine tasks, automatically stores all input/output data of the large number of individual jobs in a generic format together with the simulation protocols and the parent-child relationship of the tasks.

MM 47.19 Wed 18:30 Poster C

Ab initio electronic structure calculation of Cn element — •Hana Čenčariková[1] and Dominik Legut[2] — [1]Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovakia — [2]IT4Innovations Center, VSB Technical University of Ostrava, 17.listopadu 15, 708 33 Ostrava-Poruba, Czech Republic

The first-principle calculations in the framework of the density functional theory have been used to the study of selected properties of super-heavy element Cn. The special attention has been focused to the correct description of the energetically favored crystal structure, taken into account five basic crystal types: the body-centered, the face-centered, the simple cubic, the hexagonal cosed packed and the rhombohedral structure. The energy-volume analyses has been done usign the spin-orbit calculations with the scalar relativistic base and the extended second variational method including the relativistic $6p_{1/2}$ local orbitals for the description of the $6p$ states. Furthermore, the criteria of mechanical stability have been investigated based on the calculated elastic constants. Finally, the metal character of Cn element has been determined from the analysis of the total density of states as well as the band-structure calculations.

Acknowledgement: H.C. acknowledges support by the Slovak Research and Development Agency under Grant Nos. DS-2016-0046, APVV-16-0186 and VEGA-0043-16. D. L. acknowledges support by the Mobility grant No. 8X17046.

MM 47.20 Wed 18:30 Poster C

The nonlinear quantum Hall effect in BiTeI — •Jorge Facio[1], Inti Sodemann[2], Jhih-Shih You[1], Klaus Koepernik[1], Dmitri Efremov[1], and Jeroen van den Brink[1] — [1]IFW-Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The Berry phase has become a central ingredient in our modern understanding of Hall-like phenomena of electrons in crystals. Recently, it has been shown that time-reversal invariant metals that lack inversion symmetry can display a nonlinear version of the Hall effect whose form and strength is controlled by the dipolar distribution of the Berry curvature in momentum space.

In this work, we study the nature of Berry curvature distribution in the three-dimensional giant Rashba material Bismuth Tellurium Iodine (BiTeI). By combining first principle and simple analytical models, we study the evolution Berry curvature dipole with doping and pressure and discuss the experimental conditions for the observation of the quantum non-linear Hall effect in this material.

MM 47.21 Wed 18:30 Poster C

Ab-initio investigation of the elastic behavior of the ternary compounds $\mathrm{C}_x\mathrm{Si}_y\mathrm{Ge}_{1-x-y}$ in the cubic phase — •Tim Klose, Pasquale Pavone, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, Germany

We investigate the set of all diamond-type structures of carbon, silicon, and germanium which can be represented in a cubic unit cell containing eight atoms. Total-energy calculations are performed using density-functional theory as implemented in the full potential all-electron package **`exciting`** [1]. In conjunction with **`exciting`**, second-order elastic constants for all the considered structures are obtained using the **`ElaStic`** tool [2]. 141 geometrically distinct initial configurations are obtained by occupying each site of an fcc diamond-like lattice with a C, Si, or Ge atom, of which the 48 most relevant configurations are selected. Then, second-order elastic constants are determined for each fully relaxed configuration by applying suitable distortions to the equilibrium structures. We identify a clear distinction between three classes of configurations when analyzing the resulting equilibrium lattice and elastic constants. This classification can be correlated to the internal geometry and degree of symmetry of the corresponding configurations. This project involved thousands of individual calculations and, thus, required a careful analysis in order to extract significant findings from the generated data.

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MM 47.22 Wed 18:30 Poster C

Phase equilibria, first-principle calculations, and thermodynamic modeling of Zn-Ti system — •Songmao Liang[1], Harish K. Singh[2], Chen Shen[2], Hongbin Zhang[2], and Rainer Schmid-Fetzer[1] — [1]Institute of Metallurgy, TU Clausthal — [2]Institute of Materials Science, TU Darmstadt

The phase diagram of Ti-Zn system is of great importance for Zn alloys development and galvanizing process. The addition of Ti in Zn alloys can refine the grain size and improve the creepy resistance. Coatings with different colors can be achieved by adding Ti in the anodizing or in the galvanizing bath. However, the phase diagram of Ti-Zn system is still under debate due to the experimental difficulties such as the melting point of Ti is much higher than the boiling point of Zn which makes it challenging to prepare pure Ti-Zn alloy samples. In this work, we used quasi-harmonic approximation to calculate the finite temperature thermodynamic properties of Ti-Zn intermetallics. Based on the first-principles phonon calculations, we determined the enthalpy of formation, entropy and heat capacity, and compared with experimental phase equilibrium data. We performed a systematic CALPHAD modeling and developed a comprehensive thermodynamic description of the Ti-Zn system. The calculated phase diagram is in good agreement with experimental data than the previous modeling. Our work also sheds light on the incorporation of first-principles calculations with experimental data for CALPHAD thermodynamic assessment.

MM 47.23 Wed 18:30 Poster C

Cluster expansions with CELL: applications to simple and complex alloys — •Maria Troppenz[1], Santiago Rigamonti[1], Martin Kuban[1], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber Institut

The newly released python package CELL [1] allows for building accurate cluster expansion (CE) models. While available CE codes can tackle only small parent cells (e.g. fcc), CELL is specially suitable for studying complex alloys with large parent cells, for which a full enumeration of structures can't be performed. In this work, we show several applications of CELL to surface and bulk alloys, ranging from simple alloys with a small parent cell, as e.g. SiGe bulk and the surface alloy $\mathrm{Al_xNa_{1\text{-}x}}$/Al(100), to highly complex structures, as e.g. the thermoelectric clathrates $\mathrm{Ba_8Al_xSi_{46\text{-}x}}$ [2] and $\mathrm{Ba_8Ni_xGe_{46\text{-}x\text{-}y}\square_y}$ with 54 atoms in the parent cell. CELL implements features like Wang-Landau method and Monte-Carlo simulations. Employing them, we could discover the thermodynamic signatures of an order-disorder transition driving an insulator-to-metal transition for $Ba_8Al_{16}Si_{30}$.

[1] S. Rigamonti, M. Troppenz, M. Kuban, A. Huebner, C. Sutton, L. Ghiringhelli, M. Stournara, M. Scheffler, and C. Draxl. *CELL: python package for cluster expansions with large parent cells.* In preparation.

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MM 47.24 Wed 18:30 Poster C

The FLAPW code FLEUR: scaling and performance improvements on the route towards the exascale — •Daniel Wortmann, Uliana Alekseeva, Gregor Michalicek, and Stefan Blügel — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 54248 Jülich, Germany

While our all-electron density functional theory (DFT) code `FLEUR`[1] is used successfully since many years on a variety of different computing platforms, current developments in computer architectures and supercomputing infrastructure define new challenges and restriction on the present and future use of such comprehensive DFT codes. In particular the strong increase of additional intra-node parallelism, from the increasing number of CPU cores to the advances in GPU based computing, requires extensive adjustments of the existing code base and the reevaluation of existing implementations.

We present our recent developments of the `FLEUR` code starting from the performance analysis up to the discussion of algorithmic changes in the full-potential linearized augmented plane-wave (FLAPW) approach. We demonstrate that this enables the code to simulate systems of more than 1000 atoms efficiently using more than 6000 cores. The state of the GPU-aware implementation is also discussed and the obstacles specific to this computing platform are identified.

The work has been supported by the MaX European Center of Excellence in Computing[2] (H2020-EINFRA-2015-1 project: GA 676598).

[1] Homepage of the open-source code `FLEUR`: http://www.flapw.de

[2] http://www.max-centre.eu

MM 47.25 Wed 18:30 Poster C

Using machine learning for efficient extraction of higher order force constants in solids. — •Fredrik Eriksson, Erik Fransson, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

Higher order force constants are essential for the description of, e.g., thermal transport and metastable materials. They originate in the theory of lattice vibrations and can be used in perturbative approaches as well as atomistic simulations. Usually, the force constants of second and third order are obtained systematically by enumeration. The underlying crystal symmetry is exploited to constrain the force constants and reduce the number of independent calculations. This approach, however, scales badly with increasing order and for systems with low symmetry. This results in a steep increase of the number of reference calculations (typically based on density functional theory) whence this systematic approach is limited.

In this contribution we demonstrate how techniques from machine learning can be exploited to dramatically reduce the number of reference calculations and break the unfavorable scaling with system size and symmetry. Our implementation enables us to extract force constants (up to fourth order and beyond) even for systems with low symmetry and large primitive unitcells. This is demonstrated by applications to e.g. transition metal dichalcogenides, clathrates and the metastable phases of transition metals.

MM 47.26 Wed 18:30 Poster C

Uncertainty quantification strategies for atomistic simulations with classical effective potentials — •Peter Brommer and Sarah Longbottom — University of Warwick, Coventry, UK

Molecular dynamics (MD) simulations with classical effective potentials account for a significant fraction of current HPC usage. In those simulations, the energy of the system (and thus the forces on the atoms) depends only on the positions of the atoms; all electronic degrees of freedoms are accounted for in the interaction potential or force field. In contrast to ab-initio methods, effective potentials require the user to make some assumptions and approximations. Unfortunately, the bias, approximations and uncertainties that enter the effective potential creation process at every step (choice of interaction terms, functional form and parameter values) are badly controlled, and in most cases the confidence of the final result of a MD simulation is unknown a priori. The selection of interaction terms and functional form are often motivated by intuition and prior experience of the researcher and then validated by comparing the results in a certain situation after the fact, which is then used to justify using a potential even when such a validation is no longer feasible. However, for simulations to be truly predictive, it is essential to quantify the uncertainty one incurs by using a certain representation of the interactions between atoms. Here, I present an overview of various strategies to combat this deficit of effective potentials and the computational impact of such approaches.

MM 47.27 Wed 18:30 Poster C

Reduction of Redundant Quantum Mechanical Computations Using Machine Learning Methods for Nanocatalysts — •Eiaki Morooka, Adam Foster, and Marc Jäger — Aalto University, Helsinki, Finland

Platinum Group Metals (PGMs) are used for fuel cells, batteries and for automobile filters called autocatalysts, and Europe dominates the platinum consumption. Nevertheless, there is no primary PGM production in the EU, and recycling remains limited, while PGMs are increasingly adopted in emerging technologies for green energy conversion devices. PGMs should be substituted by inexpensive, earth-abundant catalysts, such as bimetallic transition metals with non-metallic elements. These clusters must be rationally designed and fine-tuned by using combinations of several chemical elements, different structures and sizes, which is unfeasible for both experiments and traditional quantum mechanical computations. We are developing machine learning tools to screen nanoclusters using a state-of-the-art chemical descriptor called smooth overlap of atomic positions (SOAP) to drastically reduce quantum mechanical computations. Specifically, by scanning through the similarities of local chemical environments of surface hydrogens and eliminating the surface hydrogens with similar local chemical environments.

MM 47.28 Wed 18:30 Poster C

Mechanical properties of the high-entropy alloy Au-Cu-Ni-Pd-Pt — •Felix Thiel[1], Jens Freudenberger[1,2], and Kornelius Nielsch[1] — [1]IFW Dresden, Helmholtzstr. 20, 01069, Dresden, Deutschland — [2]TU Bergakademie Freiberg, Insitut für Werkstoffwissenschaft, Gustav-Zeuner-Str. 5, 09599, Freiberg, Deutschland

High Entropy Alloys (HEAs) show outstanding mechanical and physical properties, which would not have been expected upon their simple crystal structure and the fact that they are single phased. The Au-Cu-Ni-Pd-Pt system and their including subsystems show crystallization into the same Cu-type crystal structure within the whole concentration range. Therefore, this system is unique and particularly suitable to study the alloying effect on the properties within a large concentration range without the necessity of considering other phases. The present study shows the effect of alloying a multi-component solid solution on the properties of medium and high entropy alloys in this system. In particular, effects such as solid solution hardening and work hardening are assessed.

MM 47.29 Wed 18:30 Poster C

Template-Assisted Fabrications of Nanostructure-Array-Based Gas-Sensors — •Shipu Xu, Huaping Zhao, Yang Xu, Rui Xu, Huanming Zhang, and Long Liu — Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany

Gas-sensors formed by a nanostructure array are of advanced features such as large surface area in sensing, which are also morphology- and arrangement-parameter dependent. Herein, we show a template-assisted method to fabricate nanostructure-array-based gas-sensors, by which the morphology of the arrays can be controlled on a large scale. Using colloidal monolayer and anodic aluminum oxide as a template, we get nanoporous films and nanorod arrays, respectively. By adjusting the pore size of the porous film, the SnO2 sample exhibit a low detection limit of 100 ppm ethanol gas. Additionally, a much lower detection limit of 6 ppm ethanol gas is achievable by controlling the arrayed nanorod length. Based on the above, we confirm that the template-assisted method can be used to fabricate a gas-sensor with high sensitivity.

MM 47.30 Wed 18:30 Poster C

Formation of porous nickel nanosystems under near-equilibrium condensation conditions using alumina membranes as a template for deposition — •Anna Kornyushchenko[1,2], Vyacheslav Perekrestov[1], Stefan Ostendorp[2], and Gerhard Wilde[2] — [1]Sumy State University, Laboratory of Vacuum Nanotechnologies, Sumy, Ukraine — [2]WestfälischeWilhelms-Universität, Institute of Materials Physics, Münster, Germany

Depending on morphology porous nanostructures can possess unique physical properties what can determine areas of their application. In the present work a new technological approach has been proposed to obtain ordered porous nickel nanoclusters consisting of weakly connected uniform nanocrystals of less than 10 nm in diameter. The proposed technology uses near-equilibrium condensation conditions in combination with ultra-thin alumina membranes as templates. The conditions close to thermodynamic equilibrium have been implemented by magnetron sputtering operating at a low discharge power. It is known, that alumina membranes are being widely used in order to obtain different nanostructures on surfaces, ranging from quantum-sized nanodots to nanowires and nanotubes. However, ordered systems of nano-islands which themselves consist of weakly-bound nanocrystals of almost identical shape and size have been obtained for the first time. Therefore, the deposition of weakly supersaturated vapors through the alumina membrane pores reveals new peculiarities of the self-assembly of ordered arrays of nanostructures on substrate surfaces.

MM 47.31 Wed 18:30 Poster C

Optical properties of ALD deposited ZnO as a functional sensing layer based on self-assembled mesoporous membranes — •Katharina Spangenberg, Stefan Ostendorp, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, WWU Münster, Germany

Large scale nanopatterns can be generated by using anodic aluminum oxide (AAO) masks which are porous alumina membranes fabricated in an electrochemical dissolution of aluminum in an acidic electrolyte. AAO is utilized as a self-assembled mesoporous template for producing an ordered nano-array of zinc oxide (ZnO) via atomic layer deposition (ALD). Its structure is well controllable and the correlation with optical properties can be closely studied.

The characterization of structural properties by scanning electron microscopy (SEM) and atomic force microscopy (AFM), as well as X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDX) and optical spectrometry, reveals the dependence of template based ZnO growth and microstructure on the process parameters during sample synthesis. The results show that the emission wavelength of nanostructured ZnO is tunable. The applicability of AAO embedded ZnO structures as a functional sensing layer is evaluated and discussed.

MM 47.32 Wed 18:30 Poster C

Anodic Aluminum Oxide AAO as a template for the synthesis of ZnO nanostructures via Atomic Layer Deposition — •Hanaa Seso, Stefan Ostendorp, Martin Peterlechner, and Gerhard Wilde. — Institute of Materials Physics, Westfälische-Wilhelms-University, Wilhelm-Klemm-Str.10, Münster, Germany

The anodization of aluminum can result in two different types of oxides, a Compact barrier type anodic film and a porous oxide film. The synthesis of this latter anodic aluminum oxide (AAO) and its application as a template for the fabrication of metal oxide nanostructures by atomic layer deposition (ALD) is described. the ALD is ideal for performing precise depositions of metal oxide (ZnO) nano-tubes with different diameter and wall thicknesses within the pores of AAO .the effect of the growth temperature , ranging from 100 °C to 250 °C ,on the formed ZnO is investigated . the bare and ZnO *coated AAO were characterized by scanning electron microscopy (SEM) , energy dispersive X-ray analysis (EDAX) , atomic force microscopy (AFM), X-ray diffraction electron microscopy (TEM) . The roughness and crystallinity of the as * prepared ZnO layers are discussed.

MM 47.33 Wed 18:30 Poster C

Development of an in situ photo-electric TEM holder with time correlation between photo-electrical data and imaging. — •Jonas Lindner[1], Vladimir Roddatis[1], Emanuel Ronge[1], Stefanie Mildner[1], Patrick Peretzki[2], Christian Jooss[1], and Michael Seibt[2] — [1]Institute of Materials Physics, University of Goettingen, Germany — [2]IV. Physical Institute, University of Goettingen, Germany

For an improved understanding of atomic scale processes involved in (photo-)electrochemical energy conversion, studies of electrodes and semiconductor devices under working conditions in high resolution transmission electron microscopy are highly demanded. This requires the time-correlation of TEM-images and spectroscopy-data with (photo-)electrical measurements data in an environmental transmission electron microscope (ETEM) , where systems can be studied under reactive chemical conditions, e.g. in H_2O. A measurement system has been developed by combining the program languages from Gatan Digital Mircograph (DM), Labview and C++. It provides digital ETEM-control and synchronizes the DM spectroscopy data recording with current-voltage-curves, which leads to a time correlation of the experimental results. A proof of concept experiment for the in-situ time correlation of TEM images to electrical data with time resolution of up to 100ms is presented for the Ostwald ripening of a platinum -carbon nanocomposite, typically used in Focused Ion Beam (FIB) machines for contacting. Further photo-electrical in situ TEM measurements are done on oxide heterojunctions.

MM 47.34 Wed 18:30 Poster C

A new instrument for cryo atom probe tomography — •Jonas Ott, Patrick Stender, and Guido Schmitz — Institut für Materialwissenschaft, Lehrstuhl für Materialphysik, Stuttgart, Deutschland

Atom probe tomography (APT) as well as dual beam microscopy (FIB/SEM) are powerful tools in nanotechnology with enormous scientific output. The combination of both techniques is able to deliver information up to sub-nanometer resolution of many material classes. However, sometimes the application becomes limited by the spatial separation of the two techniques. To enable the analysis of liquids and soft matter by atom probe tomography, we designed and installed a new hybrid instrument which represents a combination of a dual beam scanning microscope for FIB preparation and miniaturized APT chamber. The dual beam tool is extended by all facilities to enable cryo-preparation. The central piece of the new microscope is the APT-shuttle containing sample stage, cryo connection to reach 20 K, a piezo drive that controls the 20 *m extraction electrode and 20 kV voltage supply and insulation. Containing all these features, this shuttle is nevertheless not larger than 4x7 cm2 and can be transferred within seconds from one stage to the other. This approach enables several new possibilities with regard to measurement procedure and sample preparation. Furthermore, we could demonstrate unique APT measurements of frozen liquids and organic materials. On this poster the design and the working principle of the new tool are demonstrated. We also present calibration results in different measurement modes as achieved by the new tool.

MM 47.35 Wed 18:30 Poster C

Description of 3D polycrystalline microstructures using a tessellation model generated by ellipsoids — •Mingyan Wang[1], Lukas Petrich[2], Daniel Westhoff[2], Volker Schmidt[2], and Carl E. Krill III[1] — [1]Institute of Micro and Nanomaterials, Ulm University — [2]Institute of Stochastics, Ulm University

With 3D imaging techniques increasingly being employed to probe the microstructure of materials, we are gaining a much more comprehensive view of their internal structure, while simultaneously being confronted by an enormous amount of data! For example, in our research we have characterized polycrystalline Al-5 wt% Cu alloys by synchrotron-based 3D X-ray diffraction (3DXRD) microscopy. In this technique, the 3D microstructure is reconstructed from numerous far-field and near-field diffraction images. We obtained time-resolved information by recording a 3D snapshot after each *ex situ* annealing step. An ellipsoid-based tessellation model was then fitted to each data set to approximate complex grain morphologies. Compared to voxel-based representations of microstructure (such as those provided by 3DXRD characterization), tessellations save a considerable amount of storage space while retaining most of the information regarding the real microstructure. In addition, tessellations obviate the meshing step that must otherwise be performed in order to calculate grain boundary properties like local curvature and dihedral angle, which are critical for understanding the kinetics of grain boundary migration. Compared to meshed experimental data, the ellipsoid-based tessellation model yields consistent results for such properties.

MM 47.36 Wed 18:30 Poster C

Grain boundary thermodynamics in the iron–chromium system — Helena Solodenko, Marvin Poul, •Sebastian Eich, and Guido Schmitz — Universität Stuttgart, Stuttgart, Deutschland

We present a thorough analysis of grain boundary (GB) thermodynamics using the framework developed by Frolov and Mishin[1]. This framework *eo ipso* allows to make a prediction of GB segregation and GB free energies on the basis of the properties of the pure components in the binary system. Based on the theory and available *ab initio* as well as experimental data, we chose the iron–chromium system since it is suggested to be a candidate for stabilization against grain growth in nanocrystalline materials due to negative GB free energies. Indeed, atomistic studies utilizing an accurate thermodynamic embedded-atom potential, confirmed negative GB free energies close to the phase boundary on the chromium-rich side. Eventually, we performed atom probe tomography experiments on pre-alloyed chromium-rich iron-chromium alloys deposited by ion beam sputtering followed by subsequent heat treatment. We quantitatively compare the atomistic prediction with the experimental results.

[1] T. Frolov and Y. Mishin, Phys. Rev. B 85 (2012), 224107.

MM 47.37 Wed 18:30 Poster C

Quantitative High-resolution and Analytical TEM Investigations of Perovskite Interfaces — •Tobias Meyer[1], Patrick Peretzki[1], Birte Kressdorf[2], Christian Jooss[2], and Michael Seibt[1] — [1]IV. Physical Institute, University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Materials Science, University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The transmission of sub band gap photons as well as thermalisation losses due to phononic relaxations of hot charge carriers, resulting in the Shockley-Queisser limit of the energy conversion efficiency, are the major theoretical bottlenecks of solar cells based on classical semiconductors. However, strongly correlated materials such as perovskites are a promising candidate to exceed this limit by exploiting the nature of polaronic charge carriers, i.e. the existence of long-living intraband excitations [1]. In fact, the efficiency of halide perovskite based solar cells has increased tremendously during the last decade [2]. Nonetheless, the knowledge about their correlated transport phenomena is rather limited but highly desirable to steer the properties of prospective devices.

We investigate transition-metal oxide perovskite heterojunctions with various Transmission Electron Microscopy (TEM) techniques, i.e. High-resolution and Analytical TEM, to elucidate the character of the charge separating interface. Additionally, differences of focused ion beam and conventionally prepared specimens are discussed.

[1] Ifland, B. et al., New Journal of Physics (2017), 19(6), 063046

[2] W. S. Yang et al., Science 348 (2015), 1234-1237

MM 47.38 Wed 18:30 Poster C

Reducing the dimensionality in iron-based superconductors: quasi-one dimensional iron chalcogenide $BaFe_2S_3$ — •María Lourdes Amigó[1], Malin Lüdicke[1], Anja Wolter-Giraud[1], Christian Hess[1], Saicharan Aswartham[1], Silvia Seiro[1], and Bernd Büchner[1,2] — [1]IFW-Dresden, Germany — [2]TU-Dresden, Germany

The layered crystalline structure is a characteristic shared by most iron-based superconductors. A very interesting question is how the superconductivity evolves if the dimensionality is further reduced. Iron-chalcogen-based structures are extremely flexible and allow the exploration of dimensionality effects on the physical properties since iron atoms can form low-dimensional structures including chains (e.g. $BaFe_2S_4$) or ladders ($BaFe_2S_3$). $BaFe_2S_3$ and $BaFe_2Se_3$ are antiferromagnetic Mott insulators and have been reported to become metallic under pressure. The metallic phase presents superconductivity at low temperatures.

In this work, we focus on the synthesis of single crystals of $BaFe_2S_3$. We present a comprehensive characterization together with the resistivity and the magnetization. Above the Néel temperature (T_N ∼120K), the magnetization decreases upon cooling. This non-Curie-Weiss behavior is similar to what is found in the parent compounds of the iron-based superconductors. The resistivity presents an insulating-like behavior with a first kink at T∼200K and a second at the Néel temperature.

MM 47.39 Wed 18:30 Poster C

Reducing the dimensionality in iron-based superconductors: quasi-one dimensional iron chalcogenide $BaFe_2S_3$ — •María Lourdes Amigó[1], Malin Lüdicke[1], Anja Wolter-Giraud[1], Christian Hess[1], Sabine Wurmehl[1], Saicharan Aswartham[1], Silvia Seiro[1], and Bernd Büchner[1,2] — [1]IFW-Dresden, Germany — [2]TU-Dresden, Germany

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MM 47.40 Wed 18:30 Poster C

***In situ* experiment for selective laser melting** — •Jan Rosigkeit, Peter Staron, Florian Pyczak, and Martin Müller — Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany

We are currently developing a new industry-relevant sample environment purposefully designed for time-resolved *in situ* selective laser melting (SLM) studies using high-energy ($30-200$ keV) and high photon flux (up to 10^{12} ph/s) synchrotron radiation. The high photon flux combined with a new fast-acquisition-time (4 ms) 2D-detector for high photon energies permits time-resolved *in situ* structural analysis of the selective laser melting process. The high-energy synchrotron-radiation based X-rays result in small scattering angles (<8°), allowing large areas of reciprocal space to be imaged with a 2D detector. The device for *in situ* experiments (FlexiSLM) is planned for use at the P07 High Energy Materials Science (HEMS) beamline at the most brilliant synchrotron radiation source PETRA III at the Deutsches Elektronen-Synchrotron (DESY) in Hamburg.

MM 47.41 Wed 18:30 Poster C

XAFS on Al-alloys: an investigation of early clustering and precipitation states — •Frank Lotter, Danny Petschke, Elischa Bläss, and Torsten Staab — University Wuerzburg, Dep. of Chemistry, LCTM Roentgenring 11, 97070 Wuerzburg, Germany

X-ray absorption spectroscopy (XAS) provides a powerful tool to probe the local atomic surroundings of the absorbing element. Therefore the energy of the incoming X-ray beam is varied around the absorption edge of the specific element. The excited atom becomes origin of a spherical photo wave which interferes with neighboring atoms by multiple scattering. This results in an oscillating spectrum, the so called Fine Structure, giving information about the local structure around the probed atom.

The Al-Cu system offers a basis for alloys (Al-Cu-Mg, Al-Cu-Li, Al-Si-Cu) with important technological applications in the automotive and aerospace sector.

Differential Scanning Calorimetry (DSC) was used to confirm ageing states where one precipitate phase clearly dominates. Thus different reference states were created which then could be investigated by XAS at the Cu K-edge. Furthermore, in situ natural ageing experiments were conducted directly after quenching by using the energy dispersive XAS technique, which allows for very short measuring times, to emphasize the method's sensitivity for small changes in the local atomic configuration surrounding the Cu atoms.

MM 47.42 Wed 18:30 Poster C

Ultra-precision surface figuring of aluminium mirror devices — •Jens Bauer, Melanie Ulitschka, Frank Frost, and Thomas Arnold — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Technical aluminium alloy materials as AL6061 or AL905 are widely used in manufacturing of high performance mirror devices in the IR spectral range. However, the requirements in the optical surface quality increase tremendously for short-wavelength applications in the visible and UV range. Reactively-driven ion beam tools allow the direct surface figure error-correction of aluminium mirror optics for the first time up to 1 micron in height while preserving the surface roughness. A deterministic machining approach with a small-sized tool is applied to perform ultra-precise figuring of diversely shaped surfaces as spheres, aspheres or even freeforms. As an example the figure error correction of a deep concave parabolic mirror with an aspect ratio of central depth to open aperture of about 0.6 is presented. The contribution comprises technological aspects as the generation of a focused millimeter sized ion beam, the evaluation of different machining geometries within the particular ion beam erosion model scheme, and several trial process applications of reactive ion beam machining at aluminum sample devices.

MM 47.43 Wed 18:30 Poster C

Characterization of manganite-based building-blocks for thermal circuitry via transient thermoreflectometry — •Roland Potthast[1], Dennis Meyer[1], Alexandr Belenchuk[2], and Henning Ulrichs[1] — [1]I. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Institute of Electronic Engineering and Nanotechnology of the Academy of Sciences of Moldova, Chisinau, Moldova

We discuss the implementation and application of a transient thermoreflectometry (TTR) technique [1] for the analysis of thermal properties of multilayer samples. In TTR, a pump laser heats the surface, and the time-dependent change of the surface temperature is monitored by measuring the reflectivity of the probe laser. Our temperature-controlled setup uses a high-fluence fs-laser (1030 nm) as a pump, and a continuous wave diode laser (639 nm) as a probe. We apply the TTR-method in order to determine thermal properties of LaCaMnO-bilayers. The two manganite layers feature phase transitions at slightly different critical temperatures. We attempt to exploit this property in order to enable thermal rectification, as suggested by M. Peyrard [2], and numerical finite-difference time-domain simulation.

We acknowledge financial support by the DFG within the CRC 1073 Atomic scale control of energy conversion.

[1] F. Döring, A. Major, C. Eberl, H.-U. Krebs, Appl. Phys. A, 122, 872 (2016).

[2] M. Peyrard, EPL 76, 49 (2006).

MM 47.44 Wed 18:30 Poster C

Surface Characterization of CuCrZr-Electrodes for Resistance Spot Welding — •Philipp Moritz[1,2], Oliver Höfft[1], Hagen Kerl[2], Volker Wesling[2], and Wolfgang Maus-Friedrichs[1,2] — [1]Institute of Energy Research and Physical Technologies, Clausthal University of Technology, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Clausthal Centre of Material Technology, Clausthal University of Technology, Agricolastr. 2, 38678 Clausthal-Zellerfeld

Resistance spot welding is an established technology in the automotive industry. An important aspect in this process is the interaction of the welding electrodes with the steel body sheet. After a certain number of weldings the electrodes produce an irregular welded joint. It is presumed that adherences and diffusion processes at the interface limit the life time of the electrodes significantly.

To understand these interactions, the surfaces of CuCrZr-electrodes are studied with X-ray photoelectron spectroscopy (XPS), Scanning electron microscopy (SEM) and Energy dispersive X-ray spectroscopy (EDX). For the experiments conventional steel plates with AlSi-coatings were used for welding. The electrodes were studied after 0, 10 and 100 welding processes, respectively.

SEM and EDX measurements show that a deposition of AlSi-sheet material was formed on the CuCrZr-electrode surface. Depth profiles indicate that the elements of the steel sheet diffuse into the surface of the electrode. These effects increase with the number of welding processes.

MM 47.45 Wed 18:30 Poster C

Terahertz Spectroscopy of thin metallic films — •Natalie Kattner, Nathan Jukam, and Andreas Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

In the last decades new Terahertz (THz) sources have been developed. Many terahertz devices such as plasmonic waveguides for THz quantum cascade lasers (QCL) cavities, photonic crystals or planar metamaterial resonators incorporate metals, since they have relatively low losses and high reflectivities at terahertz frequencies.

The complex conductivity of a metal determines losses in devices. In many devices thin metallic films are used in lieu of bulk-materials. The conductivity of the thin films is in general not equal to the bulk conductivity. Thus, there has been much confusion as to the proper conductivity values and the validity of the Drude model.

Here, we examine the complex conductivity of thin films of Gold, Aluminum and Copper at terahertz frequencies in a temperature range from 4K to room temperature with Time-Domain Spectroscopy (TDS). From the TDS spectrum we determine the complex conductivity. In addition, we measure the DC conductivity of thin films as a function of temperature.

The advantages of TDS are the generation of coherent light and the possibility to determine the amplitude and the phase of the electromagnetic field. Consequently, the complex conductivity can either be determined from the reflection or the transmission coefficients without using the Kramers-Kronig relations.

MM 47.46 Wed 18:30 Poster C

New simulation method of segmented ring detector images in scanning transmission electron microscopy (STEM) analyzing medium-range order — •Sven Hilke, Jan Kirschbaum, Vitalij Hieronymus-Schmidt, Manuel Radek, Hartmut Bracht, Gerhard Wilde, and Martin Peterlechner — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster

The medium-range structure of amorphous solids at the nanometer scale is an important information for their mechanical behavior and for relaxation processes. We present in this work a new method to extract Fluctuation Electron Microscopy (FEM) normalized variance profiles - one normally gains from experimental nano-beam diffraction pattern (NBDP) - by image simulations of segmented ring detectors using STEMcl [1]. To discuss this new approach we compared experimental normalized variance profiles with the simulated ones. The segmented detector simulation and analysis of molecular dynamics (MD) simulated structures are in good agreement with the experimental data - in terms of peak position as well as peak shape in the normalized variances. These results indicate the viability of the simulation approach and opens the possibility to study e.g. small structural heterogeneities by simulations and experiments.

[1]Radek, M.; Tenberge, J.-G.; Hilke, S.; Wilde, G.; Peterlechner, M.; Ultramicroscopy (2017), submitted.

MM 47.47 Wed 18:30 Poster C

Temperaturefield-analysis of the vacuum chamber of the Planetary Emissivity Laboratory — •Maximilian Grove[1], Jörn Helbert[2], and Alessandro Maturilli[3] — [1]WWU Münster, Münster, Nordrhein-Westfalen — [2]DLR, Berlin, Berlin — [3]DLR, Köln, Nordrhein-Westfalen

The institute for planetary research of the german aerospace center [DLR] was commissioned to build the Mercury Radiometer and thermal Infrared Spectrometer [MERTIS] - an instrument for the BepiColombo mission to be launched in 2018 [1]. One task within this project was to measure spectra from heated samples in a vacuum chamber to simulate the high surface temperature and low pressure athmosphere of the Mercury for comparison [2]. The thermal behaviour of the vacuum chamber defines the signal-to-noise ratio. To estimate the influence of ambient radiation COMSOL accompanied with Finite-Element-Method [FEM] was used [3]. The geometry was simplified to a 2D-geometry due to calculation power. With the help of mesh analysis and multiple parameter sweeps an estimation of the model accuracy could be achieved. The results show expected thermal behaviour, high signal-to-noise ratios and can be used to further minimize unwanted radiation effects by changing emissivity values.

References: [1] European Space Agency, ESA - BepiColombo launch rescheduled, 25 November 2016. [2] Dr. Maturilli and Dr.rer.nat. Helbert, DLR, Characterization, testing, calibration, and validation of the Berlin emissivity database, doi: 10.1117/1.JRS.8.084985, 19 May 2014. [3] COMSOL Inc., Heat Transfer Module, 2017.

MM 47.48 Wed 18:30 Poster C

In situ Raman Spectroscopy on Paper Fibres during Tensile Testing and during Hydration — •Alena Bell[1], Sonja Wendenburg[2], Markus Biesalski[2], and Robert Stark[1] — [1]TU Darmstadt, Materialwissenschaften, Physics of Surfaces, Alarich-Weiß-Str. 16, 64287 Darmstadt, Germany — [2]TU Darmstadt, Chemie, Makromolekulare Chemie, Alarich-Weiß-Str. 8, 64287 Darmstadt, Germany

As cellulose is one of the most abundant materials in the world, it becomes more important to improve its properties, which it shows within paper, such as the wet strength. A promising approach to stabilise the mechanics of cellulose fibres against humidity is the hydrophobisation. Two kinds of cellulose, cotton linters and eucalyptus, were coated with a hydrophobic terpolymer. For the characterisation, two different kinds of measurements were applied, namely hydration and bending experiments without prestress. Both experiments were performed by Raman spectroscopy in situ.

Humidity experiments, which were performed on small strips of paper, show an increase in water band intensity with ongoing hydration and a decrease whithin the drying process for the uncoated samples.

This matched the assumption of the superposition of the paper and water Raman spectra. The coated samples do not show a clear trend for the water peak intensity. Bending experiments were performed on small fibre bundles which were extracted by hand from paper sheets and collocated on small tooth combs without prestress. We could show that a band shift of the 1095 cm-1 is observed in fibre bundles.

MM 47.49 Wed 18:30 Poster C

Sulfation kinetics of alkali chlorides and subsequent chlorine induced corrosion in waste-to-energy plants — •Sebastian Pentz[1], Daniel Ott[1], Ferdinand Haider[1], and Ragnar Warnecke[2] — [1]Universität Augsburg, Inst. f. Physik, 86159 Augsburg — [2]Gemeinschaftskraftwerk Schweinfurt GmbH, 97424 Schweinfurt

High temperature corrosion leads especially in waste-to-energy-plants to massive problems. At prevalent temperatures around 500°C-600°C corrosion is mainly chlorine induced. Responsible for the supply of chlorine at heat exchangers like superheaters or boiler walls is in majority a local release of chlorine through sulfation of solid alkali chlorides. This reaction requires an atmosphere containing SO_2, H_2O, O_2 and releases HCl/Cl_2. In this work the sulfation kinetics for different parameters, like temperature, gas stream, gas components or the influence of catalytic additives is examined. The conversion rate is strongly dependent on the transformation of SO_2 to SO_3, which is catalyzed by the presence of iron oxides like Fe_2O_3. Further experiments are done with $FeCl_2$ on top of the samples in order to directly release chlorine at the metal surface. In addition to the study of the sulfation reaction rate it is possible to characterize the metal loss of samples simultaneously. Furthermore the behaviour of chlorine during the process of the corrosion was investigated. Principles of the reaction conditions in waste-to-energy-plants, especially at the superheaters, are shown and laboratory experiments regarding the kinetics of sulfation reactions are presented.

MM 47.50 Wed 18:30 Poster C

Material Physics in Forensic Science "Recovery of Erased Markings" — Jens Balzer, Bert Weimar, and •Horst Katterwe — Kriminaltechnisches Institut, Bundeskriminalamt, 65173 Wiesbaden

The recovery of erased markings (serial numbers) is an important forensic scientific discipline that includes the physics and technology of materials (solid-state physics, metallurgy, chemistry, and engineering). Markings are applied to distinguish various items and to sign pieces in commercial use. In criminal cases, they are removed to conceal the object*s true identity. However, marking processes (die stamping: cold working for metals, warm working for plastics / engraving / laser beam markings) change the microstructure of the metals (grains, slip bands, dislocations), or in case of polymers the macromolecules around the marking become oriented (decreasing of the entropy). This poster presents methods - both destructive and nondestructive - used to recover the erased markings in metals or polymers: chemical and electrolytic etching, heat treatment, ultrasonic cavitation, magnetic particle method, hardness testing, relief polishing, swelling (memory effect by entropy elasticity), * References: 1) Voss-de Haan, Katterwe, Simross *Physik in der Kriminaltechnik*, Physik Journal 2, 2003, 35-41; 2) Katterwe *Restoration of serial numbers* in Stauffer, Bonfanti *Forensic investigation of stolen-recovered and other crime-related vehicles*, Elsevier 2006; 3) Weimar, Katterwe, Braune *Formspuren, Wiedersichtbarmachung entfernter Zeichen* in Widmaier, Müller, Schlothauer *Münchener Anwaltshandbuch Strafverteidigung*, C. H. Beck 2014.

MM 47.51 Wed 18:30 Poster C

Compressed-sensing-based feature selection strategies in materials science: Defining the "best model" — •Benedikt Hoock[1,2], Santiago Rigamonti[1], Luca Ghiringhelli[2], Matthias Scheffler[1,2], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Berlin, DE — [2]Fritz-Haber-Institut der MPG, Berlin,DE

Machine Learning (ML) methods are being currently established in materials science in order to find best models that help to better understand existing data or to identify even new materials. In this context, one needs to define what the term "best model" means. Up to now, this is far from being precisely defined, even if one confines oneself to a certain model class. We compare several approaches for cross validation (CV) based model selection strategies [1]. These differently balance between fitting accuracy and generalizability by using either training, or average training or test errors as selection criterion, respectively, and hence lead to different definitions for the "best model". We apply these strategies to a set of ab-initio calculated group-IV ternaries to predict lattice constants and energies of mixing. This is achieved by adapting a LASSO-based ML method [2] to find best descriptors constructed from simple atomic, dimer and tetrahedron data.

[1]: B. Hoock, S. Rigamonti, L. M. Ghiringhelli, M. Scheffler, and C. Draxl, "Predicting lattice constants and energies of mixing of group-IV ternary materials by compressed sensing", in preparation. [2]: L. M. Ghiringhelli, J. Vybiral, E. Ahmetcik, R. Ouyang, S. V. Levchenko, C. Draxl, New Journal of Physics 19.2, 023017 (2017).

MM 48: General Assembly of the Metal- and Materials Division

Best Poster Award

Time: Wednesday 19:45–20:45 Location: TC 006

Assembly

MM 49: Invited talk Peterlechner

Time: Thursday 9:30–10:00 Location: TC 006

Invited Talk MM 49.1 Thu 9:30 TC 006

Analysis of amorphous structures by transmission electron microscopy — •Martin Peterlechner — Institute of Materials Physics, WWU Münster, Germany

Amorphous structures are of academic and technical interest due to a wide range of applications and remarkable physical properties. In particular metallic glasses attract attention in the last decades due to their high strength and hardness, connected with their deformation mechanisms. By definition, an amorphous solid does not show long range order which is typically analyzed using conventional transmission electron microscopy (TEM). Thus new methods as e.g. fluctuation electron microscopy (FEM) have been developed, able to detect medium range order. Additionally, a correlative microscopy approach using high-angle annular dark field (HAADF) and electron energy loss spectroscopy (EELS) was developed in collaboration to quantify density changes within an amorphous phase. In this talk, the sensitivity and limitations of currently applied TEM based methods and their results are discussed with the help of image simulations. A custom built GPU-supported code was applied to shed light on the sensitivity and ability of TEM methods. TEM is an excellent tool to detect density changes and structural changes, occurring upon deformation and relaxation. New instrumentational developments moreover facilitate time series, analyzing relaxation and related atomic mobility. This opens new possibilities to study the difference between differently processed amorphous phases.

MM 50: Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales

Plasticity and Fracture

Time: Thursday 10:15–11:30 Location: H 0106

Topical Talk MM 50.1 Thu 10:15 H 0106
New Insights into the Ductility of Freestanding Metallic Thin Films — •Benoit Merle — Department of Materials Science and Engineering, Institute I, Friedrich-Alexander-University Erlangen-Nürnberg, Germany

Little is known about the ability of freestanding films to accommodate plastic deformation, which is detrimental to the design of future generations of MEMS and integrated sensors. New insights are provided by investigations on 100-300 nm PVD copper, gold and silver thin films by means of in-situ tensile tests in a TEM and in-situ bulge tests in an AFM. They revealed that small specimens can accommodate a remarkable level of strain (10% or more) due to the grain-boundary mediated dominated deformation and the associated high strain-rate sensitivitya. This is in sharp opposition to the behavior of larger samples, which typically fail around 1% strain, because they contain defects that act as crack initiators. Suppressing them at all is hardly achievable in practice, which is why the most promising strategy to improve the ductility of thin films consists into improving their resistance to fracture. The bulge test offers a convenient way to measure the fracture toughness and observe the associated mechanisms. Against expectations, it was found that the thickness hardly influences the toughness of the films within the investigated range and that the microstructure does not play such a critical role as assumed. The resistance to fracture was shown to mostly depend on the resistance to necking ahead of a crack tip, suggesting new possibilities to increase the ductility of the films.

MM 50.2 Thu 10:45 H 0106
In situ TEM deformation studies of the Bauschinger effect in nanocrystalline thin films — •Ankush Kashiwar[1,2], Aaron Kobler[3], Horst Hahn[1,2], and Christian Kübel[1] — [1]Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Technische Universität Darmstadt, 64287 Darmstadt, Germany — [3]Nanoscribe GmbH, 76344 Eggenstein-Leopoldshafen, Germany

Nanocrystalline (nc) metals with grain sizes smaller than about 100 nm exhibit outstanding mechanical strength and fatigue properties compared to their coarse grained counterparts. Recent studies on this class of materials have reported an extended elastic-microplastic regime upon loading and unloading. With the aim of investigating the deformation mechanisms governing these elastic plastic transitions, we perfomed in situ cyclic loading-unloading experiments on sputtered nc Pd thin films inside a TEM. As the strain is progressively increased during each cycle, the stress strain curves show an increasingly nonlinear unloading, deviating from an elastic unloading behavior, which is a characteristic of the Bauschinger effect (BE) in thin metal films. The corresponding ACOM-STEM series indicate local orientation changes in several grains, which are often fully or partially reversible. In addition, there is an evidence of partially reversible dislocation activity during loading and unloading from BF-TEM analysis. In our current experiments, we are combining the different imaging modes for the same sample in cyclic deformation experiments to correlate dislocation activity and grain orientation changes to systematically understand the deformation processes governing the BE in nc thin films.

MM 50.3 Thu 11:00 H 0106
Plasticity in three-point bent Au nanowires studied by in situ Laue micro-diffraction — •Thomas Cornelius[1], Zhe Ren[1], Gunther Richter[2], and Olivier Thomas[1] — [1]Aix-Marseille Univ, Univ Toulon, CNRS, IM2NP UMR 7334, Marseille, France — [2]Max-Planck Institute for Intelligent Systems, Stuttgart, Germany

In the recent past, in-situ experimental setups are being designed for monitoring the evolution of nanostructures during mechanical deformation. Compared to electron microscopy, X-ray diffraction has the benefit of being non-destructive, penetrating (no special need for sample pre-thinning) and extremely sensitive to elastic strains and defects. Thanks to the development of new synchrotron sources, increasingly efficient focusing optics, and advanced 2D detectors X-ray diffraction is becoming a major tool for investigating the structure of nano-objects in situ during mechanical deformation. In particular, Laue microdiffraction with its high sensitivity on crystal orientation and geometrically necessary dislocations (GND) is a predestined method for in-situ nano-mechanical testing. Here, we present in-situ Laue microdiffraction studies on the plasticity of three-point bent Au nanowires revealing the activation of unexpected slip systems and the storage of GNDs in contrast to MD simulations that predict the formation of wedge-shaped twins in purely bent nano-beams which escape the crystal after unloading.

MM 50.4 Thu 11:15 H 0106
X-ray nanodiffraction for in-situ mechanical studies — •Anton Davydok and Christina Krywka — Helmholtz-Zentrum Geesthacht, Hamburg, Germany

Huge scientific interest to mechanical properties of nano- and microscale non-organic materials requires appropriate experimental techniques with commensurate tools for detail investigations. For complete understanding of the deformation process in-situ experiments are necessary. P03 nanofocus endstation at PETRA III in DESY operated by Helmholtz Zentrum Geesthacht provides highly stabile experimental setup with high spatial resolution using a nanosized beam. It is one of only few places in the world where the experimental conditions for scanning X-ray nanodiffraction are provided and it offers a hard X-ray beam with a size of only 250 x 350 nm^2. The strong focus on materials science at P03 is demonstrated by the wide range of experiments already performed with in-situ sample environment including mechanical testing with strain resolution of 10^{-5}. In this presentation the setup for in-situ experiments at the Nanofocus Endstation of P03 beamline (PETRA III, DESY) will be presented with technical characteristic and examples of successful experiments will be shown.

MM 51: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data II

Time: Thursday 10:15–11:45 Location: H 0107

MM 51.1 Thu 10:15 H 0107
Towards a Roadmap of Chemical Space — •Johannes Margraf and Karsten Reuter — Technische Universität München

Data-driven research in materials science and chemistry is typically focused on the properties of individual compounds. If the value of some property is known for a representative part of chemical space, the remaining values can be estimated by interpolation. In this context, it is essential to understand what compounds make up the chemical space of interest. This can be trivial to define (e.g. all binary octet semiconductors) or require significant effort (e.g. all organic molecules up to a certain size). With this contribution, we want to shift the focus from individual compounds to chemical reactions. This means that chemical space is transformed from a list of compounds to a network of reactions connecting them (i.e. a map).

To this end, we will show how the space of chemical reactions can be constructed and organized in a systematic and exhaustive manner. We will further discuss how these reaction networks can be applied in the prediction of reaction mechanisms. Finally, we will compare how machine learning of reaction energies performs in reaction and compound space.

MM 51.2 Thu 10:30 H 0107

CritCat (H2020): Rational design of catalyst materials from first-principles — •Jaakko Akola — Tampere University of Technology, Finland — NTNU Trondheim, Norway

The H2020-project CritCat aims to provide solutions for the substitution of critical metals, especially rare platinum groupmetals (PGMs), used in heterogeneous and electrochemical catalysis. CritCat explores the properties of ultra-small transition metal (TM) nanoparticles to achieve optimal catalytic performance with earth-abundant materials. The emphasis is on industrially-relevant chemical reactions and emerging energy conversion technologies in which PGMs play an instrumental role, particularly in the context of hydrogen energy. The goal is to tailor optimal nanoparticle catalysts for selected (electro)chemical reactions.

The CritCat project includes all the aspects for rational catalyst design including novel catalyst synthesis, characterization, and performance testing together with large-scale computational simulations of the relevant catalysts, substrates and model reactions using the latest computational methods. The DFT data is collected in a descriptor database and used for materials screening at later stages. We have developed new machine learning algorithms for neural network (NN) force fields for generating catalyst structures, descriptor-based efficient hydrogen adsorption site scanning and prediction, and effective charge and energy level prediction based on xyz-files. The new tools pave way for much more efficient catalyst simulations with DFT accuracy.

MM 51.3 Thu 10:45 H 0107

Machine Learning Structural Descriptors on Nanocluster Catalysts — •Marc Jäger[1], Eiaki Morooka[1], and Adam Foster[1,2] — [1]Aalto University, Helsinki, Finland — [2]Kanazawa University, Japan

Scientists have advanced significantly in producing nanoparticles with defined composition, size and morphology in the last decade. Due to this and because of their remarkable properties, nanoclusters have gained attention in heterogeneous catalysis. Nanoclusters differ from bulk metal behaviour, their catalytic properties are sensitive to changes in size and morphology. Nanoparticles like molybdenum disulfide are known to catalyze the hydrogen evolution reaction (HER). The combinatorial and structural space of nanoclusters is vast, so extensive modelling is difficult. Structural descriptors are used to describe the geometry of an adsorption site and to predict properties which indicate a high catalytic activity, in particular the hydrogen adsorption free energy. We analysed the performance of state-of-the-art structural descriptors (SOAP, MBTR and ACSF). Simulations can provide energetic and kinetic analysis of HER using DFT. The vast amount of possible nanoclusters, all potential candidates for catalysing the HER, requires reduction and interpolation of DFT calculations. This is tackled by merging the combinatorial space with the chemical compound space and applying machine learning on diverse datasets.

MM 51.4 Thu 11:00 H 0107

Automatic Selection of Atomic Fingerprints for Machine-Learning Potentials — •Giulio Imbalzano — École polytechnique fédérale de Lausanne, Lausanne, Switzerland

Machine learning of atomic-scale properties is revolutionizing the way simulations are performed, making it possible to evaluate interatomic potentials with first-principles accuracy, at a fraction of the cost. The accuracy, speed and reliability of a machine-learning potential, however, depend strongly on the way atomic configurations are represented before being used as inputs. The raw Cartesian coordinates are typically transformed in ”fingerprints” that are designed to better encode the symmetries of the problem and the physics of the interactions. I discuss an automatic protocol to select a reduced number of fingerprints out of a large set of candidates, based on the intrinsic correlations of the training data. This procedure can greatly simplify the construction of neural-network potentials that strike the best balance between accuracy and computational efficiency, and has the potential to accelerate by orders of magnitude the evaluation of Gaussian Approximation Potentials based on the Smooth Overlap of Atomic Positions kernel.

MM 51.5 Thu 11:15 H 0107

Data-driven assessment of the transferability of effective interatomic potentials — •Y.V. Lysogorskiy, T. Hammerschmidt, and R. Drautz — Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Many materials properties are directly accessible with high-precision by quantum-mechanical calculations using density-functional theory (DFT). However, the computational costs of the DFT calculations make many important materials properties difficult to calculate. To tackle this problem interatomic interaction potentials are widely used. A large number of interatomic potentials is available for a wide range of chemical elements and their mixtures. A central difficulty for applying potentials is the typically very limited information about their reliability for a particular simulation. We performed high-throughput calculations using DFT and interatomic potentials in order to investigate the transferability of interatomic potentials statistically. The results of our calculations are collected in a specially designed database for further analysis. The consequent statistical and correlation analysis of properties and their deviations with respect to reference values allow us to quantify the errors and transferability of interatomic potentials.

MM 51.6 Thu 11:30 H 0107

Data-driven approach to accelerate the development of Bond-Order-Potentials — •Jan Jenke, Aparna P.A. Subramanyam, Alvin Ladines, Thomas Hammerschmidt, and Ralf Drautz — ICAMS Ruhr-Universität Bochum, Bochum, Germany

Interatomic potentials provide a means to simulate extended length and time scales that are outside the reach of ab-initio calculations. However, the transferability of interatomic potentials to atomic environments which were not included in the parameterization of the potential is often unknown and a (re-)parameterization usually very time consuming. We suggest a data-driven approach to overcome these problems for the development of tight-binding (TB) based bond-order-potentials (BOP). The parameterization is mapped to a multi-dimensional optimization problem, which is initialized by a comprehensive database of TB parameters across the periodic table. Using a 2d structure map we systematically sample the possible atomic environments during the parameterization process. This also allows us to predict and analyse the transferability to structures which were not included in the parameterization process. We demonstrate that our method accelerates the development of BOPs with a transparent parameterization process and at the same time provides a direct and quantitative measurement of transferability.

MM 52: Methods in Computational Materials Modelling (methodological aspecst, numerics)

Atomistic sampling techniques

Time: Thursday 10:15–11:30 Location: TC 006

MM 52.1 Thu 10:15 TC 006

Finding reaction coordinates for crystal nucleation in Ni — •Grisell Diaz Leines, Ralf Drautz, and Jutta Rogal — Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany

Despite the technological importance of crystal nucleation, fundamental insight into the early stages of solidification is often hampered by the long timescales and complexity of the process. In this work we employ transition path sampling simulations together with a maximum likelihood analysis of the committor function to identify the reaction coordinates that best describe the nucleation mechanism in nickel. The analysis of the reweighted path ensemble on a set of candidate structural order parameters shows that the nucleation pathway in Ni is governed by the initial formation of mesocrystal regions and a subsequent emergence of fcc-hcp crystallites embedded within the core of these prestructured clusters. Our findings indicate that the prestructured liquid cloud is an order parameter that enhances the reaction coordinate and therefore has an essential role in the structural description of the nucleus and its interfacial free energy. Moreover, we show that the prestructured regions predetermine the coordination of the fcc-hcp polymorphs selected, acting as precursors of the crystallization. These results shed light not just on the atomistic mechanism of nucleation during solidification in Ni but also on the process of polymorph selection.

MM 52.2 Thu 10:30 TC 006

A Preconditioning scheme for Minimum Energy Path finding methods. — •Stela Makri[1], James Kermode[1], and Christoph Ortner[2] — [1]Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry, UK — [2]Mathematics Institute, University of Warwick, Coventry, UK

In transition state theory, the study of thermally activated transitions between energy minima is achieved by finding transition paths connecting the minima. These paths provide information on the energy barrier and reaction rates of the system without going through long and expensive simulations. To find them, current techniques use steepest descent-like minimisation to relax a discretised initial guess. However, steepest descent typically gives slow convergence rates in the presence of ill-conditioned potentials. In this talk I will be discussing how to reduce the condition number of the potential of an arbitrary system and improve the convergence speed and robustness of transition path finding methods, using a preconditioning scheme.

Our key assumption is that the cost of constructing a preconditioner is much smaller than the cost of computing the potential; for density functional theory the cost of single point evaluations is much more expensive than the computation of a preconditioner and thus the proposed approach improves computing times significantly. We have developed a local preconditioning scheme, where the preconditioner acts as a coordinate transformation on the discrete images along the path and a global preconditioning scheme is currently in development, in which the entire path is preconditioned as one entity.

MM 52.3 Thu 10:45 TC 006

One shot calculation of multicomponent phase diagrams with combined umbrella and nested sampling — •Robert Baldock[1], Christopher Sutton[2], Luca Ghiringhelli[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, Switzerland — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The automated calculation of complete phase diagrams, directly from a first-principles or empirical potential energy function, is one of the outstanding challenges in computational materials science. Here we show how nested sampling, a Bayesian Markov chain Monte Carlo algorithm, can be transformed into a powerful tool for exactly this task. In particular, the introduction of umbrella sampling within nested sampling enables the efficient, one-shot calculation of composition-temperature phase diagrams, including for materials that exhibit a miscibility gap whereby the material separates into domains of different composition. Since our nested sampling algorithm does not require previous information about the location of phase transitions, or the atomic structures of phases formed by the material, it can be used as a black-box tool for phase diagram calculation. I will showcase the efficacy of the approach by presenting the binary phase diagrams of a Lennard-Jones alloy (continuous atomistic state space) and gallium indium phosphide as described using a lattice model (discrete atomistic state space).

MM 52.4 Thu 11:00 TC 006

Accurate free energies from *ab initio*: Applications of the TU-TILD technique — •Xi Zhang[1], Dominique Korbmacher[1], Lifang Zhu[1], Albert Glensk[1], Andrew Duff[3], Fritz Körmann[1,2], Blazej Grabowski[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany — [2]Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628 CD Delft, Netherlands — [3]Scientific Computing Department, STFC Daresbury Laboratory, Hartree Centre, Warrington, UK

Calculations of free energies have been long pursued to predict and understand many important phenomena in materials, e.g., thermodynamic properties, defect properties, or phase transitions. Computing free energies with sufficient accuracy fully from *ab initio* is a demanding challenge requiring special methodological techniques. Based on density functional theory, the recently developed TU-TILD (*two-stage upsampled thermodynamic integration using Langevin dynamics*) [Phys. Rev. B 91, 214311 (2015)] technique provides a very efficient framework retaining the desired accuracy in the free energies, capturing in particular explicit anharmonicity. We show the efficiency and accuracy of the TU-TILD technique by focussing on stacking fault Gibbs energies. Successful extensions to point defect Gibbs energies, dynamically unstable phases, phonon lifetimes and liquid free energies within the TOR-TILD technique will be briefly highlighted.

MM 52.5 Thu 11:15 TC 006

Approach for ab initio simulations of materials under extreme conditions — •Jacob Wilkins and Matthew Probert — University of York, York, United Kingdom

To date, the ab initio exploration of materials in extreme conditions has been primarily focussed on equilibrium studies of heat and pressure to a stable crystal structure which fails to capture the methods used to produce these conditions in experiments. In order to attempt to more accurately reproduce the mechanisms present we have adopted a partially self-parametrising fire-and-forget approach for application to moderately sized systems to induce a series of independent shock-waves into a sample medium for testing shock response of the material.

Using the approach of the Hugoniostat, optimised for application to ab initio time-scales we apply a number of isolated shocks at stactic volumes and use a predictor-corrector algorithm to approach the target pressure in even steps. This method allows us to extract the material response to the compression in order to predict the ideal coupling, allowing the method to minimise convergence times even for extreme compressions.

MM 53: Liquid and Amorphous Metals

Processing

Time: Thursday 10:15–11:30 Location: TC 010

MM 53.1 Thu 10:15 TC 010

Cluster-assembled Metallic Glasses — •Cahit Benel[1], Arne Fischer[1], Aline Léon[2], Anna Zimina[2], Mohammed Reda Chellali[1], Robert Kruk[1], and Horst Hahn[1,3] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany — [2]Institute for Photon Science and Synchrotron Radiation, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen, Germany — [3]Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt, 64287, Darmstadt, Germany

Contrary to rapidly quenched metallic glasses, cluster-assembled metallic glasses (CAMGs) have precisely controlled building blocks in terms of their chemical composition and cluster size. Our state-of-the-art cluster ion beam deposition system allows us to deposit various cluster-based films under well-defined conditions. Furthermore, different compaction scenarios can be realized by varying the impact energies of the clusters. A series of amorphous FeSc samples were deposited with various impact energies. The magnetic properties of the samples can be tailored by the impact energy, which affects the ferromagnetic to paramagnetic transition temperature. No evidence of oxidation was found by the X-ray absorption fine structure spectroscopy analyses. The distinct difference in magnetism of chemically identical amorphous alloys is an evidence for a novel atomic structure existing in CAMGs and can provide a fundamental understanding of the structure-material property relation.

MM 53.2 Thu 10:30 TC 010

Ni-Ti nanoglasses: amorphous structure, and magnetic properties — •Mohammed Reda Chellali[1], Sree Harsha Nandam[1], Suzhi Li[1], Leonardo Velasco Estrada[1], Robert Kruk[1], and Horst Hahn[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]KIT-TUD Joint Research Laboratory Nanomaterials, Institute of Materials Science, Technische Universität Darmstadt (TUD), Jovanka-Bontschits-Str. 2, D-64287 Darmstadt, Germany

The so-called nanoglasses display very spectacular properties, such as highly catalytic activity, mechanical performance, or magnetic characteristics, which differ significantly from any known amorphous mixtures. Here, Ni50Ti50 the nanometer-sized glassy particles are generated by means of inert-gas condensation (IGC). Elemental segregation of Ni and Ti is observed in consolidated nanoglasses. The structure of the nanostructured metallic glasses is found to consist of nanometer-sized amorphous regions which are connected by glass-glass interfaces. It is shown that Ni50Ti50 nanoglass is a ferromagnetic whereas the amorphous and crystalline samples with the same chemical composition (Ni50Ti50) are paramagnetic. The ferromagnetism is clarified by the existence of such regions of low atomic density.

MM 53.3 Thu 10:45 TC 010

Metallic nanoglasses from nanoparticle consolidation: A computational study — •Omar Adjaoud and Karsten Albe — Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Otto-Berndt-Str. 3, D-64287 Darmstadt, Germany

Metallic nanoglassses are amorphous materials with an inhomogeneous microstructure, which can be produced by consolidating nanometer-sized glassy spheres and consist of glassy grains connected by glass-glass interfaces. Experiments [1,2] and simulations [3,4] have revealed that glass-glass interfaces are chemically and topologically different from the grain intererior, but the influence of the consolidation process on the microstructure is still under debate. In this contribution, we present molecular dynamics simulations of the consolidation process of nanometer-sized metallic glassy spheres. Our results reveal that during cold compaction most of the glassy spheres deform by homogeneous plastic flow, while in some glassy spheres strain localization occurs. For all studied materials, the porosity is typically closed if the hydrostatic pressure exceeds 4 GPa. Structural analysis shows that the width of the resulting interfaces is significantly larger than in atomistic models based on planar interfaces. Moreover, structural changes occur not only in the interfaces but also in the glassy regions.

1. J. Jing *et al.*, J. Non-Cryst. Solids **113**, 167-170 (1989). 2. J.X. Fang *et al.*, Nano Lett. **12**, 458-463 (2012) . 3. Y. Ritter *et al.*, Acta Mat. **59**, 6588-6593 (2011) . 4. O. Adjaoud *et al.*, Acta Mat. **113**, 284-292 (2016).

MM 53.4 Thu 11:00 TC 010

Consolidation of amorphous powder by thermoplastic forming and subsequent mechanical testing — •Benedikt Bochtler[1], Moritz Stolpe[1,2], Benedikt Reiplinger[1], and Ralf Busch[1] — [1]Lehrstuhl für Metallische Werkstoffe, Universität des Saarlandes, Saarbrücken, Germany — [2]Heraeus Deutschland GmbH & Co. KG, Hanau, Germany

Bulk metallic glasses combine extraordinary strength with a large elastic limit, making them interesting for industrial applications. However, the casting of parts is complicated by the high cooling rates that are necessary. Alternatively, the production and subsequent consolidation of amorphous powder can decouple the production of an amorphous pre-material from the forming of the final part.

Here, amorphous powder of the commercially available Zr-based glass-forming alloy AMZ4 (Zr59.3Cu28.8Al10.4Nb1.5) is consolidated by thermoplastic forming (TPF), where the glassy powder is processed in the supercooled liquid state. Various time and temperature protocols are tested and evaluated regarding the powder compaction and the conservation of the amorphous structure. Compact and amorphous samples are obtained and are subsequently tested by three-point beam bending. The results show that the consolidated samples are still outperformed by as-cast bulk material in bending, however reach the hardness of bulk material. The experimental observations in combination with isothermal crystallization times and viscosity measurements allow to determine a generic TPF processing window that can be used as a tool to assess the thermoplastic formability of different alloys.

MM 53.5 Thu 11:15 TC 010

Synthesis, analysis and deformation of co-sputtered multilayers of amorphous CuZr and nanocrystalline Cu — •Farnaz Abdollahzadeh Davani, Sven Hilke, Martin Peterlechner, and Gerhard Wilde — Materials Physics, Münster,Germany

Metallic glasses are of scientific and technical interest due to their high strength and hardness. Upon deformation, it is expected that soft spots deform locally, finally leading to localized shear in so-called shear bands. In this work, multi-layers of amorphous CuZr and nanocrystalline Cu have been prepared by magnetron co-sputtering of pure Zr and Cu. The as processed structures were analyzed using scanning electron microscopy and transmission electron microscopy. Upon deformation of the layered system, the deformation can be analyzed in the crystalline and amorphous regions. The processing and the deformation are discussed.

MM 54: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 10:30–12:45 Location: HL 001

MM 54.1 Thu 10:30 HL 001

Core-level spectroscopy with the *GW* approximation — •Dorothea Golze and Patrick Rinke — Department of Applied Physics, Aalto University, Espoo, Finland

Inner-shell spectroscopy is an important tool to characterize molecules, liquids and adsorption processes at surfaces. We present a new, accurate method for computing X-ray photoelectron spectra based on the *GW* approximation that overcomes the limitations of density functional theory based approaches. Green's function theory in the *GW* approximation has become the method of choice for addition and removal energies of valence electrons in solids and is now increasingly being applied to molecules. However, *GW* core-level spectroscopy has thus far not received any attention. In most *GW* implementations, the self-energy is computed in the imaginary frequency domain followed by an analytic continuation to the real frequency axis. However, our calculations show that the analytic continuation becomes highly inaccurate for frequencies far away from the Fermi level and is not suitable for the computation of core excitations. Thus, we evaluate the self-energy on the real-frequency axis using the contour deformation (CD) technique. We implemented CD in combination with a resolution-of-the-identity approximation for the screened Coulomb interaction in the FHI-aims program package. Test calculations reveal that our implementation reproduces Turbomole reference calculations [1] perfectly. Furthermore, we present benchmark studies of small and medium-sized gas-phase molecules and discuss the potential of our method for more complex systems. [1] M. J. van Setten et al. JCTC, 2013, 232

MM 54.2 Thu 10:45 HL 001

***GW* and beyond from matrix resolvents** — •Jan Gesenhues[1], Dmitrii Nabok[2], Michael Rohlfing[1], and Claudia Draxl[2] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Theoretische Festkörperphysik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Typically GW calculations make use of either plasmon pole models or numerical integration in order to determine the screened Coulomb interaction W. We demonstrate how to obtain an analytical representation of W with the help of a matrix resolvent and present some standard GW results which have been obtained with the method. The analytical W is a useful starting point for subsequent calculations involving vertex corrections. On the other hand, the matrix resolvent technique itself can be applied upon a BSE-like equation of motion for the polarizability to include vertex corrections.

MM 54.3 Thu 11:00 HL 001

Electron-Magnon Scattering in Elementary Ferromagnets from First Principles: Lifetime Broadening and Kinks — Mathias C. T. D. Müller, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We study the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the two-particle (electron-hole) Green function, where single-particle Stoner excitations and collective spin-wave excitations (magnons) are treated on the same footing. We employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. In the case of Co and Ni, the renormalization gives rise to kinks in the electronic band dispersion at low binding energies, which we attribute to electron scattering with spatially extended spin waves. Furthermore, we find a band anomaly at larger binding energies in iron, which results from a coupling of the quasihole with single-particle excitations that form a peak in the Stoner continuum. This band anomaly has, in fact, been observed in recent photoemission experiments at the same energy and momentum.

MM 54.4 Thu 11:15 HL 001

Effects of the Tamm-Dancoff approximation on the optical spectra of organic molecules — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

When calculating excited state properties of electronic systems within the many-body perturbation theory (MBPT), the Bethe-Salpeter equation (BSE) needs to be solved. This is often done within the so called Tamm-Dancoff approximation (TDA), neglecting the coupling of resonant and anti-resonant excitations.

It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for some organic semiconductors[1]. In this talk we discuss the effects of the TDA on the resulting optical spectra of organic molecules of different sizes and investigate for which cases the TDA may still be justified.

[1] B. Baumeier et al: *J Chem. Theory Comput.*, 2012, **8**, 997

MM 54.5 Thu 11:30 HL 001

Ab-initio treatment of non-local electronic correlations with the dynamical vertex approximation — •Anna Galler[1], Patrik Thunström[2], Patrik Gunacker[3], Josef Kaufmann[3], Matthias Pickem[3], Jan M. Tomczak[3], and Karsten Held[3] — [1]Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France — [2]Department of Physics and Astronomy, Materials Theory, Uppsala University, 75120 Uppsala, Sweden — [3]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Recently, approaches such as the dynamical vertex approximation (DΓA) or dual-fermion method have been developed. These diagrammatic approaches are going beyond dynamical mean-field theory (DMFT) by including non-local electronic correlations on all length scales as well as the local DMFT correlations. Here we present our efforts to extend the DΓA methodology to ab-initio materials calculations (AbinitioDΓA). Our approach is a unifying framework which includes both, GW and DMFT-type of diagrams, but also important non-local correlations beyond, e.g. non-local spin fluctuations. In our multi-band implementation we are using a worm sampling technique within continuous-time quantum Monte Carlo in the hybridization expansion to obtain the DMFT vertex, from which we construct the reducible vertex function in a ladder approximation. As a first application we show results for transition metal oxides. Support by the ERC project AbinitioDGA (306447) is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, Jan M. Tomczak, and K. Held, Physical Review B 95, 115107 (2017)

MM 54.6 Thu 11:45 HL 001

Non-local correlations in effectively reduced spatial dimensions — •Jan M. Tomczak[1], Matthias Pickem[1], Benjamin Klebel[1], Anna Galler[2], Josef Kaufmann[1], Patrik Gunacker[1], Patrik Thunström[3], Thomas Schäfer[2], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Austria — [2]Centre de Physique Théorique, Ecole Polytechnique, Palaiseau, France — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Using the dynamical vertex approximation and its recent extension for electronic structure calculations, AbinitioDΓA[1], we explore the impact of spatial dimensions onto non-local correlations: (a) we compare magnitude and manifestations of non-local self-energies in ultra-thin films of transition-metal oxides to those in the bulk material. (b) we track the evolution of non-local correlations in the doped Hubbard model when continuously going from 3D to 2D. In particular we probe the limits of the "space-time separation" of electronic correlations evidenced in 3D[2]. Support by the ERC project AbinitioDGA (306447) and the Austrian Science Fund (FWF) projects I 2794-N35 and P 30213-N36 is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, JMT, K. Held, PRB 95, 115107 (2017), [2] T. Schäfer, A. Toschi, JMT, PRB 91, 121107R (2015)

MM 54.7 Thu 12:00 HL 001

Does the optical signature of oxidized polyethylene stem from saturated or unsaturated carbonyl defects? — •Guido Roma[1], Fabien Bruneval[1], and Layla Martin-Samos[2] — [1]DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif sur Yvette, France — [2]CNR-Demokritos, Trieste, Italy

Polyethylene (PE), one of the simplest and most used aliphatic polymers, is generally provided with a number of additives, in particular antioxidants, because of its tendency to get oxidized. Carbonyl defects, a product of the oxidation of PE, are occurring in various forms, in particular saturated ones, known as ketones, where a C=O double bond substitutes a CH_2 group, and various unsaturated ones, i.e., with further missing hydrogens. Many experimental investigations of the optical properties in the visible/UV range mainly attribute the photoluminescence of PE to one specific kind of unsaturated carbonyls, following analogies to the emission spectra of similar small molecules. However, the reason why saturated carbonyls should not be optically detected is not clear. We investigated the optical properties of PE with and without carbonyl defects using perturbative GW and the Bethe-Salpeter equation in order to take into account excitonic effects. We discuss the calculated excitonic states in comparison with experimental absorption/emission energies and the stability of both saturated and unsaturated carbonyl defects. We conclude that the unsaturated defects are indeed the best candidate for the luminescence of oxidized PE, and the reason is mainly due to oscillator strengths.

MM 54.8 Thu 12:15 HL 001

Bethe-Salpeter equation beyond the Tamm-Dancoff approximation at finite momentum transfer: Absorption and loss spectra including excitonic effects — •Benjamin Aurich, Caterina Cocchi, and Claudia Draxl — Humboldt-University, Berlin, Germany

The state-of-the-art ab-initio method for computing optical properties of semiconductors is based on the Bethe-Salpeter equation (BSE) which describes the excitations of the system in terms of interacting electron-hole (e-h) pairs. For absorption spectra, typically no momentum transfer from light to the e-h pairs is considered, and the coupling between excitations and de-excitations of e-h pairs is usually neglected by using the Tamm-Dancoff approximation (TDA). This approach yields excellent agreement with experiment for many materials, but may break down for confined systems [1]. The TDA is also known to fail to describe the electron energy loss spectra for materials as simple as silicon [2]. We report on the extensions of the open-source code `exciting` [3] allowing for BSE calculations beyond the TDA and at finite momentum transfer using an exact diagonalization scheme [4]. We demonstrate the differences between TDA and non-TDA spectra at vanishing and finite momentum transfer for periodic molecular systems.

[1] M. Grüning et al., Nano Lett **9**, 2820 (2009)
[2] V. Olevano and L. Reining, Phys. Rev. Lett. **86**, 5962 (2001)
[3] A. Gulans et al., J. Phys. Condens. Matter **26**, 363202 (2014)
[4] T. Sander et al., Phys. Rev. B **92**, 045209 (2015)

MM 54.9 Thu 12:30 HL 001

Calculations of charge and spin susceptibilities and quasiparticle energy shifts within the CASTEP plane-wave DFT code — •Vincent Sacksteder[1], Evgeny Plekhanov[2], Phil Hasnip[3], Matt Probert[3], Stewart Clark[4], Keith Refson[1], and Cedric Weber[2] — [1]Royal Holloway University of London, UK — [2]Kings College London, UK — [3]University of York, UK — [4]University of Durham, UK

CASTEP is a pseudopotential based plane wave code which scales to the largest supercomputers and offers a wide feature set. Within CASTEP we have implemented calculation of the charge and spin susceptibility tensor, which describes the response to a perturbing charge or spin. We present corrections to the Kohn-Sham energies obtained by using the susceptibility tensor to screen Hartree-Fock exchange. In the static limit this is the SEX part of the COHSEX approximation, and if instead the dynamic susceptibility is used one obtains the GW approximation.

Our memory and CPU consumption scales linearly with the plane wave basis size, allowing thorough exploration of convergence with basis size, not only of the susceptibility itself, but of the SEX and GW quasiparticle shifts. We emphasize that our calculations are heavily parallelized, in exactly the same way as a standard DFT ground state calculation.

This work will allow first principles calculations of magnon spectra, exchange couplings, ionization potentials, and KKR and DMI coefficients.

MM 55: Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales

Layered Structures

Time: Thursday 11:45–13:00 Location: H 0106

Topical Talk MM 55.1 Thu 11:45 H 0106

Deformation mechanism map of Cu/Nb nanoscale metallic multilayers as a function of temperature and layer thickness — •Jon Molina-Aldareguia[1], Jeromy Snel[1], Miguel Monclús[1], Nathan Mara[2], Irene Beyerlein[3], and Javier Llorca[1,4] — [1]IMDEA Materials Institute, c/Eric Kandel 2, 28906 Getafe (Madrid), Spain — [2]University of Minnesota, Minneapolis, MN 55455-0132 — [3]University of California, Santa Barbara, CA 93106-5070 — [4]Universidad Politécnica de Madrid, 28040 Madrid, Spain

The mechanical properties and deformation mechanisms of Cu/Nb nanoscale metallic multilayers (NMMs) manufactured by accumulative roll bonding (ARB) are studied at 25 °C and 400 °C. Cu/Nb NMMs with individual layer thicknesses between 7 and 63 nm were tested by in-situ micropillar compression inside a scanning electron microscope. Yield strength, strain-rate sensitivities and activation volumes were obtained from the pillar compression tests. The deformed micropillars were examined under scanning and transmission electron microscopy in order to examine the deformation mechanisms active for different layer thicknesses and temperatures. A remarkable transition in deformation mechanism occurred at 400 °C as the layer thickness decreased, from dislocation glide to dislocation climb at interfaces, which resulted in temperature-induced softening. A deformation mechanism map, in terms of layer thickness and temperature, is proposed from the results obtained in this investigation.

MM 55.2 Thu 12:15 H 0106

Cu/Fe Nanocomposites produced by Accumulative Roll Bonding — •Maher Ghanem, Benoit Merle, Heinz Werner Höppel, and Mathias Göken — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Werkstoffwissenschaften, Lehrstuhl Allgemeine Werkstoffeigenschaften (WW I); Martensstraße 5, 91058 Erlangen, Deutschland

The accumulative roll bonding (ARB) process has been applied to produce multilayered composites with layer thickness in the range of submicron to nanometer. Such multilayered composites show a strong increase in strength as the grain sizes are refined down to the submicron range. CuSn4/Fe multilayered nanocomposites with alternating layers of CuSn4 and Fe (99.88%) were roll bonded with 50% reduction and a post heat treatment at 400 °C following each pass. The rolling was repeated at least 10 times in order to achieve a layer thickness less than 1 um. Microstructure and texture of the nanocomposites were evaluated using backscatter electron (BSE) imaging and electron backscatter diffraction (EBSD), respectively. Mechanical properties were investigated through tensile and nanoindentation tests in order to observe the changes in the mechanical properties both locally and globally as the number of ARB passes increased. Furthermore, the layer interfaces of the nanocomposite at different rolling cycles were analyzed using Atom Probe Tomography (APT).

MM 55.3 Thu 12:30 H 0106

Severe Microscale Deformation of Pearlitic Steel During Tribology — •Steffen Brinckmann[1], Caroline Fink[1], Haleh

Taghinejadi[2], and Gerhard Dehm[1] — [1]Max-Planck-Insitut für Eisenforschung, Düsseldorf, Germany — [2]University of Cambridge, Cambridge, UK

Tribology at the macroscale is determined by the interaction of the microasperities that result in the wear of the counter surface and the subsurface microstructure evolution. State of the art macroscale tribology experiments investigate the convoluted interaction of a thousands of asperities and phases. We focus on a single asperity with micrometer size and study how the pearlite microstructure is deformed. The pearlite consists of hard cementite lamellae and soft ferrite matrix, each of which has a unique deformation mechanisms. We study both deformation mechanisms and discuss how the alignment of the microstructure influences the residual deformation, the wear of the microstructure. We determine the cementite deformation mechanisms and quantify the grain refinement in the ferrite matrix as a function of the wear loading. The development of a microstructure based understanding of the wear mechanisms would allow in the future to design wear resistant surfaces for engineering components.

MM 55.4 Thu 12:45 H 0106

Local Fatigue Testing by Dynamic Micropillar Compression of ARB Processed Bimodal Copper Sheets — •Sebastian Krauss, Mathias Göken, and Benoit Merle — Department of Materials Science and Engineering, Institute I, Friedrich-Alexander-University Erlangen-Nürnberg, Germany

Local fatigue experiments on microscale testing geometries offer the opportunity to isolate microstructure contributions to mechanical deformation behavior. In contrast to macroscopic fatigue testing, it is therefore possible to characterize the effect of individual features of interest independently. In this study Accumulative Roll Bonding (ARB) processed copper sheets with a bimodal microstructure were analyzed. Micropillars were milled by FIB structuring, producing testing geometries in individual layers of the material. Due to the bimodal microstructure, the different microsamples in each layer show varying grain sizes, which results in a change of the respective fatigue properties. Additionally micropillars at the interface were prepared to study interface contributions on the fatigue behavior. The investigations were executed by a novel approach that combines dynamic nanoindentation and micropillar compression. With this technique the high cycle fatigue range is easily accessible for microscale samples. Observation of the underlying deformation processes was performed by recording SEM micrographs of the deformed samples. Continuative investigations were realized by FIB milling of the deformed samples to create a cross-sectional view of the deformed microstructure.

MM 56: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data III

Time: Thursday 11:45–13:15 Location: H 0107

Topical Talk MM 56.1 Thu 11:45 H 0107

On the need for a digital representation of materials data along scientific and industrial processes — •Christoph Schweizer, Eva Augenstein, Heiner Oesterlin, and Adham Hashibon — Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

In the field mechanics of materials and material science and engineering in general, an ongoing challenge is to identify process-structure-property relationships. Due to the vast amount of manufacturing processes, mechanical properties as well as characterization and simulation methods on all scales, the resulting research data is extremely heterogeneous in nature. In this work, first steps are undertaken to set up an ontological knowledge base, which can be used to manage and analyze a large amount of material histories and provides the flexibility, which is needed to work on a scientific level. The ontology provides the structure and logical relations, which are needed to set up and later analyze the knowledge base. A small domain ontology is created based on the upper level Basic Formal Ontology (BFO) and the European Materials Modelling Ontology (EMMO), which are currently under development. The knowledge base which can be represented as a network graph is created and filled with research data from available public funded projects dealing with metallic high temperature materials, the underlying manufacturing processes, characterization methods, the microstructure and the mechanical properties. It is demonstrated, that the resulting network graph can be analyzed to identify process-structure-property relationships.

MM 56.2 Thu 12:15 H 0107

Probabilistic neural network design of an alloy for direct laser deposition — Bryce Conduit[1], Trevor Illston[2], Divya Vadgadde Duggappa[3], Scarlett Baker[1], Steve Harding[4], Howard Stone[5], and •Gareth Conduit[6] — [1]Rolls-Royce plc, PO Box 31, Derby, DE24 8BJ, United Kingdom — [2]Materials Solutions, Worcester, WR4 9GN, United Kingdom — [3]Rolls-Royce plc, Bangalore, India — [4]Rolls-Royce plc, PO Box 3, Bristol, BS34 7QE, United Kingdom — [5]Department of Materials Science & Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge, CB3 0FS, United Kingdom — [6]Cavendish Laboratory, University of Cambridge, J.J. Thomson Avenue, Cambridge, CB3 0HE, United Kingdom

A neural network tool was used to discover and characterize the new nickel-base alloy for direct laser deposition most likely to simultaneously satisfy targets of processibility, cost, density, phase stability, creep resistance, oxidation, and resistance to thermal stresses. Experimental testing confirms that the physical properties of the proposed alloy exceed those of other commercially available Ni-base alloys for combustor liner applications.

MM 56.3 Thu 12:30 H 0107

ab initio Phase Stability: From 0 K to Relevant Temperatures — •Moritz to Baben, Chandrahaasan Kattuputhur, and Klaus Hack — GTT-Technologies, Herzogenrath, Germany

Today, large repositories with ab initio calculation results for over a million compounds exist [1,2,3]. However, these contain only data from calculations at 0 K. Phase stability predictions on the other hand requires information on the Gibbs energy at elevated temperatures. Here, the current state of the art relies on CalPhaD (Calculation of Phase Diagrams) databases which have been derived mostly from experiments at high temperatures and contain only some thousands of compounds. In this contribution it will be discussed how ab initio phase stability data can be used at relevant temperatures -introducing the new aiMP database in FactSage [4]- and the veracity of the data is benchmarked. Systematic discrepancies between energy of formation from ab initio calculations and experiments e.g. for nitrates are discussed and the accuracy of high-throughput ab initio calculations for energy of formation of metallic systems is challenged. [1]: materialsproject.org [2]: aflowlib.org [3]: oqmd.org [4]: C.W. Bale et al., FactSage thermochemical software and databases, 2010-2016, CALPHAD 54 (2016) 35

MM 56.4 Thu 12:45 H 0107

Damage classification in DP steel using neural networks — •Tom Reclik[1], Carl F. Kusche[1], Ulrich Kerzel[2], and Sandra Korte-Kerzel[1] — [1]Institut für Metallkunde und Metallphysik, RWTH Aachen, Germany — [2]Lehrstuhl für Operations Research, RWTH Aachen, Germany

To this day, various methods are used in order to reveal the micromechanical mechanisms of damage in materials. Post-mortem analysis at different stages of stress reveals only snapshots of the material, while in-situ methods are spatially limited to observing the evolution of only a few damage events. A limiting factor in all those methods is the amount of work involved in controlling the microscope and the image analysis. In this work, we implement different structures and architectures of neural networks for the localization and classification of damages. As a sample material dual-phase steels are chosen, due to the different responses of the ductile ferrite matrix and the brittle martensite islands to stress, resulting in the formation of damage sites belonging to distinct classes at early stages of deformation. The developed algorithms can on the one hand be used in order to automate the statistical evaluation of post-mortem micrographs, while on the other hand enabling in-situ experiments to generate statistically relevant data. Due to the computational nature of this method, a high throughput of data is possible, enabling a more complete understanding of failure mechanisms in many materials.

MM 56.5 Thu 13:00 H 0107

A machine-learning approach for finding new hard-magnetic phases — Johannes J. Möller, Anna J. Lehner, Daniel F. Urban, and •Christian Elsässer — Fraunhofer IWM, Freiburg, Germany

Data-mining and machine-learning (ML) techniques play an increasingly important role in the discovery and development of new materials. In this contribution, we use kernel-based learning methods to predict optimal chemical compositions for new permanent magnets, which are key components in many green-energy technologies. The magnetic-property data used for training and testing the ML models were obtained by a combinatorial high-throughput screening (HTS) using density-functional theory calculations. For encoding the structural and chemical information of the HTS data in a machine-readable format, we use several existing and newly developed material descriptors and assess the predictive power of the ML models built with them. The accuracy of the ML models with an optimal choice of descriptor and model parameters enables the prediction of promising structure-composition combinations for substitutes of state-of-the-art magnetic materials like $Nd_2Fe_{14}B$ - with similar intrinsic hard-magnetic properties but no or less amounts of critical rare-earth elements.

MM 57: Methods in Computational Materials Modelling (methodological aspecst, numerics)

Advances in Electronic Structure Calculations

Time: Thursday 11:45–13:15 Location: TC 006

MM 57.1 Thu 11:45 TC 006

DFT+U for molecular orbitals — •Christoph Freysoldt and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40273 Düsseldorf

Density functional theory with Hubbard-U corrections (DFT+U) is a standard technique to perform electronic-structure calculations for correlated materials at relatively low computational cost. Standard implementations use projection onto localized atomic orbitals, e.g., the d-orbitals for transition metals or f-orbitals for lanthanides. However, for materials containing superoxide ions (O_2^-), the correlated sites are the molecular π^* orbitals (MOs) of the O_2 unit rather than the p-orbitals of single O atoms. I will present our implementation of DFT+U for molecular sites in the SPHInX code[1]. It is based on projectors for the atomic orbitals and a subsequent geometry-defined contraction to MO space. This setup allows to derive analytical forces with only minor additions to a standard DFT code, and therefore makes the approach available for standard simulation protocols such as geometry optimization, molecular dynamics, or cluster expansion.

[1] https://sxrepo.mpie.de

MM 57.2 Thu 12:00 TC 006

Assessment of the GLLB-SC potential for solid-state properties and attempts of improvement — •Fabien Tran, Sohaib Ehsan, and Peter Blaha — Vienna University of Technology, Vienna, Austria

Based on the work of Gritsenko *et al.* (GLLB) [Phys. Rev. A **51**, 1944 (1995)], the method of Kuisma *et al.* [Phys. Rev. B **82**, 115106 (2010)] to calculate the band gap in solids was shown to be much more accurate than the common methods of the local density approximation (LDA) and generalized gradient approximation (GGA). The main feature of the GLLB-SC potential (SC stands for solid and correlation) is to lead to a nonzero derivative discontinuity that can be conveniently calculated and then added to the Kohn-Sham band gap for a comparison with the experimental band gap. In this work, a thorough comparison of GLLB-SC with other methods, e.g., the modified Becke-Johnson (mBJ) potential [F. Tran and P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009)], for electronic, magnetic, and density-related properties is presented. It is shown that for the band gap, GLLB-SC does not perform as well as mBJ for systems with a small band gap and strongly correlated systems, but is on average of similar accuracy as hybrid functionals. The results on itinerant metals indicate that GLLB-SC overestimates significantly the magnetic moment (much more than mBJ does), but leads to excellent results for the electric field gradient, for which mBJ is in general not recommended. In the aim of improving the results with the idea of GLLB, variants of the GLLB-SC potential are also tested.

MM 57.3 Thu 12:15 TC 006

Basis Set Selection for Advanced Density Functionals and Quantum Chemistry via Compressed Sensing — •Niklas Menzel[1], Luca M. Ghiringhelli[1], Gitta Kutyniok[2], and Matthias Scheffler[1,3] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]Technische Universität, Berlin, DE — [3]UC Santa Barbara, USA

The selection of basis functions is an important issue in density functional theory and quantum chemistry. The main task is to minimize the computational costs while maintaining the accuracy. Commonly used basis sets are not sufficiently accurate to represent the eigenfunctions for advanced exchange-correlation treatments. This leads to basis set extensions, such as the correlation-consistent basis sets by Dunning [JCP 90, 1007 (1989)]. We propose a new method based on Compressed Sensing (CS), a recently developed signal processing technique. In CS, sparse signals are recovered using ℓ_0-norm or ℓ_1-norm regularization. Similarly, the key component of our approach is to find sparse real-space representations of self-consistently converged eigenfunctions (reference orbitals). We have developed a method for the selection of continuously parametrized basis functions (like Gaussian- or Slater-type basis functions). For the reference orbitals we used numeric atom-centered orbital basis functions. The reference orbitals are generated for the free atom and homonuclear dimers.

With our new approach we can robustly determine accurate basis sets for all atoms.

MM 57.4 Thu 12:30 TC 006

A Compressed Sensing Approach to Kohn-Sham Density Functional Theory — •Ingo Roth[1], Adrian Steffens[1,2], Christian Krumnow[1], Luca Ghiringhelli[2], Matthias Scheffler[2], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, FU Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

In density-functional theory calculations, the choice of basis sets plays a crucial role, determining the accuracy and computational cost of the simulation. The use of standardized basis sets and schemes which exploit the locality of the problem explicitly by assuming the Fock matrix to be banded often restrict the allowed states too much. Moreover, choosing an optimal basis set is a nontrivial task for many systems of interest, and large basis sets to compensate for this do not only increase computational time, but may also lead to numerical instability. In a more flexible approach, we propose a scheme that employs central notions of compressed sensing, a signal processing paradigm that has revolutionized the recovery of signals by efficiently identifying their underlying sparsity patterns, which makes it possible to massively undersample, yet fully recover a signal. In this spirit, we have developed an algorithm based on multi-task regularized Stiefel-manifold optimization that enforces sparsity basis function coefficients, thus identifying those basis functions that carry the most relevant information of the system.

MM 57.5 Thu 12:45 TC 006

Full Configuration Interaction Quantum Monte Carlo study of the spin polarized three dimensional uniform electron gas — •Michele Ruggeri[1], Pablo Lopez Rios[1,2], and Ali Alavi[1,3] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Theory of Condensed Matter Group, Cavendish Laboratory, J. J. Thomson Avenue, Cambridge CB3 0HE, UK — [3]University Chemical Laboratory, Lensfield Road, Cambridge, CB2 1EW, UK

The uniform electron gas is system consisting in electrons in a uniform positive background, which can be used to model electrons in a metal and to study electronic correlations. Quantum Monte Carlo methods, especially DMC with the fixed node approximation, proved to be a powerful tool to study the uniform electron gas, but due to the sign problem these QMC results are only variational. It is however possible to obtain essentially exact estimates of the energy of electronic systems using Full Configuration Interaction Quantum Monte Carlo (fciqmc).

We compare fixed node DMC and fciqmc energies for the three dimensional spin polarized uniform electron gas in the high density regime ($r_S = 0.5$ and 1.0) for different system sizes ($N = 7$ to 33 electrons), giving an estimate of the fixed node error. We show that it is possible to improve the fixed node energies using multi-determinant trial wave functions, obtaining results in agreement with fciqmc if a large enough number of determinants is used. Twist averaged boundary conditions are in use to reduce finite size effects.

MM 57.6 Thu 13:00 TC 006

Vibrational modes, phonons, and atomic relaxation in Diffusion Monte Carlo — Yu Yang Liu, •Bartholomew Andrews, and Gareth Conduit — University of Cambridge, Cambridge, United Kingdom

Diffusion Monte Carlo methods are a prime candidate for high-accuracy electronic structure calculations. Determining atomic forces and the matrix of force constants is important for relaxing structures, calculating vibrational properties, and performing molecular dynamics simulations. We develop a quantum mechanical expectation value to evaluate the matrix of force constants directly in Diffusion Monte Carlo. The proposed formalism captures the full Van der Waals force, and thus opens new applications to molecules and solids in condensed matter.

MM 58: Liquid and Amorphous Metals

Mechanical Properties and Fracture

Time: Thursday 11:45–13:15 Location: TC 010

MM 58.1 Thu 11:45 TC 010

Mechanical and thermal properties of PdNiP based bulk metallic glasses — •Niklas Nollmann, Vitalij Hieronymus-Schmidt, Jonas Lübke, Harald Rösner, and Gerhard Wilde — WWU Münster

At low temperatures and high stresses bulk metallic glasses (BMGs) deform inhomogeneously and suffer from a lack of ductility making BMGs unsuitable for many applications. This inhomogeneous deformation can be described in the frame work of a 'fictive temperature' concept with free volume as a key parameter. An increment or redistribution of the present free volume can be achieved in different ways: i) cryogenic rejuvenation or ii) micro-alloying [2]) may lead to enhanced ductility. In our study we investigated $Pd_{40}Ni_{40}P_{20}$ based bulk metallic glasses in detail: Adding small amounts of Iron or Cobalt to the $Pd_{40}Ni_{40}P_{20}$ metallic glass leads to huge changes in ductility. These effects on the mechanical properties by micro-alloying were monitored in bending and compression tests. We also calculated the critical fictive temperature for these different $Pd_{40}Ni_{40}P_{20}$ based BMGs to show the influence of annealing on the plasticity which is directly linked to the influence of free volume. Moreover, the effects of different degrees of cryogenic rejuvenation due to changes in cycle numbers and resting times at different temperatures of the same metallic glass were investigated with respect to the amount of free volume and the mechanical properties.

MM 58.2 Thu 12:00 TC 010

Novel atomic-level mechanism governing shear banding in metallic glasses — •Daniel Şopu[1,2], Alexander Stukowski[1], Mihai Stoica[3], and Sergio Scudino[4] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, Otto-Berndt-Straße 3, D-64287 Darmstadt, Germany — [2]ErichSchmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, A-8700 Leoben, Austria — [3]ErichSchmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, A-8700 Leoben, Austria — [4]IFW Dresden, Institut für Komplexe Materialien, Helmholtzstraße 20, D-01069 Dresden, Germany

The most conceivable scenario of shear band formation is the percolation of shear transformations zones (STZ) along a viable plane of maximum shear stress. However, despite the recent research progress, how an autocatalytic chain reaction of STZ takes place in a metallic glass remains a critical question that has not been resolved so far in the field. Here, by using molecular dynamics simulations, we provide a new atomic-level mechanism underlying the STZ percolation process. The mechanism is based on the autocatalytic generation of successive strong strain and rotation fields, leading to STZ percolation and, ultimately, to the formation of a shear band. The results build a bridge between the discrete nature of STZs at the atomic-level and the rather continuous character of shear bands at the microscale. We suggest that our results may have significant implications for understanding several aspects characterizing the process of shear banding in metallic glasses and other disordered materials.

MM 58.3 Thu 12:15 TC 010

Effect of elemental segregation on mechanical properties of metallic nanoglasses — •Sree Harsha Nandam[1], Ruth Schwaiger[2], Di Wang[1], Reda Chellali[1], Yulia Ivanisenko[1], and Horst Hahn[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Institute for Applied Materials, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Metallic nanoglasses represent a new class of non-crystalline solids with excess free volume at the interfaces. Because such interfaces can act as nucleating sites for shear during plastic deformation, nanoglasses have enhanced plasticity compared to a conventional metallic glass. In this paper, the effect of elemental segregation at the interfaces on mechanical properties of Pd-Si and Cu-Zr binary metallic nanoglasses synthesized by inert gas condensation is studied. The amorphous nature and nanosize of the particles is confirmed by X-ray diffraction and transmission electron microscopy. Elemental segregation in nanoscale is observed in Cu-Zr system while no such segregation is found in Pd-Si nanoglasses by atom probe tomography. Deformation behavior is studied by nanoindentation and micropillar tests. Homogeneous deformation is observed in Cu-Zr metallic nanoglasses whereas inhomogeneous deformation is observed in Pd-Si system. The effect of elemental segregation and the free volume in the metallic nanoglasses on their deformation behavior will be discussed in the present paper.

MM 58.4 Thu 12:30 TC 010

Local atomic order of a metallic glass made visible by scanning tunneling microscopy — •Yuansu Luo and Konrad Samwer — I. Physikalisches Institut, Georg-August-Universität, D-37077 Göttingen, Germany

STM investigations on quasi low-dimensional ultrathin films Zr65Cu27.5Al7.5 were carried out to explore atomic level structure of a locally ordered system. The highly oriented pyrolytic graphite (HOPG) was chosen as substrate. It creates imaging contrasts between long-range and short-range orders, so that the structural heterogeneousness arising from competition between the glass former and the epitaxy can be ascertained. For this purpose, the film is ultrathin in an order of magnitude corresponding to the scale of short range order (SRO). A chemical order predicted for this system was observed in atomic ordered regimes, accompanied with a charge density wave. This implies a chemical short range order (CSRO) in atomic disordered regimes, where polyhedral clusters are dominant with Cu(Al) in the center. An attempt was made for structural modeling based on high resolution STM images, giving icosahedral orders on surface and different Voronoi clusters in 3-D space.

MM 58.5 Thu 12:45 TC 010

Sensitivity for density change detection studied by scanning transmission electron microscopy image simulations — •Sven Hilke, Vitalij Hieronymus-Schmidt, Gerhard Wilde, and Martin Peterlechner — University of Münster, Institute of Materials Physics, Wilhelm-Klemm-Str. 10, 48149 Münster

Amorphous solids and metallic glasses have been in the focus of research for decades. Local diffraction experiments collecting many nano-beam diffraction patterns (NBDP) present a powerful tool to analyze amorphous structures. Recently the methods of Fluctuation Electron Microscopy (FEM) [1] as well as electron correlation microscopy (ECM) [2] were introduced in transmission electron microscopy (TEM). In the present study, the sensitivity of TEM methods to measure missing atoms in solids are analyzed. High angle annular dark field (HAADF) scanning TEM (STEM) is sensitive enough to detect signals of single atoms. It is the aim of this work to show that density changes can be quantitatively analyzed in crystalline silicon and amorphous copper zirconium (Cu64Zr36) by STEMcl [3], a STEM image simulation program.

[1] Voyles, P.M.; Muller, D.A.; Ultramicroscopy (2002), Volume 93, Issue 2, Pages 147-159.

[2] He, L.; Zhang, P.; Besser, M. F.; Kramer, M. J.; Voyles, P. M.; Microscopy and Microanalysis (2015), 21(04), 1026-1033.

[3]Radek, M.; Tenberge, J.-G.; Hilke, S.; Wilde, G.; Peterlechner, M.; Ultramicroscopy (2017), submitted.

MM 58.6 Thu 13:00 TC 010

In-situ observation of electron beam induced nanocrystallization of an ultra thin W foil — •Stefan Noisternig[1], Clemens Mangler[1], Christian Ebner[1], Christian Rentenberger[1], Hans-Peter Karnthaler[1], and Willem Tichelaar[2] — [1]University of Vienna, Physics of Nanostructured Materials, 1090 Vienna, Austria — [2]CEOS-GmbH, 69126 Heidelberg, Germany

An amorphous 2nm thin tungsten (W) foil supported by 3 nm carbon on a QUANTIFOIL grid is studied in an UltraSTEM 100 Nion dedicated scanning transmission electron microscope (STEM).

During the observation in the STEM the amorphous structure of W converts to a partially nanocrystalline one. The time to form the crystalline structure depends on the radiation dose of the electron beam. A Fast Fourier Transformation analysis of High Angle Annular Dark Field (HAADF) images reveals that WC0.82 and W3C0.375 nanocrystals formed during the radiation of the amorphous W foil under the electron beam.

During the continuous acquisitions a movement of bright dots is observed in HAADF images. We interpret this phenomenon as an observed surface diffusion of W atoms which is here activated well below the knock-on energy (above 1 MeV) for W. Mean square displacements of bright dots are measured at amorphous areas and at crystalline areas. The calculated diffusion parameters are then compared to literature values obtained with different methods.

We kindly acknowledge financial support by the Austrian Science Fund (FWF): [I1309].

MM 59: Invited talk Sprengel

Time: Thursday 15:00–15:30 Location: TC 006

Invited Talk MM 59.1 Thu 15:00 TC 006

Dilatometric Techniques for Atomic Scale Analysis of Defects and Processes in Solids — •Wolfgang Sprengel — Institute of Materials Physics, Graz University of Technology, Graz, Austria

Basic material parameters such as the relaxation volume of a lattice vacancy [1] or the grain boundary expansion [2] are related to volumetric changes of the solid. The same holds for processes governing changes in the microstructure such as recrystallization, the formation, transformation and dissolution of precipitates [3, 4] or, e.g., the glass transition in an amorphous alloy [5]. It will be demonstrated that all the above mentioned parameters and processes are experimentally accessible with high-precision on an absolute atomic scale by applying novel developments of specific dilatometric techniques. Financial support by the Austrian Science Fund (FWF) is appreciated (P21009-N20, P22645-N20, P25628-N20).

[1] J.A. Kotzurek, et al., Appl. Phys. Lett. **109** (2016) 021906.

[2] E.-M. Steyskal et al., Phys. Rev. Lett., **108** (2012) 055504.

[3] M. Luckabauer et al., Magnesium Technology, TMS Series Springer, Cham (2017), 669-674.

[4] M. Luckabauer et al., Rev. Sci. Instrum. **87** (2016) 075116.

[5] M. Luckabauer et al., Phys. Rev. B **89** (2014) 174113.

MM 60: Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales

Functional Mechanics

Time: Thursday 15:45–16:45 Location: H 0106

MM 60.1 Thu 15:45 H 0106

Interpenetrating-phase metal-polymer composites mimicking mechanical behavior of bone — •Ilya Okulov[1], Artem Okulov[1,2], Jörg Weissmüller[1,3], and Jürgen Markmann[1,3] — [1]Helmholtz-Zentrum Geesthacht,Geesthacht, Germany — [2]Institute of Metal Physics of the Ural Branch of the Russian Academy of Sciences, Ekaterinburg, Russia — [3]Hamburg University of Technology, Hamburg, Germany

The close match of stiffness between an orthopedic implant material and cortical bone is critically important to ensure fast healing of injured tissues. However, due to its complex composite microstructure, bone exhibits quite a unique mechanical response. In order to mimic bone's mechanical properties, we developed interpenetrating-phase metal-polymer composites. The composites were fabricated by impregnation of epoxy resin into biocompatible open porous metallic scaffolds. The metallic scaffolds were synthesized by liquid metal dealloying - a metallurgical process for synthesis of porous materials by means of selective corrosion in a liquid metal [1,2]. The yield strength of the composites exceeds that of cortical bone while its stiffness remains in a range of that for cortical bone. Moreover, the composites exhibit high strain rate sensitivity similar to bone. These findings suggest advantages for biomedical applications of the current composites, e.g. as materials for orthopedic implants.

[1] T. Wada, K. Yubuta, A. Inoue and H. Kato, Materials Letters 65, 1076-1078 (2011). [2] I.V. Okulov, J. Weissmüller and J. Markmann, Scientific Reports 7, 20 (2017).

MM 60.2 Thu 16:00 H 0106

Structural investigations of spider attachment hairs — •Silja Flenner[1], Imke Greving[1], Emanuel Larsson[1], Clemens Schaber[2], Christina Krywka[1], Stanislav N. Gorb[2], Martin Rosenthal[3], Manfred Burghammer[3], and Martin Müller[1] — [1]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany — [2]Institute of Zoology, Kiel University, Germany — [3]ESRF, Grenoble, France

The hairy attachment system of spiders enables these animals to walk upside-down on rough and smooth surfaces without the use of glue. These outstanding biological structures comprise of pads including hundreds to thousands of specially designed hairs that are made of composite materials consisting of proteins and reinforcing chitin fibres.

The goal of our study is to gain an in-depth understanding of the structure-function mechanism of the attachment and detachment processes of single hairs to a surface. X-ray Tomographic Microscopy and Scanning X-ray nanobeam diffraction are ideal tools to reveal the inner structure of the spider hairs and allow to determine the gradient of the mechanical properties which is essential for the attachment process.

With both techniques we found that the shaft of the attachment hair is hollow. Wide Angle X-ray scattering of the shaft revealed, that in contrast to the tip region, oriented α-chitin was present, indicating the presence of chitin crystals in the shaft region. These results suggest that the tube-shaped hollow part of the hair in combination with the presence of chitin crystals along the tube is needed to withstand the strong forces which occur during attachment/detachment process.

MM 60.3 Thu 16:15 H 0106

Influence of flexoelectricity on nanomechanical properties of ferroelectrics — •Gustau Catalan[1], Kumara Cordero-Edwards[2], Fabian Vasquez-Sanchez[2], Amir Abdollahi[3], and Neus Domingo[2] — [1]ICREA-Institucio Catalana de Recerca i Estudis Avançats, Barcelona, Catalonia — [2]ICN2-Institut Catala de Nanociencia i Nanotecnologia, Barcelona, Catalonia — [3]Universitat Politecnica de Catalunya (UPC), Barcelona, Catalonia

Flexoelectricty is a coupling between strain gradients (inhomogeneous deformations) and electric polarization. It is allowed by symmetry in all materials, but it is strongest in those with high dielectric constants, such as ferroelectrics. Because of flexoelectricity, the electrostatic energy cost of very inhomogeneous deformations, such as those that can be induced at the nanoscale due to e.g. nanoindentation or cracking, can be enormous. Flexoelectricity thus has a strong impact on the mechanical response of materials (and particularly ferroelectrics) at the nanoscale.

Here I will present results that have profound implications for our understanding of solid state mechanics and fracture physics. Specifically, due to flexoelectricity the indentation response and also the fracture propagation in ferroelectrics can be asymmetric: cracks travelling parallel to the ferroelectric polarization become much longer than tose travelling against it. This discovery challenges the general notion that mechanical properties of matter are symmetric with respect to space inversion. Some implications and possible applications of this discovery will be discussed.

MM 61: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data IV

Time: Thursday 15:45–17:15 Location: H 0107

Topical Talk MM 61.1 Thu 15:45 H 0107

Big Data of Materials Science: Interpretability of Machine Learning — Luca M. Ghiringhelli[1], •Jan Vybiral[2], Sergey V. Levchenko[1], Claudia Draxl[3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem, Germany — [2]Czech Technical University, Dept. of Mathematics FNSPE, Prague, Czech Republic — [3]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany

An important part of every machine learning approach to statistical learning is the representation of the input data. This representation usually assumes an implicit (and largely unchallenged) choice of right descriptors. To allow for human interpretability of learned structures in the data, their choice is crucial. Trustful prediction of new promising materials, identification of anomalies, and scientific advancement are doubtful if the connection between the descriptor and the actuating mechanisms is unclear.

We use the techniques of compressed sensing and feature selection to analyze this issue, define requirements for useful descriptors, and propose a practical algorithm for their identification. It selects suitable descriptors from a large set of physically meaningful quantities, which is created in a human-guided process.

For a classical example, the energy difference of zincblende/wurtzite and rocksalt semiconductors, we demonstrate how a meaningful descriptor can be found systematically.

MM 61.2 Thu 16:15 H 0107

Cluster expansions with CELL: a novel python package with a focus on complex alloys — •Santiago Rigamonti[1], Maria Troppenz[1], Martin Kuban[1], Axel Huebner[1], Christopher Sutton[2], Luca Ghiringhelli[2], Matthias Scheffler[2], and Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber Institut

The cluster expansion (CE) technique allows for obtaining compact models of configuration-dependent properties in alloys with *ab initio* accuracy, by expanding these properties in terms of clusters (sets of crystal sites). In this work, we present the code CELL [1] which is an object-oriented, modular and user-friendly python package for building accurate CE models. Its focus is on complex surfaces and bulk alloys possessing large parent cells (>30 atoms), for which a full structure enumeration is impossible. We note, though, that CELL is not limited to complex alloys. The creation of training data-sets is incorporated into a user-friendly setup of parent- and supercell objects. For selecting the optimal set of clusters, compressed-sensing schemes, such as LASSO and the split Bregman method, and various cross-validation strategies are available. In addition, finite-temperature properties and the characterization of phase transitions are achieved by applying the Wang-Landau method and diffusive nested sampling. We will demonstrate CELL's capabilities by selected examples.

[1] S. Rigamonti, M. Troppenz, M. Kuban, A. Huebner, C. Sutton, L. Ghiringhelli, M. Stournara, M. Scheffler, and C. Draxl. *CELL: python package for cluster expansions with large parent cells.* In preparation.

MM 61.3 Thu 16:30 H 0107

***Ab-initio* study of the clathrate $Ba_8Ni_xGe_{46-x-y}\Box_y$: Stability, structure, and electronic properties** — •Martin Kuban, Santiago Rigamonti, Maria Troppenz, and Claudia Draxl — Humboldt-Universität zu Berlin

The type-I clathrate $Ba_8Ni_xGe_{46-x-y}\Box_y$ is a prototypical example of the phonon-glass–electron-crystal concept and thus promising for thermoelectric applications. Recent experimental studies [1] show that either *n*- or *p*-type conductivity can be achieved by tuning its composition around the charge-compensation ($x+y=4$). This is important in view of building enhanced *n*-*p* thermoelectric junctions with the same base material. Upon the addition of Ni, the stable phases tend to form less vacancies ($\Box$), while the lattice constants stay almost unchanged. In this work we perform an *ab-initio* cluster-expansion [2] study in the composition range $0 \leq x \leq 6$ and $0 \leq y \leq 4$. This allows us to investigate the configurational ground-states (GS) at zero temperature. For these GS-structures, we observed the transition of a minimum in the electronic density of states (DOS) from below the Fermi level for $x+y<4$, to above the Fermi level for $x+y>4$, thus confirming the experimentally observed change from *n*- to *p*-type conductivity. From the calculation of the phase diagram, we find good agreement with experiment regarding the lattice constant and the formation of vacancies for increasing Ni content.

[1] U. Aydemir *et al.*; Dalton Trans **44**, 7524 (2015).

[2] S. Rigamonti *et al.*, in preparation.

MM 61.4 Thu 16:45 H 0107

SISSO: a Compressed-Sensing Method for Systematically Identifying Efficient Physical Models of Materials Properties — •Runhai Ouyang[1], Stefano Curtarolo[2], Emre Ahmetcik[1], Matthias Scheffler[1], and Luca M. Ghiringhelli[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem, Germany — [2]Materials Science, Duke University, Durham, NC, USA

We present a systematic data-driven approach for discovering physically interpretable descriptors and predictive models, within the framework of compressed sensing. SISSO (sure independence screening and sparsifying operator) tackles immense and correlated features spaces, and converges to the optimal solution from a combination of features relevant to the materials' property of interest. The methodology is benchmarked with the quantitative prediction of the ground-state enthalpies of octet binary materials (using *ab initio* data) and applied to the showcase example of predicting the metal-insulator classification (with experimental data). Accurate predictive models are found in both cases. For the metal-insulator classification model, the interpretability and predictive capability are tested beyond the training data: It perfectly rediscovers the available pressure-induced insulator to metal transitions and it allows for the prediction of yet unknown transition candidates, ripe for experimental validation.

MM 61.5 Thu 17:00 H 0107

From autonomous subspace selection of material properties to physically meaningful predictions — •Benjamin Regler, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

In data-driven materials science, the discovery of functional relationships is an inverse problem on finding subsets of materials properties (features) which relate to physical observables.

The inverse problem can be solved by statistical-learning algorithms that require manual adjustment and are thus based on ongoing experience and the knowledge being built. This makes ensuring the physical interpretability of the generated data-based models a demanding task.

Therefore, we highlight an autonomous systematic feature-subspace construction and selection method using information-theoretic concepts. We use a generalization of the Shannon entropy to select physically meaningful subsets (sharing the same notion of uncertainty as the Gibbs entropy in statistical thermodynamics) and use compressed sensing to find the best approximate models without prior knowledge.

Then, we apply the framework and highlight key problems such as stability predictions of zinc-blende vs. rock-salt octet binary semiconductors and band-gap predictions of topological insulators. Finally, we discuss the physical interpretation of the generated models and identify the strongest correlated materials properties with the actuating mechanism.

MM 62: Methods in Computational Materials Modelling (methodological aspecst, numerics)

QM-based interaction models

Time: Thursday 15:45–17:15 Location: TC 006

MM 62.1 Thu 15:45 TC 006

Uncertainty Quantification for Classical Effective Potentials — •Sarah Longbottom and Peter Brommer — University of Warwick, Coventry, UK

Effective potentials are an essential ingredient of classical molecular dynamics simulations. Little is understood of the errors incurred in representing the complex energy landscape of an atomic configuration by an effective potential containing considerably fewer parameters. The probabilistic sloppy model method [1] has been implemented in the potfit force matching code [2]. This introduces uncertainty quantification into the interatomic potential generation process. Uncertainties in the effective potential are propagated through MD to obtain uncertainties in quantities of interest, which are a measure of the confidence in the model predictions.

We demonstrate the technique using three potentials for nickel: two simple pair potentials, Lennard-Jones and Morse, and a local density dependant EAM potential. A sloppy model fit to DFT reference data is constructed for each potential to calculate the uncertainties in lattice constants, elastic constants and thermal expansion. These can be used to show the unsuitability of pair potentials for nickel. In contrast, with EAM we observe a decreased uncertainty in the model predictions. This shows that our method can capture the effects of the error incurred in the potential generation process without resorting to comparison with experiment or DFT.

[1] S. L. Frederiksen, et al., Phys. Rev. Lett., 93 (16), 2004.

[2] P. Brommer, et al., Modell. Simul. Mater. Sci. Eng., 23 (7), 2015.

MM 62.2 Thu 16:00 TC 006

Combination of machine learning and high-throughput DFT calculations for the prediction of thermodynamic stability — •Jonathan Schmidt[1], Jingming Shi[4], Pedro Borlido[2], Liming Chen[3], Silvana Botti[2], and Miguel Marques[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena and European Theoretical Spectroscopy Facility, Germany — [3]Département MI, Laboratoire ICTT, Ecole Centrale de Lyon, France — [4]Institut Lumière Matière, Université de Lyon, France

We perform a large-scale benchmark of machine learning methods for the prediction of the thermodynamical stability of solids. We start by constructing a data set that comprises density functional theory calculations of around 250,000 cubic perovskite systems. Incidentally, around 500 of these are thermodynamically stable but are not present in crystal structure databases. This data set is then used to train and test a series of machine learning algorithms to predict the distance to the convex hull of stability. In particular, we study the performance of ridge regression, random forests, extremely randomized trees (including adaptive boosting), and neural networks. We find that extremely randomized trees give the best results and use this method in combination with DFT to explore ternary compounds with the AB_2C_2 composition. By using machine learning we reduce the overall calculation cost by around 75% and find that there may be 10 times more stable compounds in these phases than previously known.

MM 62.3 Thu 16:15 TC 006

Improving the training of force-fields based on neural networks — •Mário Marques and Miguel Marques — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

The evaluation of potential energy surfaces lies at the heart of many problems in materials science. Density functional theory is often used for this task, but it quickly becomes impractical for systems with hundreds or thousands of atoms.

In this contribution we describe a methodology, based on Behler-Parrinelo approach for artificial neural networks, to solve this problem. We obtain training and test sets from a fully unbiased approach based on global structural prediction techniques.

We extend the back propagation method to consider the error in the forces and stress and we discuss the suitability of a few activation functions. Finally, we develop force fields for Si and Ge, and present some applications to the calculation of point defects and phase diagrams.

MM 62.4 Thu 16:30 TC 006

DFTB for lazy theorists: automatic transferable parametrization with particle swarm optimization — •Chiara Panosetti[1], Reinhard J. Maurer[2], and Karsten Reuter[1] — [1]Technische Universität München — [2]University of Warwick

In terms of numerical efficiency and accuracy, tight-binding is intermediate between first-principles and empirical methods. Among the many flavors used in materials modelling, Self-Consistent Charge Density Functional Tight Binding (SCC-DFTB)[1] is particularly geared to cover a broad range of bonding situations while retaining access to electronic properties. This renders it appealing for use, *e.g.*, as a lower-level pre-screening technique in hierarchical approaches. However, its pairwise parametrization requires a procedure which constitutes an N^2 effort within the periodic table and is not only tedious, but also rather arbitrary and difficult to document and reproduce.

Building on the work of Chou *et al.*,[2] we here propose, extend and critically discuss a new parametrization strategy where all the quantities determining the SCC-DFTB interaction are optimized with a particle swarm algorithm to minimize a generalized observable-based cost function. Careful use of such a powerful tool should facilitate reproducibility and provide a straightforward recipe to fine tune the balance between transferability and accuracy.

[1] M. Elstner, Theor. Chem. Acc. 116, 316 (2006).

[2] C. P. Chou *et al.*, J. Chem. Theory Comput. 12, 53 (2016).

MM 62.5 Thu 16:45 TC 006

Systematic development of analytic bond-order potentials for W, Re and Os — •Aparna P. A. Subramanyam, Jan Jenke, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr University Bochum, Bochum, Germany

The limited applicability of accurate quantum mechanical simulations to extended time and length scales calls for approximate interatomic interaction models in order to perform large-scale atomistic simulations. In this work we show the coarse graining of the electronic structure to tight binding and analytic bond-order potentials (BOPs).

We present the systematic parameterization of BOPs for the transition metals W, Re and Os. In particular we demonstrate the systematic parameterisation from downfolding the DFT eigenspectrum to a TB basis that is then solved on the BOP level. The accuracy of the BOPs is validated with respect to the structural stability, to the formation energies of point defects and the formation energies of planar defects like stacking faults and twin boundaries. We furthermore validate the transferability of the BOPs with a comprehensive set of different atomic environments.

MM 62.6 Thu 17:00 TC 006

Charge transport in organic semiconductors: Towards an ACKS2-based polarization in force fields. — •Patrick Gütlein[1], Harald Oberhofer[1], Karsten Reuter[1], and Jochen Blumberger[2] — [1]Technische Universität München, Germany — [2]University College London, UK

Charge carrier transport, an integral part of diverse reactions and devices, is generally subject to the non-negligible response of the surrounding environment. Especially in organic semiconductors the accurate theoretical treatment of dynamic electronic rearrangements in dense media is a complex task. The high anisotropy and comparatively low dielectric screening require system sizes that challenge even efficient first-principles approaches like density-functional theory (DFT). In this situation the recently proposed atom-condensed Kohn-Sham density functional theory approximated to second order (ACKS2) approach[1] could represent a computationally undemanding, yet accurate extension to conventional force field methods. In this approach, the linear response of the electron density and Kohn-Sham potential are captured by an atom-centered series expansion up to second order.

For a range of molecular model systems we systematically compute the ACKS2 parameters with DFT and discuss linear response properties obtained by a Gaussian type orbital basis set representation. This marks an important first step in making ACKS2 applicable as a polarizable force field. [1] T. Verstraelen et al., J. Chem. Phys. 138, 7 (2013); ibid 141, 19 (2014).

MM 63: Transport (Diffusion, conductivity, heat)

Transport I

Time: Thursday 15:45–17:00 Location: TC 010

MM 63.1 Thu 15:45 TC 010

Atomic transport in Si/Al interfaces — •Kevin-Patrick Treder, Efi Hadjixenophontos, Sebastian Eich, and Guido Schmitz — Institut für Materialwissenschaft, Lehrstuhl für Materialphysik, Stuttgart, Deutschland

The crystallization temperature for semiconductors such as Si and Ge can be drastically lowered when in contact with a metal. Metal induced crystallization (MIC) or the layer-exchange processes were tried to be understood by different thermodynamic or kinetic approaches in the recent years. The direct comparison of the reactions of amorphous or crystalline Si with Al inside a single sample may provide further insight into the mechanisms. In a new experimental approach, we produce artificial nano-sized triple junctions at which the Al/c-Si, the Al/a-Si and the c-Si/a-Si interfaces merge. Samples are prepared via RF-Sputtering, followed by ex-situ annealing in Ar-atmosphere and subsequent post processing via FIB-lift-outs. Full cross-section characterization and analysis was provided by HRTEM and local EDX-analysis. Clear evidence is provided for ˜ 2 nm temperature-independent amorphous interlayer formed at the c-Si/Al interface. The diffusion phenomena across and along the related interfaces are demonstrated and measured in direct comparison.

MM 63.2 Thu 16:00 TC 010

Magnetotransport and Quantum Oscillation Phenomena in Dirac Semimetal Na_3Bi — •Mohammad Pakdaman, Alimamy Bangura, Claus Mühle, and Hidenori Takagi — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Three dimensional Dirac semimetals are a three dimension analogue of Graphene where the conduction band and valance band touch at discrete points in reciprocal space with linear dispersion. In this class of materials Na_3Bi has a uniquely simple band structure compared to other example discovered so far. A consequence of this unique band structure is the realization of unusual electronic properties that are predicted to be manifest in the transport properties. In order to probe the exotic electronic properties of this material, the magnetotransport measurement have been done on single crystal of Na_3Bi. The results were compared to the *ab initio* calculations and predictions of the physical properties for this recently predicted state of matter, and these experiments give further evidence for the realisation of this exotic state of matter.

MM 63.3 Thu 16:15 TC 010

Plasma charge carrier attachment induced transport in electrolytes — •Jan Wiemer and Karl-Michael Weitzel — Philipps Universität Marburg, Chemistry Department

A new approach for measuring the electrical conductivity properties of solid electrolytes over a wide range of total pressures applicable for any thickness of the sample is presented. The approach is based on generating a plasma by femtosecond laser ionization of e.g. air. Charge carriers of different polarity are separated in a static electric field. Charge carriers of the selected polarity are attached to the front side of a sample which is in contact with a single metal electrode inducing a well defined surface potential. This induces charge carrier transport in the sample which is detected at the metal electrode. We present different examples of glasses demonstrating that the approach allows measuring conductivities and activation energies in full agreement with reference measurements. The advantages are that the sample is i.) only in contact with a single electrode, ii.) the pressure range is from fine vacuum up to high pressures, iii.) the chemical identity of the charge carrier can be chosen by choosing the plasma medium and iv.) the polarity can be easily switched by switching static fields.

MM 63.4 Thu 16:30 TC 010

On bottleneck areas for ionic transport in NASICON materials — •Kaustubh Bhat, Stefan Blügel, and Hans Lustfeld — Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

Among ionic conductors, NASICON [1] materials are receiving attention for large-scale energy storage applications. We first use the Nudged Elastic Band (NEB) method for calculating the energy barrier for sodium ion transport in $Na_6Sc_4\,(PO_4)_6$ (NSP). Experimental results point towards the existence of certain bottlenecks which reportedly determine the ionic conductivity of a given material [2]. We have developed a novel method using second order force constants to model the influence of these bottlenecks – interionic distances and in particular areas – to the migration barriers of sodium ions. Using our model we test the bottleneck hypothesis [3]. Furthermore, we use the information gained from the model to identify ionic substitutions to NSP that reduce the energy barrier.

[1] H.Y.P. Hong, Mat. Res. Bull. **11**, 173 (1976).
[2] M. Guin and F. Tietz, J. Power Sources **273**, 1056 (2015).
[3] M. Guin, PhD Thesis, ISBN 978-3-95806-229-0 (2017)

MM 63.5 Thu 16:45 TC 010

Improvements in thermoelectric material performance — •Genadi Naydenov, Philip Hasnip, Vlado Lazarov, and Matthew Probert — Department of Physics, University of York, York, YO10 5DD, UK

Thermoelectric technology has the potential to convert waste heat into useful electricity, dramatically improving energy efficiency. Optimising thermoelectric materials focuses on increasing their power factor and decreasing their thermal conductivity. Recent experimental and theoretical studies have shown that half-Heusler systems, e.g. NbFeSb, can reach a high power factor ($\sim$10 mWm^{-1}K^{-1}) even at room temperature, and that the thermal transport is dominated by phonons. The phonon thermal conductivity may be lowered by substitution with heavier elements, which introduce point scatterers. Recently the half-Heusler TaFeSb has also been predicted to be an excellent thermoelectric material, but has yet to be investigated thoroughly. We will present the results of our first-principles materials modelling investigation into the thermoelectric properties of pure TaFeSb, NbFeSb and $Ta_xNb_{1-x}FeSb$, and show how the power factor and ZT may be optimised by judicious choices of x and doping concentration. We show that p-type $Ta_xNb_{1-x}FeSb$ is an excellent candidate thermoelectric material.

MM 64: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France Paul R. Kent, Oak Ridge National Laboratory, USA Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 15:00–17:45 Location: HL 001

Invited Talk MM 64.1 Thu 15:00 HL 001

Recent developments in FCIQMC: real-time propagation and improved convergence with walker number — •Ali Alavi — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Full Configuration Interaction QMC method samples Slater determinants using an imaginary-time propagation of walkers, and can yield essentially exact ground- and excited states energies and wavefunctions for Fermionic systems. Recently we have extended this methodology to real-time propagation, enabling the calculation of spectral functions along the real-frequency axis. This method will be described in the talk, together with representative examples from molecular and lattice models. We will also describe a second development in the FCIQMC methodology which substantially improves the rate of convergence of the ground-state technique with respect to the number of walkers. With the new method, we can compute essentially the exact ground state energy of the benzene molecule, correlating 30 electrons (the entire valence) in the full set of 108 orbitals of a VDZ basis. Perspectives of the new methods will be discussed.

MM 64.2 Thu 15:30 HL 001

Quasi-Continuous LDA+DMFT calculations for SrVO3. — •Evan Sheridan, Christopher Rhodes, Evgeny Plekhanov, and Cedric Weber — King's College London, Theory and Simulation of Condensed Matter (TSCM), The Strand, London, United Kingdom.

The Dynamical Mean Field Theory (DMFT) is an extremely powerful tool in the treatment of strongly correlated electron systems and many DMFT calculations suffer from a computational bottleneck when it attempts to solve the Anderson Impurity Model (AIM).

Common among the early Anderson Impurity solvers was the Auxiliary Field Quantum Monte Carlo (AF-QMC) approach which relies on a discretisation of the imaginary time grid. AF-QMC solvers suffer from the notorious Suzuki-Trotter error,as a result of this , that has largely been ignored in recent years with the advent of Continuous Time-QMC (CT-QMC) solvers.

Here, we present a systematic study of how this issue can be overcome for realistic material properties using LDA+DMFT. We find that our quasi-continuous time method compares well to the state-of-the-art CT-QMC calculations for SrVO3, with the added advantage of linear scaling in temperature. The theoretical framework proposed is quite general and can be extended to cluster DMFT calculations.

MM 64.3 Thu 15:45 HL 001

High temperature superconducting oxychlorides: a light element model for cuprates — •Matteo d'Astuto[1,2], Blair Lebert[2,3], Ikuya Yamada[4], and Masaki Azuma[5] — [1]Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — [2]IMPMC, UMR7590 UPMC-Sorbonne Universités - CNRS, Paris, France — [3]Synchrotron SOLEIL, Gif-sur-Yvette, France — [4]Nanoscience and Nanotechnology Research Center (N2RC), Osaka, Japan — [5]Materials and Structures Laboratory, TITech, Yokohama, Japan

The copper oxychloride cuprate $Ca_2CuO_2Cl_2$ (CCOC) system, with vacancy or Na doping on the Ca site, is unique among the high temperature superconducting cuprates (HTSCs) since it: lacks high Z atoms; has a simple I4/mmm 1-layer structure, typical of 214 (LSCO) cuprates, but which is stable at all doping and temperatures; and has a strong 2D character due to the replacement of apical oxygen with chlorine. It also shows a remarkable phase digram, with a superconducting T_C growing to the optimal doping without any minimum around 1/8 doping, despite the observation of charge modulations by near-field spectro-microscopy. Due to the reduced number of electrons, advanced calculations that incorporate correlation effects, such as quantum Monte Carlo are easier, but relatively little is known about CCOC (for a cuprate) from an experimental point of view. We are now filling this gap by a comprehensive experimental study covering the whole phase diagram, in particular of the (para)magnon and phonon dispersion..

MM 64.4 Thu 16:00 HL 001

Antiferromagnetic correlations in the metallic strongly correlated transition metal oxide $LaNiO_3$ — •Hanjie Guo[1], Zhiwei Li[1], Li Zhao[1], Zhiwei Hu[1], Chunfu Chang[1], Changyang Kuo[1], Wolfgang Schmidt[2], Andrea Piovano[2], Tunwen Pi[3], Oleg Sobolev[4], Daniel Khomskii[1], Liu Hao Tjeng[1], and Alexander Komarek[1] — [1]MPI CPfS, Dresden, Germany — [2]ILL, Grenoble, France — [3]NSRRC, Taiwan — [4]FRMII, Munich, Germany

The material class of rare earth nickelates with high Ni^{3+} oxidation state is generating continued interest due to the occurrence of a metal-insulator transition with charge order and the appearance of non-collinear magnetic phases within this insulating regime. The recent theoretical prediction for superconductivity in $LaNiO_3$ thin films has also triggered intensive research efforts. $LaNiO_3$ seems to be the only rare earth nickelate that stays metallic and paramagnetic down to lowest temperatures. So far, centimetre-sized impurity-free single crystal growth has not been reported for the rare earth nickelates material class since elevated oxygen pressures are required for their synthesis. Here, we report on the successful growth of centimetre-sized $LaNiO_3$ single crystals by the floating zone technique at oxygen pressures of up to 150 bar. Our crystals are essentially free from Ni^{2+} impurities and exhibit metallic properties together with an unexpected but clear antiferromagnetic transition.

MM 64.5 Thu 16:15 HL 001

First-principles quantum Monte Carlo study of correlated materials — •Huihuo Zheng — Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont, USA

Strongly correlated electronic systems have become an important subject of condensed matter physics, because of many fascinating phenomena arising in these systems such as metal-insulator transition, high temperature superconductivity, etc. Accurate characterization of the electron-electron correlations in these systems from first principles is essential for us to understand how these phenomena emerge from microscopic interactions. I will present our efforts in modeling correlated materials using the first-principles quantum Monte Carlo (QMC) method by showing two representative *ab intio* studies (vanadium dioxide and graphene) and a density-matrix downfolding theory for constructing low energy effective models from *ab initio* simulations. Using QMC, we correctly characterized the electronic structure of vanadium dioxide and unveiled the electronic origin of the metal-insulator transition which has been a mystery for decades. For graphene, we computed the electron screening from σ bonding electrons and illustrated how the emergent physics from underlying Coulomb interactions results in the observed weakly correlated semimetal. On the other hand, the downfolding approach we developed provides a way to quantitatively identify important microscopic interactions relevant to the macroscopic physics.

MM 64.6 Thu 16:30 HL 001

Reduced Density Matrix Theory for Coupled Fermion-Boson Systems — •Florian Buchholz[1], Iris Theophilou[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]MPSD, Hamburg, Germany — [2]CCQ, The Flatiron Institute, New York, United Sates — [3]Nano-bio Spectroscopy Group, San Sebastián, Spain

Reduced density matrix (RDM) theory proved to be successful in describing a wide range of many-body problems that are not easily accessible by the more common many-body perturbation theories or density functional theory. Especially as RDM theories are non-perturbative, they are advantageous in strong coupling scenarios.

However, RDM theory was to our knowledge never applied to systems with more than one active particle type. The focus of this talk is to analyze the possibilities and problems of an extension to coupled fermion-boson theories. Comparing a typical bilinear interaction term of the form $c_i^+ c_j (a_k^+ + a_k)$, where c^+/c and a^+/a indicate fermion and boson creation/annihilation operators, respectively and the fermionic 2-body interaction term $c_i^+ c_j^+ c_k c_l$, the former should have a considerably reduced definition space, which we hope to be exploitable. On the other hand, the bilinear interaction has a very different structure than the 2-body interaction and it is not clear at all, how to define a RDM that carries all information to compute experimental observables of a coupled fermion-boson system.

Specifically, I will illustrate some of the peculiarities of the fermion-boson interaction for simple model systems and present some ideas to deal with those.

MM 64.7 Thu 16:45 HL 001

Critical temperatures as function of magnetic anisotropy in two-dimensional systems from first-principles calculations — •Daniele Torelli — Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in monolayer CrI_3 highlights the importance of a microscopic understanding of anisotropy in ground state magnetic systems. Single-ion anisotropy accounts mainly for spin-orbit coupling interaction and, in particular for two-dimensional (2D) materials, it's crucial to escape the Mermin-Wagner theorem. Here we investigate the variation of critical temperatures as functions of anisotropy in Heisenberg model systems using Metropolis Monte Carlo simulations. Results for square, hexagonal and honeycomb lattices are compared with equivalent simulations in the Ising model, which is confirmed to represent the limit with infinite anisotropy. Based on a new developed computational 2D materials database, we predict a vast number of 2D structures with high critical temperatures. As testing system, relevant Heisenberg exchange couplings and magnetic anisotropy energy in CrI_3 monolayer are extracted from first principle calculations and energy mapping analysis, yielding to an estimation of Curie temperature in good agreement with experimental results.

MM 64.8 Thu 17:00 HL 001

Oxygen vacancy-induced absorption of visible light in SrNbO3 — •Marcello Turtulici, Steffen Backes, and Silke Biermann — Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau, France

SrNbO3 has recently attracted attention as a bright red photocatalyst. Several, mutually contradicting, models have been proposed in the literature in order to explain the strong absorption in the visible spectrum, and no consensus even on the basic nature of the mechanism has been reached. In this work we investigate the optical properties of this material by means of state-of-the-art Density Functional Theory and many-body perturbation theory techniques. We evidence a high sensitivity of the optical properties on deviations from the ideal crystal structure. In particular, the optical properties should strongly depend on the presence of oxygen vacancies, which give rise to additional absorption channels in the visible frequency range. Most notably, the experimentally observed red color is likely due to transitions between orbitals of dominant Nb-eg character, which are enhanced by the strong hybridization of the quite extended 4d-states of Nb with oxygen p-states.

MM 64.9 Thu 17:15 HL 001

Transient charge and energy flow in the wide-band limit — Fabio Covito, •Florian Eich, Riku Tuovinen, Michael Sentef, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Thanks to recent advances in ultra-fast pump-probe spectroscopies and nano-thermometry it is possible to study charge and energy flow at atomic time and length scales. In order to analyze the transient dynamics of nanoscale devices theoretically, the wide-band limit is a commonly used approximation. Here we investigate the applicability of the wide-band limit to the study of charge and heat transport through nanojunctions exposed to voltage biases and temperature gradients. We find that while this approximation faithfully describes the long-time steady-state charge and heat transport, it fails to characterize the short-time transient behavior of the junction. In particular, we find that the charge current flowing through the device shows a discontinuity when a temperature gradient is applied, while the energy flow is discontinuous when a voltage bias drives the dynamics and even diverges when the junction is exposed to both a temperature gradient and a voltage bias. We discuss this pathological behavior and propose two possible solutions.

MM 64.10 Thu 17:30 HL 001

From DFT to Coupled Cluster Theory - Understanding Oxygen Activation on Coin Metal Nanoparticles — •Wilke Dononelli and Thorsten Klüner — Institut für Chemie, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

In this study we focus on one of the most fundamental catalytic model reactions, the oxidation of CO on a metal catalyst. We studied the activation of molecular oxygen via dissociation or direct reaction of CO and O_2 within density functional theory (DFT) and high level CCSD(T) calculations. Therefore we use Au_{13} and Au_{55} nanoparticles (NPs) and a periodic Au(321) surface as model systems and compare the catalytic activity of the gold substrates to Ag and Cu based, as well as bimetallic NP catalysts. Part of the DFT calculations were performed, using the well-established PBE functional as implemented in the Vienna ab initio simulation package (VASP). Hybrid and double hybrid DFT calculations on the NPs were performed in Gaussian09. CCSD(T) calculation were performed in Gaussian09 using conventional CCSD(T) for the M_{13} (M=Au,Ag,Cu) NPs and CCSD(T)/PBE in a QM/QM embedding scheme using the ONIOM approach for M_{55} NPs. For systems of 55 metal atoms PBE gives the same results as double hybrids or even CCSD(T). For smaller M_{13} NPs interaction energies differ between PBE and higher levels of theory, which might be explained by the molecule like character of these NPs.

MM 65: Functional Materials (Actuators, filters, sensors, shape memory)

Time: Thursday 17:30–19:00 Location: H 0106

MM 65.1 Thu 17:30 H 0106

Thermosalient ('jumping') crystals — •Ivor Lončarić[1], Jasminka Popović[1], Vito Despoja[2], and Željko Skoko[2] — [1]Ruđer Bošković Institute, Bijenička 54, HR-10000 Zagreb, Croatia — [2]Department of Physics, Faculty of Science, University of Zagreb, Bijenička 32, HR-10000 Zagreb, Croatia

Thermosalient materials when heated or cooled are characterized by a fast and energetic phase transition in which crystals experience macroscopic change in dimensions and jump to distances much larger than their own dimension. Since the first systematic study [1], there has been a rising intrest for these interesting, and potentially useful, acutating materials. As a one example, N-2-propylidene-4-hydroxybenzohydrazide shows irreversible thermosalient phase transition from Form I to Form II and reversible thermosalient phase transition from Form II to Form III. We combine experiments and first-principles electronic structure calculations to elucidate this interesting and technologically useful phenomenon[2].

[1] Skoko et al., J. Am. Chem. Soc. 132, 14191 (2010)
[2] Lončarić et al., Cryst. Growth Des. 17(8), 4445-4453 (2017)

MM 65.2 Thu 17:45 H 0106

Analysis of different methods for methylammonium lead iodide perovskite deposition into nanoporous anodic-aluminum oxide membranes — •Mirko Gabski, Martin Peterlechner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

Organometal-trihalide perovskites are organo-metal salts which have gained popularity as a light harvesting material in thin film solar cells in recent years due its favorable properties (e.g. cheap and simple processing, high absorption coefficient, direct band gap, high charge carrier mobility) and led to solar cells with efficiencies up to ~20 %. Anodic-aluminum oxide (AAO) provides a highly ordered nanoporous template consisting of hexagonally arranged pores with tunable pore diameters ranging from ~10 to ~200 nm and a thickness between ~10 nm and 100 μm which is easily synthesized using a simple anodization procedure and is thus excellently suited for the synthesis of quasi-one-dimensional nanostructures. By choosing a suitable deposition method the AAO template can be used to fabricate an array of quasi-one-dimensional perovskite nano-rods in parallel circuit where the direction of charge carrier flow is guided by the confinement imposed by the surrounding AAO. In this work, different deposition methods (e.g. drop-coating, dip-coating, spin-coating and co-evaporation) are investigated for their applicability for perovskite deposition into AAO membranes with varying thicknesses and pore diameters since changing aspect ratios impose different constraints on the choice of the most suitable deposition method.

MM 65.3 Thu 18:00 H 0106

Role of Hydrogen Bonds in Organic Ferroelectrics using Neutron Scattering and First principles Simulations — •Sanghamitra Mukhopadhyay — ISIS Facility, Rutherford Appleton Laboratory-STFC, Harwell Science and Innovation Campus, Oxfordshire OX11 0QX, UK

Hydrogen bonded organic ferroelectrics are important functional materials for potential technological applications in flexible electronics. Role of hydrogen bonds is important in this class of materials for designing new functionalities. Microscopic knowledge of structure and dynamics of those hydrogen bonds are thus crucial. In this work I will present structure and dynamics of few organic ferroelectrics using neutron diffraction, spectroscopy and first principles simulations.

Neutron scattering experiments are done on IRIS and OSIRIS spectrometers at ISIS to understand the structures and hydrogen bond motifs in these ferroelectrics. inelastic and quasielstic neutron scattering spectroscopies are employed to investigate the pico-second dynamics in those materials.

State-of-the-art calculations based on plane wave pseudo potential density functional theory to predict the structure. Inelastic neutron scattering spectrum are interpreted using first principles lattice dynamics and the quasielastic neutron spectrum are calculated by analysing the trajectory of the molecular dynamical simulations.

Correlating structure and dynamics of these functional materials, it is shown that the in-plane strains on hydrogen bonds are responsible for high ferroelectric polarisation of these organic solids.

MM 65.4 Thu 18:15 H 0106

In situ observations on dynamic reconfiguration of bilayer defects in van der Waals bonded Ge-Sb-Te based alloys — •Andriy Lotnyk[1], Ulrich Ross[1], Torben Dankwort[2], Isom Hilmi[1], Lorenz Kienle[2], and Bernd Rauschenbach[1,3] — [1]Leibniz Institute of Surface Engineering (IOM), Permoserstr. 15, 04318 Leipzig, Germany — [2]Institute for Materials Science, Faculty of Engineering, University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany — [3]Felix Bloch Institute for Solid State Physics, Leipzig University, Linnéstr. 5, 04103 Leipzig, Germany

Ge-Sb-Te (GST) based phase change alloys are well-known materials from optical data storage applications and are emerging contenders for non-volatile data storage applications. In the present work, atomic structure and dynamics of layered defects frequently reported in van der Waals bonded GST based alloys and superlattices are investigated using aberration-corrected STEM. The defects are confined into two atomic layers of GeSb and Te and represent special type of stacking fault. In situ experiments showed that the bilayers can be easily reconfigured into such bilayer stacking faults with subsequent formation of a new van der Waals gap. Depending on the beam dose, the newly formed stacking fault can either reconfigure back to the initial state or move in later direction within the faulty stacking plane. The results of the present work shed insight into mechanism of structural reconfiguration of building blocks in van der Waals bonded GST compounds, also relevant for an understanding of switching mechanisms in iPCMs.

MM 65.5 Thu 18:30 H 0106

Stability of the Shape Memory Effect and Transformation Temperatures in Ti-Ta-X Alloys — •Alberto Ferrari, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44801 Bochum, Germany

Ti-Ta-based alloys exhibit a high-temperature shape memory effect (SME) due to a martensitic transformation between an orthorhombic phase (α'') and a body-centered cubic phase (β). The stability of the SME in binary Ti-Ta is compromised by the formation of detrimental phase (ω). It has been observed experimentally that alloying a third component to pure Ti-Ta hinders the formation of the ω phase. Both the stability of the SME and the transformation temperature depend strongly on the chemical composition; the underlying mechanism is, however, not fully understood. In this contribution, the stability and the transformation temperature are analyzed systematically as a function of composition of Ti-Ta-X by means of *ab-initio* calculations; in particular, it is examined how different elements and different concentrations affect the formation energy of the α'', β and ω phases. The trends in formation energies are found to be related to the electronic properties and the size of the alloying elements. Simpler models that describe the compositional dependence of the transformation temperature are derived from first principles data and allow us to gain chemical insight into the effect of alloying on the relative phase stability. Our model is exploited to guide the experimental design of new stable and high-temperature shape memory alloys.

MM 65.6 Thu 18:45 H 0106

Functionalized gold electrodes for sensing DNA mutations — Ganesh Sivaraman[1], Frank C. Maier[1], Rodrigo Amorim[2], Ralph H. Scheicher[3], and •Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Universidade Federal Fluminense, Departamento de Física, Volta Redonda/RJ, Brazil — [3]Department of Physics and Astronomy, Materials Theory, Uppsala University, Sweden

Derivatives of small diamond-like nanostructures, the diamondoids, are used to functionalize fold electrodes. Within the gap of these functionalized electrodes, different DNA units are placed. These are native nucleotides, as well as modified nucleotides, such as mutations and epigenetic markers. Using quantum-mechanical calculations together with the non-equilibrium Green's functions formalism, we investigate the electronic transport properties across the functionalized electrodes for the cases of all nucleotides place in the electrode gap. Distinct electronic signals were found, which give rise to different coupling strengths across the electrode gap. These signals occur at distinct values of the gating voltage and can uniquely characterize the nucleotide in the metallic gap. Specifically, they can clearly distinguish between the native and the mutated nucleotides. Accordingly, diamondoid functionalized electrodes can be used as a sensing setup within nanopore materials.

MM 66: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data V

Time: Thursday 17:30–19:00 Location: H 0107

Topical Talk MM 66.1 Thu 17:30 H 0107

Discovering Interpretable Patterns, Correlations, and Causality — •Jilles Vreeken — Max Planck Institute for Informatics, Saarbrücken, Germany — Saarland University, Saarbrücken, Germany

To gain non-trivial insight from data using machine learning, we need to be able to interpret what these results mean. This we can either do by staring long and hard at the highly complex and non-linear models that methods such as support vector machines or deep learning provide when we run them on our data. This most often ends in us throwing the towel, as these models are extremely difficult to understand. Alternatively, we can require the learning method to report in a language we can (much) (more) easily understand, instructing it to discover things beyond what we already know.

In this talk, I will give an introduction to this latter, interpretable approach. In particular, I will explain the power of local modeling, that of non-parametric correlation discovery, that of pattern languages, will give examples of recent discoveries we made on materials science data using a technique called subgroup discovery, and an outlook on very recent approach to discover causal dependencies in data without having to make (almost) any assumptions.

MM 66.2 Thu 18:00 H 0107

Subgroup Discovery for Finding Local Patterns in Materials Data — •Mario Boley[1], Bryan R. Goldsmith[2], Christopher Sutton[3], Jilles Vreeken[1], Matthias Scheffler[3], and Luca M. Ghiringhelli[3] — [1]Max-Planck-Institut für Informatik, Saarbrücken — [2]University of Michigan, Ann Arbor — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

We establish that subgroup discovery (SGD), a form of local pattern discovery for labeled data, can help find interpretable descriptors from materials-science data obtained by first-principles calculations. In contrast to global modelling algorithms, SGD finds descriptions of subpopulations in which, locally, the target property takes on an interesting distribution. First, we formulate the SGD algorithm for applications in scientific domains. Subsequently, SGD is applied to configurations of neutral gas-phase gold clusters to discern general and interesting patterns between their geometrical and physicochemical properties. For example, SGD uncovers that van der Waals interactions within gold clusters are linearly correlated with their radius of gyration and are weaker for planar clusters than for nonplanar clusters. Moreover, we explore SGD for finding descriptors that predict both the formation and bandgap energies of transparent conducting oxides as well as descriptors that classify the octet binary semiconductors as either rock salt or zincblende; in both settings using only information of their chemical composition. Lastly, an efficient optimal solver using branch-and-bound is developed for dispersion-corrected objective functions to facilitate the discovery of interpretable subgroups.

MM 66.3 Thu 18:15 H 0107

Generation of ab initio datasets with predefined precision using uncertainty quantification — •Jan Janssen, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

A major challenge in multiscale materials simulation is the ab initio prediction of phase stabilities in multi-phase materials. To extend the ab initio accuracy to larger length and time scales the fitting of machine learning potentials seems promising, but this approach is intrinsically limited to the accuracy of the input data. Therefore it is essential to quantify the different sources of uncertainty in ab initio calculation, including the systematical error of convergence, the statistical or numerical error and the model error for derived quantities. Already the determination of the equilibrium lattice constant and bulk modulus requires a careful analysis of the fitting of energy-volume curves, going beyond the consideration of standard convergence parameters like cutoff and k-points. In order to handle this delicate interplay of uncertainties, we introduce the concept of uncertainty phase diagrams. Based on the uncertainty phase diagrams we model the convergence gradients of the contributing errors, to automate the convergence process not only for the error in energy. The modelling of uncertainties in relation to the corresponding ab initio calculation is enabled by our recently developed Python based workbench pyiron. Our investigations revealed that commonly used rules of thumb for fitting ground state materials properties become invalid for high precision calculations.

MM 66.4 Thu 18:30 H 0107

Numerical-Error Estimates for DFT Calculations and Materials Databases — C. Carbogno[1], K.S. Thygesen[2], B. Bieniek[1], C. Draxl[1,3], L. Ghiringhelli[1], A. Gulans[3], O.T. Hofmann[4], K.W. Jacobsen[2], •S. Lubeck[3], J.J. Mortensen[2], M. Strange[2], E. Wruss[4], and M. Scheffler[1] — [1]FHI Berlin, Germany — [2]DTU, Lyngby, Denmark — [3]HU Berlin, Germany — [4]TU Graz, Austria

Density-functional theory (DFT) has become an invaluable tool in materials science. Whereas the precision of different approaches has been scrutinized for the PBE functional using extremely accurate numerical settings [1], little is yet known about code- and method-specific errors that arise under more commonly used numerical settings. Recently, this has become a severe issue, since it prevents repurposing publicly available DFT data created using different settings and/or codes. To overcome this, we study the convergence of different properties (geometries, total and relative energies) in four conceptually-different DFT codes (exciting, FHI-aims, GPAW, VASP) for typical settings. Specifically, we discuss relative and absolute errors as a function of the numerical settings, e.g., basis sets and **k**-grids, for 71 elemental solids [1]. Using this data, we propose analytical models that allow for reliable error estimates for *any* compound, as we explicitly demonstrate for binary and ternary solids. We discuss the extensibility of our approach towards more complex materials properties and its applicability in computational materials databases.

[1] K. Lejaeghere *et al.*, *Science* **351**, aad3000 (2016).

MM 66.5 Thu 18:45 H 0107

An Electronic Transport Properties Database From High-Throughput Ab-initio Computations — •Francesco Ricci[1], Wei Chen[2,4], Umut Aydemir[3,5], Jeffrey Snyder[3], Gian-Marco Rignanese[1], Anubhav Jain[2], and Geoffroy Hautier[1] — [1]Institute of Condensed Matter and Nanosciences (IMCN), Université catholique de Louvain, Louvain-la-Neuve, Belgium — [2]Lawrence Berkeley National Lab, Berkeley, CA, USA — [3]Department of Materials Science and Engineering, Northwestern University, Evanston, USA — [4]Department of Mechanical, Materials and Aerospace Engineering, Illinois Institute of Technology, Chicago, USE — [5]Koç University, Department of Chemistry, Turkey

Nowadays the state-of-the-art DFT codes and the high-throughput (HT) frameworks allow us to compute materials properties at a large scale. As recently made by Materials Project (MP) for elastic and piezoelectric tensors, we will present a large and freely accessible data set of transport properties as effective mass and Seebeck coefficient. This transport data has been computed on top of energy band structures available in MP, using the well-known BoltzTraP code inserted in a HT framework. Given the importance of electronic transport properties, the whole community of material science researcher will benefit from this database. We will present the work flow to obtain the data and the data set. Some correlations between the transport properties and some applications in the field of transparent conducting oxides and thermoelectric materials will be presented.

MM 67: Methods in Computational Materials Modelling (methodological aspecst, numerics)

Method development

Time: Thursday 17:30–19:00 Location: TC 006

MM 67.1 Thu 17:30 TC 006

Linear Scaling first-principles constant pressure molecular dynamics in Conquest — •Zamaan Raza[1], Shereif Mujahed[2], David Bowler[2], and Tsuyoshi Miyazaki[1] — [1]National Institute for Materials Science (NIMS), Tsukuba, Japan — [2]London Centre for Nanotechnology (LCN), University College London, United Kingdom

Density functional theory (DFT) calculations have become commonplace in the characterisation, design and prediction of materials, but conventional implementations scale poorly. Conquest (http://ordern.github.io) is a first principles electronic structure code that can perform DFT calculations that scale linearly with the number for atoms, and is capable of almost ideal parallel efficiency even when using more than 200,000 cores to deal with million-atom systems. Its capabilities include Born-Oppenheimer molecular dynamics (MD) in the micro-canonical and canonical ensembles, and extended-Lagrangian MD which includes electronic degrees of freedom in the equations of motion, solving fundamental problems involving time-reversibility.

Constant pressure MD provides a closer match to experimental and planetary interior conditions than constant volume, and facilitates the modeling of polymorphic phase transitions. Moreover, it is often difficult to choose the correct volume when modeling complex amorphous or biological systems. In this talk, we discuss the implementation of isobaric-isothermal (NPT) molecular dynamics in Conquest, and demonstrate that efficient and robust NPT simulations are now possible for systems containing 10,000+ atoms.

MM 67.2 Thu 17:45 TC 006

Treatments of disorder within electronic structure calculations — •Alberto Marmodoro and Hubert Ebert — Dept. Chemie, LMU, München

The coherent potential approximation (CPA) has proved to be a powerful tool to account for disorder in solid state systems. Among reasons for its success one can enumerate the ability to describe both diagonal [1] and off-diagonal [2] breakdown of long range order (LRO); suitability to account for an arbitrary concentration of defects, not constrained to the diluted limit; flexibility of the underlying alloy analogy model to also set up a first principles description of finite temperature effects in the magnetic [3] and positional [4] degrees of freedom. Additional aspects coming over the years under scrutiny have concerned the single-site nature of the theory, to also incorporate short-range order (SRO) effects [5]; and its effective medium construction in terms of a self-consistent arithmetic average procedure, as opposed to other statistics mainly proposed in the study of localization problems [6-7]. We look into this line of developments through examples spanning from model hamiltonians to multiple scattering adaptations.

(1) P. Soven, Phys.Rev. **156**, 809, (1967) (2) G. Bouzerar et al. Phys.Rev.B **66**,1, (2002)

(3) J. Staunton et al., JMMM, **45**, 15-22, (1984); (4) H. Ebert et al., Phys.Rev.B **91**, 165132, (2015)

(5) D. Rowlands et al., Phys.Rev.B, **67**, 115109, (2003)

(6) V.Dobrosavljevic et al., Phys.Rev.Let. **78**, 3943, (1997); (7) H.Terletska et al., Phys.Rev.B **95**, 134204, (2017)

MM 67.3 Thu 18:00 TC 006

Multilevel Adaptive Sparse Grids for parametric stochastic materials models — •Sandra Döpking[1], Daniel Strobusch[2], Christoph Scheurer[2], and Sebastian Matera[1] — [1]Freie Universität Berlin — [2]Technische Universität München

Many material models require sampling to obtain the desired model output, e.g. molecular dynamics or Monte Carlo sampling. Most of these models depend on a number of parameters which show a high variability. This can be an effect of uncertainties due to the limited accuracy of the underlying method. Or, the model might represent a class of materials with different material parameters. We present a Multilevel Adaptive Sparse Grid approach to explore the parameter space and to construct a surrogate of the often expensive original model. In this approach, the points in the parameter space are adaptively chosen which reduces the total number of costly model evaluations. Moreover, the multi-level structure of the sparse grids allows us to reduce the sampling accuracy and therefore the cpu-time spend for the model evaluation in each refinement step. We demonstrate the methodology for a first-principles kinetic Monte Carlo (1p-kMC) model for heterogeneous CO oxidation, where we address the impact of the uncertain reaction energetics derived from Density Functional Theory. We find that the multi-level approach reduces the computational cost significantly compared to non-adaptive, single level sparse grids – without compromising the accuracy of the results. For this model, we observe that DFT uncertainty can have a tremendous impact on the simulation output and that 1p-kMC predictions have to be interpreted carefully.

MM 67.4 Thu 18:15 TC 006

How to simulate nuclear quantum effects accurately at the cost of molecular dynamics — •Venkat Kapil[1], Jörg Behler[2], Joost VandeVondele[3], and Michele Ceriotti[1] — [1]EPFL, Lausanne, Switzerland — [2]Universität Göttingen, Göttingen, Germany — [3]CSCS, ETH Zurich, Zurich, Switzerland

The precise description of quantum nuclear fluctuations in atomistic modelling is possible by employing path integral techniques, which involve a considerable computational overhead due to the need of simulating multiple replicas of the system. Consequently, the cost is still prohibitive when combined with advanced electronic structure methods. An elegant way of reducing the number of replicas is by applying a correction based on a high order factorization of the Boltzmann operator. However, the high cost of computing the correction has prevented the use of this technique to condense phase systems. In this work, we present a molecular dynamics scheme which alleviates the cost of explicitly computing the expensive correction, that allows us to utilize the improved efficiency of the high order scheme. Furthermore, we demonstrate how to synergically use multiple time step integration in real and imaginary time to reduce down to zero, the cost of modelling quantum effects while describing inter atomic interactions at high levels of electronic structure theory.

MM 67.5 Thu 18:30 TC 006

Workflows and provenance tracking for high-throughput computational materials discovery — •Martin Uhrin, Sebastiaan Huber, Giovanni Pizzi, and Nicola Marzari — EPFL STI IMX THEOS, Lausanne, Switzerland

The last decade has seen a push in computational materials science towards cementing high-throughput approaches as a cornerstone of materials discovery and understanding. This in turn requires the development of new tools to enable researchers to shift from running individual calculations to manage thousands, if not millions of these, in a reliable, intuitive and reproducible way. In order to answer these needs, we have developed AiiDA, a python platform, to enable domain experts to encode their scientific expertise in highly customisable workflows that are easy to write, document, debug and share ensuring that such expertise is retained and can be built upon. Meanwhile, a database backend is used to automatically store the full provenance as a graph of inputs, calculations and corresponding outputs, allowing the user to see exactly where any result came from, or continue to work from any intermediate step. I will show how one can write and run AiiDA workflows in ipython notebooks and highlight the many advantages over the more traditional, 'throwaway script', approach and highlight some published high-throughput computational materials modelling projects that have been performed using AiiDA.

MM 67.6 Thu 18:45 TC 006

Effective treatment of formation energies for automated high-throughput computational materials design — •Rico Friedrich[1], Cormac Toher[1,2], Andrew Supka[3,4], Marco Fornari[1,3,4], Marco Buongiorno Nardelli[1,5], and Stefano Curtarolo[1,2] — [1]Center for Materials Genomics, Duke Univ. — [2]Mat. Sci., Elec. Eng., Phys. and Chem., Duke Univ. — [3]Dept. of Phys., Central Michigan Univ. — [4]Science of Advanced Materials Program, Central Michigan Univ. — [5]Dept. of Phys. and Dept. of Chem., Univ. of North Texas

Automated high-throughput computational materials design, as implemented in the AFLOW framework [1], aims at the systematic prediction and optimization of materials properties for technological applications. The approach requires an accurate and efficient description of formation energies to assess the thermodynamic stability of new compounds. This presents a major challenge to standard computational materials science approaches such as density functional theory (DFT). Significant errors arise when calculating total energy differences between chemically dissimilar materials due to incomplete error cancellation [2]. This is particularly the case for oxides (and other chalcogenides), where the chemical natures of diatomic (O_2) molecules, elemental metals and solid oxides are very different. We discuss various approaches to compute the formation energies of materials and compare their accuracy with respect to experimental reference data.

[1] S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012).
[2] V. Stevanović *et al.*, Phys. Rev. B **85**, 115104 (2012).

MM 68: Transport (Diffusion, conductivity, heat)

Transport II

Time: Thursday 17:30–18:30 Location: TC 010

MM 68.1 Thu 17:30 TC 010

Radiotracer self-diffusion experiments in CoCrFeNi and CoCrFeMnNi high entropy alloy single crystals — •Daniel Gaertner[1], Jonas Lübke[1], Josua Kottke[1], Yury Chumlyakov[2], Gerhard Wilde[1], and Sergiy Divinski[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Department of Physics of Metals, Tomsk State University, 36 Lenin Ave., Tomsk 634050, Russia

High entropy alloys are multicomponent alloys, which have a large number of constituting elements in equiatomic or nearly equiatomic concentrations. These materials are hypothesized to show significantly decreased self diffusivities. For the first time, diffusion of all constituent elements in equiatomic CoCrFeNi and CoCrFeMnNi single crystals is investigated using the radiotracer technique, thereby the tracer diffusion coefficients of Cr-51, Co-57, Fe-59, Mn-54 and Ni-63 are determined at a temperature of 1100 °C. Two contributions to the long-range atom transport are observed and their nature is elucidated by varying the diffusion times. In addition to the bulk diffusion transport, short-circuit diffusion seems to be prominent due to a high density of grown-in dislocations. The components are characterized by significantly different diffusion rates, with Mn being the fastest element and Ni and Co being the slowest ones.

MM 68.2 Thu 17:45 TC 010

Volume diffusion in high-entropy Al$_x$CoCrFeNi alloys — •Josua Kottke[1], Simon Trubel[1], Daniel Gaertner[1], Louis J. Santodonato[2], Peter K. Liaw[2], Sergiy V. Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, USA

High-entropy alloys (HEAs), i.e. multicomponent alloys with a large number of constituting elements in equiatomic or nearly equiatomic composition, attract an increased attention as potential structural materials due to their favorable mechanical and physical properties, especially at elevated temperatures. Hereby, we contribute to a debate about hypothetical sluggish diffusion phenomena in HEAs by investigating self-diffusion in Al$_x$CoCrFeNi ($x = 0.5$, 1 and 2) alloys.

Tracer diffusion in the Al$_x$CoCrFeNi alloys is measured between 800 °C and 1100 °C by applying the ^{51}Cr, ^{57}Co and ^{59}Fe radioisotopes. As the Al content x in the Al$_x$CoCrFeNi alloys is increased, a two-phase FCC+BCC microstructure replaces the single phase FCC one at $x < 0.3$ and the material becomes single phased BCC at $x = 2$. A careful microstructure examination using XRD, SEM and EBSD analysis allowed quantifying the measured diffusion profiles in terms of two separate contributions to long-range diffusion in FCC and BCC phases. The results indicate that the number of alloying elements in HEAs affects diffusion in FCC or BCC HEAs differently.

MM 68.3 Thu 18:00 TC 010

Effect of stoichiometry on self-diffusion in triple-defect binary intermetallics: Semi Grand Canonical and Kinetic Monte Carlo simulations. — •Rafal Kozubski[1], Jan Betlej[1], Piotr Sowa[1], Graeme Murch[2], and Irina Belova[2] — [1]M. Smoluchowski Institute of Physics, Jagiellonian University in Krakow, Lojasiewicza 11, 30-348 Krakow, Poland — [2]Centre for Mass and Thermal Transport in Engineering Materials, School of Engineering, The University of Newcastle, Callaghan, Australia

Vacancy-mediated self-diffusion and chemical short- and long-range ordering in triple-defect binary intermetallics was modelled with Ising nn and nnn pair interactions and simulated in atomistic scale. The Kinetic Monte Carlo (KMC) algorithm was implemented with local-configuration-dependent migration barriers and temperature-dependent equilibrium vacancy concentration determined by means of Semi Grand Canonical Monte Carlo (SGCMC) simulations. The resulting concentration dependence of the component tracer diffusivities in a triple-defect B2-ordering A-B system mimicking Ni-Al was in a very good agreement with the experimental results obtained for that system. In particular, inversion of the relationship between the Ni and Al-diffusivities in Al-rich Ni-Al systems deduced from the features of interdiffusion in Ni-Al was perfectly reproduced by direct self-diffusion simulations. The origin of the phenomenon is elucidated in terms of an increase of the nnn Al jump frequency resulting from specific atomic and vacancy configurations originating from the triple-defect character of disordering.

MM 68.4 Thu 18:15 TC 010

electronic transport coefficients from first principles — •zhenkun yuan, christian carbogno, and matthias scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6,14195 Berlin

The Kubo-Greenwood formalism has been employed successfully for the first-principles calculation of electrical conductivities at elevated temperature and/or for disordered systems [1]. It relies on *ab initio* molecular dynamics simulations to include electron-phonon scattering, which is the most important scattering mechanism for electronic transport in bulk materials. However, this approach suffers from severe finite-size effects for crystalline solids close to room temperature, since accounting for the dominant scattering with long-wavelength phonons would require extremely large supercells. In this work, we propose possible strategies to overcome this limitation. In particular, we assess to which extent the asymptotically exact extrapolation scheme [2] that we recently developed to correct for finite-size effects in the calculation of vibrational thermal conductivities can be extended to electronic transport. To this end, *ab initio* calculations are performed both for direct (GaAs) and indirect (Si) semiconductors and the obtained results are compared to the existing experimental and theoretical data [3].

[1] M. French and T. R. Mattsson, *Phys. Rev. B* **90**, 165113 (2014).
[2] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).
[3] J. Zhou, B. Liao, and G. Chen, *Semicond. Sci. Technol.* **31**, 043001 (2016).

MM 69: Structural Materials (Steels, light-weight materials, high-temperature materials)

Structural Materials I

Time: Friday 9:30–10:45 Location: H 0106

MM 69.1 Fri 9:30 H 0106

Dislocation dissociations in C11b MoSi2 and their impact on its plastic deformation — Václav Paidar[1], Miroslav Čák[2], •Mojmír Šob[3,4,5], and Václav Vitek[6] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czechia — [2]ICAMS, Ruhr-Universität Bochum, Germany — [3]Central European Institute of Technology, CEITEC MU, Masaryk University, Brno, Czechia — [4]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno, Czechia — [5]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czechia — [6]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, U.S.A.

Using the DFT calculated γ-surfaces possible metastable stacking faults have been found for the most common slip planes {013) and {110) in MoSi2. These calculations reveal three distinct stacking faults on {013) planes and one stacking fault on {110} plane. Owing to such multiplicity of metastable stacking faults there is a large number of possible dislocation dissociations. These dislocation splittings are analysed using the anisotropic elasticity and relevant stacking faults. The results show that the only dissociations of the <331] dislocations favoured over the complete undissociated dislocations are on {013) planes either in one or two planes of this type. Splitting into {110) planes are never favored. For loading along the [001] axis the dislocation glide may take place at high temperatures when the cross slip releases the sessile screw dislocations on two {013) planes.

MM 69.2 Fri 9:45 H 0106

Evaluation of Fermi surfaces, single and two-particle spectral properties for FeSe using Quasi-particle self consistent GW + DMFT — •Swagata Acharya, Dimitar Pashov, and Mark van Schilfgaarde — King's College London, London, United Kingdom

Most of the first principles techniques, based on DFT or DFT+DMFT frameworks, fails to reproduce the spectral properties of the FeSe both in the tetragonal and orthorhombic phases. Within our recently developed quasi-particle self-consistent GW coupled to DMFT, we show how proper estimations of the non-local and local spin fluctuations reproduce the spectral properties in very good agreement with the experiments. We also compute the spin-wave excitation spectra and find momentum dependent shifts in spin-fluctuation weights across the structural transition at 90 K. We rigorously show how these compare with the extant experimental findings.

MM 69.3 Fri 10:00 H 0106

Chromium and iron based zeta phases - lattice dynamics from first-principles — •Petr Dvořáček and Dominik Legut — VSB Technical University of Ostrava

It was shown [1] that the Z-phase precipitates at higher rate in Cr-rich steels than in Cr-depleted ones and this precipitation correlates with the presence of Niobium. Recently, the lectronic structure and mechanical properties of Z-phases, namely CrNbN and CrVN, were investigated employing first-principles calculations [2]. In this contributions we extend our understanding for dynamical and thermodynamical properties of the Cr-(V/Nb/Mo)-N and Fe-(V/Nb/Mo)-N Z-phases based on the lattice vibrations computed within the quasi-harmonic approximations[3]. The requested Hellman-Feynman forces acting on atoms along the atomic vibrations were computed emlopying density functional theory via the Vienna Ab Initio Simulation package[4]. The results are following: CrNbN, CrVN, CrNbVN, FeNbN, FeNbVN are thermodynamically stable, CrMoN, FeVN are thermodynamically unstable, but are stable in gamma-point and FeMoN is completely thermodynamically unstable.

References: 1. H. K. Danielsen and J. Hald, Energy Mater. 1, 49 (2006). 2. D. Legut and J. Pavlů, J. Phys.: Condens. Matter. 24 , 195502 (2012). 3. A. Togo and I. Tanaka, Scr. Mater., 108, 1-5 (2015). 4. G. Kresse and J. Furthmueller, Comput. Mater. Sci. 6, 15 (1996).

This work was supported by Czech National Foundation grant No. 17-27790S and Path to Exascale project No. CZ.02.1.01/0.0/0.0/16_013/0001791.

MM 69.4 Fri 10:15 H 0106

Theoretical and experimental investigation of mixing and clustering thermodynamics of Ti1-xAlxB2 alloys with age-hardening potential — •Erik Johansson, Nils Nedfors, Annop Ektarawong, Johanna Rosén, and Björn Alling — Linköping University - The Department of Physics, Chemistry and Biology (IFM)

Our project investigates phase stability and temperature dependence of structural parameters of Ti1-xAlxB2 metastable ceramic alloys. These alloys were predicted to exhibit a tendency for isostructural decomposition despite the fact that binary TiB2 and AlB2 are structurally very similar. Due to the reported high hardness of TiB2 and the prospect of age-hardening through isostructural clustering, these alloys could be good candidates for hard protective coatings on industrial cutting tools. In our work, we present theoretical predictions based on first-principles density functional theory. The phase diagram for this ternary system is derived and shows an isostructural miscibility gap. Phonon vibrational contributions to the free energies within harmonic and quasiharmonic approximations are calculated for the ordered binaries and disordered alloys, and we show their effect on the phase diagram. Non-isotropic thermal expansion beyond the standard implementation of the quasiharmonic approximation is investigated, and we discuss the methodological differences. Experimental synthesis of Ti1-xAlxB2 thin films using physical vapour deposition demonstrates the feasibility of growing the alloys, and after heat treatments at 1000 °C isostructural decomposition can be observed in the films confirming the theoretical predictions.

MM 69.5 Fri 10:30 H 0106

Influences of temperature and configurational disorder on electronic properties of boron carbide — •Annop Ektarawong[1], Sergei Simak[1], and Björn Alling[1,2] — [1]Department of Physics, Chemistry and Biology (IFM), Linköping University, SE-581 83 Linköping, Sweden — [2]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Long-standing controversial issues, concerning the electronic properties of boron carbide, are emphasized by large discrepancies between experiments and theoretical calculations. One of these is the overestimation of the bandgap of B_4C by standard DFT functionals, known to underestimate the bandgaps of all other materials. Another is the predicted metallic state of $B_{6.5}C$ in conflict with its experimental semiconducting state. With the aim of resolving such discrepancies, we investigate from first principles influences of temperature and configurational disorder, induced by low-energy defects, on electronic properties of the material. Regardless of the temperature, our results reveal a large variation in size of the bandgap and the appearance of the midgap states, both depending on the material's atomic configuration and composition, and also yield a fairly good agreement, compared to the experiments. The *ab initio* molecular dynamics simulations reveal the volumetric thermal expansion due to the lattice vibrations has a minimal impact on the bandgap of the material, while a major decrease of the bandgap is caused by explicit atomic displacements, induced by the vibrations. The temperature-dependent bandgaps of boron carbides, especially, B_4C and $B_{4.3}C$, will also be presented and discussed.

MM 70: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data VI

Time: Friday 9:30–11:00 Location: H 0107

Topical Talk MM 70.1 Fri 9:30 H 0107
Transmission Electron Microscopes as a tool generating Big Data: challenges ans opportunities — •Cécile Hébert — LSME, Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Switzerland

Modern state of the art transmission electron microscopes have become versatile tools fitted with a great variety of detectors. Thanks to tremendous improvement in the stability of components, a single instrument can be operated in various modes. Typically it is possible to operate it in conventional TEM mode or in scanning TEM mode. In TEM mode, cameras are used to reccord images or diffraction patterns. In STEM mode, detectors are used to collect signal as a function of probe position. This signal can be the scattered electrons at various angles, the direct electron beam, eventually analyzed in energy (electron energy loss spectrometry), X-Rays emmited by the specimen or even full diffraction pattern at each probe position. With the ability to scan area of 100 to several 1000 squared pixel, rapid CCD camera (1000 fps) for dynamical experiments, every mid-sized lab can generate data volumes up to petabytes/year. An additional challenge is posed by the fact that several signals are captured by detectors of various brands and delivered in closed undocumented formats. With the current trend towards open science, this poses new challenges but give also opportunities to address the topic on a global level.

MM 70.2 Fri 10:00 H 0107
High-throughput classification and categorization of structures from atomistic simulations — •Lauri Himanen, Patrick Rinke, and Adam Foster — Department of Applied Physics, Aalto University, Espoo, Finland

Our capability of producing, storing and analysing computational materials science data has grown tremendously. As the high-throughput screening of materials is becoming ever more popular, materials databases are being filled with atomic and electronic structure data.

To enable structure-related database queries, specific structural classes need to be defined. Unfortunately the required information is not always provided, and when it is, it is often based on an unspecified definition. To cope with large heterogeneous datasets of atomistic calculations, automated and verifiable methods for analyzing and categorizing atomistic structures are becoming necessary.

We discuss different methods that can be used in extracting structural information from various structural classes. These techniques involve finding a standardized unit cell, finding a translational basis for periodic materials within complex atomic environments and cluster analysis for separating different structural components. We also propose a material map that can be used to categorize the structural space and apply the introduced methods in the automatic classification of pristine crystals, surfaces and 2D materials.

MM 70.3 Fri 10:15 H 0107
Compact representation of crystal structures using three-dimensional diffraction patterns and deep learning — •Angelo Ziletti, Matthias Scheffler, and Luca M. Ghiringhelli — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Big data is emerging as a new paradigm in materials science. A vast amount of three-dimensional structural data is provided by both computational repositories (e.g. http://nomad-coe.eu) and experiments (e.g. atom probe tomography). Computational methods that automatically and efficiently detect long-range order are of paramount importance for materials characterization and analytics. Current methods are either not stable with respect to defects, or base their representation on local atomic neighbourhoods, which in turn makes it difficult to detect "average" longe-range order. In the proposed approach, for a given crystal structure we first calculate its diffraction pattern, expand it on spherical harmonics, and then use a neural-network model to obtain a compact, low-dimensional representation. We apply this workflow to a subset of materials from the Novel Materials Discovery (NOMAD) Archive, and show that our deep-learning-based approach compactly encodes structural information, is robust to defects (e.g. point defects, and/or strain), and allows to build easily interpretable structural-similarity maps. This work received funding from the NOMAD Laboratory, a European Center of Excellence.

MM 70.4 Fri 10:30 H 0107
Cluster analysis of chemical libraries based on molecular fingerprinting — •Annika Stuke[1], Lei Xie[2], Milica Todorović[1], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, Finland — [2]Department of Computer Science, Hunter College, the City University of New York, USA

Machine learning models promise to greatly accelerate the process of discovering new and better materials. However, it is difficult for learning models to achieve a robust and high prediction performance with imbalanced chemical datasets, in which certain classes of chemical structures are overrepresented. Learning algorithms are easily influenced by the larger classes, leading to biased results. We present an efficient method to generate diverse subsets from large chemical databases with cluster analysis. Databases are split into different clusters with an extended exclusion sphere algorithm based on the pairwise Tanimoto similarity calculated from Morgan fingerprints [1]. A diverse subset is then generated by picking molecules with different substructures from each cluster. The method has been successfully employed to select structurally diverse subsets of a dataset of 64k organic molecules from the Cambridge Crystal Structure Database [2]. We demonstrate the effect of this method on the prediction performance of machine learning models based on kernel ridge regression and neural networks for spectral properties of molecules. [1] D. Butina, J. Chem. Inf. Comput. Sci. 39, 747 (1999), [2] C. Schober et al., J. Phys. Chem. Lett. 7, 3973 (2016)

MM 70.5 Fri 10:45 H 0107
Identifying synthesisable ice structures from first principles — •Edgar Engel[1,2], Andrea Anelli[1], Michele Ceriotti[1], Chris Pickard[2], and Richard Needs[2] — [1]TCM Group, Cavendish Laboratory, UoCambridge, UK — [2]Laboratory of Computational Science and Modeling, IMX, EPFL, Lausanne, Switzerland

We present a comprehensive density-functional-theory study of the crystalline phases of water ice. We construct candidate ice structures on the basis of more than five million tetrahedral networks listed in the Treacy, Deem, and IZA databases, collecting 15,882 locally-stable ice structures. The search for the few synthesisable structures among them is a needle-in-a-haystack kind of problem, which is conventionally tackled using a convex hull construction to identify structures which are stabilised by manipulation of a particular constraint (such as density) chosen on the basis of experimental evidence or intuition. This heavily constrains which stabilisable structures are identified and does not account for the uncertainties inherent to computed structure properties. Hence, we instead employ a recently developed probabilistic generalised convex hull construction to stochastically sample the likelihood of each structure to be stabilised by application of appropriate thermodynamic constraints. We thereby recover (entirely a priori) all known ice phases except the known-to-be metastable ice IV. We further identify several new promising candidates for experimental synthesis, providing a much needed starting point for the determination of accurate structural properties and possible synthetic pathways.

MM 71: Methods in Computational Materials Modelling (methodological aspecst, numerics)

Determination of Defect Properties

Time: Friday 9:30–11:00 Location: TC 006

MM 71.1 Fri 9:30 TC 006

Computing the Absolute Gibbs Free Energy in Atomistic Simulations: Applications to Defects in Solids — Bingqing Cheng and •Michele Ceriotti — Laboratory of Computational Science and Modeling, Institute of Materials, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland

The Gibbs free energy is the fundamental thermodynamic potential underlying the relative stability of different states of matter under constant-pressure conditions. However, computing this quantity from atomic-scale simulations is far from trivial, so the potential energy of a system is often used as a proxy. Here we use a combination of thermodynamic integration methods to accurately evaluate the Gibbs free energies associated with defects in crystals, including the vacancy formation energy in BCC iron, and the stacking fault energy in FCC nickel, iron and cobalt. We quantify the importance of entropic and anharmonic effects in determining the free energies of defects at high temperatures, and show that the potential energy approximation as well as the harmonic approximation may produce inaccurate or even qualitatively wrong results.Our calculations manifest the necessity to employ accurate free energy methods such as thermodynamic integration to estimate the stability of crystallographic defects at high temperatures.

MM 71.2 Fri 9:45 TC 006

First-principles calculations of lattice-vacancy diffusion coefficients via non equilibrium ab initio molecular dynamics — •Igor A. Abrikosov[1,2], Davide G. Sangiovanni[1,3], Davide Gambino[1], and Björn Alling[1,4] — [1]Linköping University, Sweden — [2]National University of Science and Technology "MISIS", Moscow, Russia — [3]Ruhr-Universität Bochum, Germany — [4]Max-Planck-Institut für Eisenforschung GmbH, Germany

We revisit the color-diffusion (CD) algorithm in non equilibrium ab initio molecular dynamics (NE-AIMD) and propose substantially more efficient approach for the estimation of monovacancy jump rates in crystalline solids at temperatures well below melting [1]. Considering bcc Mo between 1000 and 2800 K as a model system, NE-AIMD results show that the colored-atom jump rate increases exponentially with the force intensity F, up to F values far beyond the linear-fitting regime employed previously. At the same time, equilibrium rates extrapolated by NE-AIMD results are in excellent agreement with those of unconstrained dynamics. The gain in computational efficiency increases rapidly with decreasing temperatures and reaches a factor of 4 orders of magnitude at the lowest temperature considered in the present study. Moreover, we demonstrate the applicability of the CD algorithm in simulations of Ti monovacancy jump frequencies in a compound, NaCl-structure titanium nitride (TiN), at temperatures ranging from 2200 to 3000 K [2].

[1] D. G. Sangiovanni, et al., Phys. Rev. B 93, 094305 (2016).

[2] D. Gambino, et al., Phys. Rev. B 96, 104306 (2017).

MM 71.3 Fri 10:00 TC 006

Modelling diffusion in non-dilute Ni-Re alloys: A combined kinetic Monte Carlo and cluster expansion approach — •Maximilian Grabowski, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Deutschland

Ni is a base component in high-temperature superalloys and Re is one of the key ingredients to improve mechanical properties in Ni-based alloys, in particular creep resistance. It is, however, not fully understood how Re affects creep in Ni-based superalloys.

Previous studies showed that in the dilute limit there is almost no effect of Re on the diffusivity of the atoms or the mobility of the vacancies. In this study, we extend our investigation to the non-dilute limit of Re by including Re-Re interactions. This enables us to investigate atomic mobilities and segregation behaviour over the entire composition range.

We use a kinetic Monte Carlo (KMC) approach to simulate diffusion in Ni-Re alloys. The key parameter in the KMC model are the diffusion barriers, which are strongly dependent of the local atomic configuration. To obtain an accurate and fast evaluation of the configuration-dependent diffusion barriers, we combine the KMC model with a cluster expansion (CE) approach. The CE is parametrised using energies from density-functional theory (DFT) calculations for a large number of possible Ni-Re configurations. From the KMC simulations, we then extract diffusion coefficients, evaluate the vacancy mobility as a function of Re concentration.

MM 71.4 Fri 10:15 TC 006

First-principles calculations of field evaporation in atom probe tomography — •Michael Ashton, Arpit Mishra, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40273 Düsseldorf

Atom probe tomography (APT) has developed into a key technique for studying 3D element distribution in complex microstructures at near-atomic resolution. At the heart of the technique is the evaporation of single atoms from a very sharp tip exposed to huge electric fields (10^{11} V/m). However, commonly used geometric reconstruction algorithms fail to take into account any details of the evaporation mechanism, such as differences in evaporation between chemical species or from different sites. To shed light on the factors influencing field evaporation, we study desorption from various sites (ad-atom, steps, kinks) on prototypical metal surfaces (Al, W) by means of density-functional theory calculations. From these calculations, we obtain the field-dependent evaporation barriers, which will be used in subsequent APT simulations. We also find evidence for the roll-over effect at steps, that has been proposed to explain orientational bias in evaporation trajectories.

MM 71.5 Fri 10:30 TC 006

Free Energy of Cu/Ag Heterophase Interfaces — •Marvin Poul, Sebastian Eich, and Guido Schmitz — Universität Stuttgart, Stuttgart, Deutschland

The properties of nanocrystalline materials are influenced by the thermodynamics of their interfaces. In particular we are interested in incoherent heterophase interfaces. Using the Frenkel-Ladd[1] method and the framework of interface thermodynamics developed by Frolov and Mishin[2], we present a Monte Carlo method to compute the free interface energy of incoherent Cu/Ag interfaces. All calculations are performed with the thermodynamically accurate Embed-Atom method potential developed by Williams et al.[3], which is known to reproduce the energies of planar defects very well. In general the procedure should be applicable to arbitrary incoherent interfaces.

[1] Frenkel, D., and Anthony JC L. J. Chem. Phys. 81 (1984): 3188-3193. [2] Frolov, T., and Y. Mishin. Phys. Rev. B 85 (2012): 224107. [3] Williams, P. L., Y. Mishin, and J. C. Hamilton. Model. Simul. Mater. Sci. Eng. 14 (2006): 817.

MM 71.6 Fri 10:45 TC 006

Modeling defects and grain boundaries with the amplitude expansion of the phase field crystal model — •Marco Salvalaglio[1], Rainer Backofen[1], Ken Elder[2], and Axel Voigt[1] — [1]Institute of Scientific Computing, Technische Universität Dresden, 01062 Dresden, Germany — [2]Department of Physics, Oakland University, Rochester, 48309 Michigan, USA

The Phase-Field Crystal (PFC) approach describes the dynamics of local atomic probability density on diffusive time scales. It is restricted to relatively small systems as it requires fine spatial discretizations. The Amplitude expansion of the PFC model (APFC) is a coarse-grained approach allowing for tackling larger systems. However, it has limitations on the quantitative description of material properties and on 3D systems. We present the realistic modeling and simulations of grain boundary morphologies between tilted/twisted and strained crystals by means of the APFC model. This is achieved through a Finite Element Method framework with advanced computational features and an extension of the model allowing for the control over the energy of defects, grain boundaries and interfaces. Typical planar and spherical grain boundaries are illustrated for different lattice symmetries, namely triangular/honeycomb in 2D as well as body-centered cubic and face-centered cubic in 3D. Moreover, new results concerning the dynamics of spherical grain boundaries are discussed.

MM 72: Magnetic Shape Memory Alloys (joint with MA)

Time: Friday 9:30–10:30 Location: TC 010

MM 72.1 Fri 9:30 TC 010

Magnetic ground state and compositional stability of epitaxial strain induced martensites in $\mathbf{Fe_xRh_{1-x}}$ thin films — •Ralf Witte[1], Markus E. Gruner[2,3], Richard A. Brand[1,2], Di Wang[1,4], Heiko Wende[2], Robert Kruk[1], and Horst Hahn[1,5] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [3]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München — [4]Karlsruhe Nano Micro Facility (KNMF), Karlsruhe Institute of Technology — [5]KIT-TUD-Joint Research Laboratory Nanomaterials, Technical University Darmstadt

Recently we reported on the formation of an adaptive martensite structure observed in chemically disordered, equiatomic FeRh thin films which were subject to large epitaxial strains [1]. A magnetically disordered ground state of the resulting structure was predicted from density functional theory (DFT) calculations. In this contribution we will show by means of low temperature conversion electron Mössbauer spectroscopy that the strain induced structural change leads to a magnetic spin glass state at low temperature in agreement with DFT calculations. Additionally, structural and magnetic characterization of thin films with different Fe_xRh_{1-x} composition will be presented. The observed magnetic and strain adaption behavior is discussed with respect to the equilibrium binary alloy phase diagram and the existing metastable phases. We acknowledge funding by the DFG via HA1344/28-1. [1] R. Witte *et al.*, PRB 93, 104416 (2016).

MM 72.2 Fri 9:45 TC 010

Ab initio design strategies for NiMn-based magnetocaloric materials: The effect of Co and Fe — •Biswanath Dutta, Fritz Körmann, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

In the quest to improve magnetocaloric properties of NiMn-based Heusler alloys, doping with ferromagnetic elements is found to be a promising strategy. Recent experiments show a large magnetization drop also known as metamagnetic transition and a giant inverse magnetocaloric effect (MCE) upon martensitic transformation in Co and Fe substituted NiMn-based Heusler alloys. In spite of this huge potential, a complete understanding of the role of different substitutional elements in these materials is still missing. Using ab initio calculations, we study the impact of Co and Fe on the martensitic transformation and the magnetic properties in Mn-excess Ni-Mn-Al alloy (B. Dutta et al., Phys. Status Solidi B 1700455 (2017)). Our calculations reveal an antiferromagnetic to ferromagnetic transition above a critical amount of Co or Fe doping in the austenite phase. The martensite phase, however, remains antiferromagnetic, which explains the experimentally observed metamagnetic transition in these alloys. The obtained magnetic properties are explained on the basis of magnetic exchange interactions. We also find that both Co and Fe substitution reduces the martensitic transformation temperature with the effect being larger in the case of the Fe containing alloy. Based on the achieved results on saturation magnetization and transformation temperature, Co containing alloys are found to be more promising for future MCE applications.

MM 72.3 Fri 10:00 TC 010

Martensitic transformations in $\mathbf{Ni_2MnGa}$ alloy: a first-principles study — •Martin Zelený[1,2], Ladislav Straka[2,3], Alexei Sozinov[4], and Oleg Heczko[2,3] — [1]NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [3]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [4]Material Physics Laboratory, Lappeenranta University of Technology, Savonlinna, Finland

The martensitic transformation paths in Ni_2MnGa alloy from cubic austenite to several low-symmetry martensitic structures have been studied by first-principles calculations combined with the generalized solid state nudged elastic band method. We determined the minimum energy path and corresponding changes in crystal lattice leading to the four-, five-, and seven-layered modulated phases of martensite (4O, 10M, and 14M) described as the relaxed nanotwinned non-modulated (NM) phase. In the transformation to the 10M phase there is no energy barrier on the path and energy decreases with a large negative slope. Initially, these transformations are driven by a softening of the TA_2 $[\xi\xi0]$ phonon branch corresponding to the shift of (110) planes. Transformation paths to other structures exhibit more or less significant barriers in the beginning of the path, hindering such a transformation from austenite. This finding corresponds to experiment and demonstrates that the kinetics of the transformation is decisive for the selection of the particular low-symmetry structure of martensite.

MM 72.4 Fri 10:15 TC 010

Timedependent effects in martensitic transformations of Ni-Mn-X Heussler alloys with X = Ga, In and Snd — •Peter Entel — University Duisburg-Essen, Lotharstrasse, 47048 Duisburg

Martensitic transformation of rapidly and less rapidly cooled Heusler alloys of type Ni-Mn-X with X = Ga, In, and Sn are investigated by ab initio calculations. For the rapidly cooled alloys, we obtain the magnetocaloric properties near the magnetocaloric transition. For the less rapidly cooled alloys hese magnetocaloric properties start to change considerably. This shows that none of the Heusler alloys is in thermal equilibrium. Instead each alloy tranforms during temper annealing into a dual-phase composite. The two phases are identified to be cubic Ni-Mn-X and tetragonal NiMn.

MM 73: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Friday 10:30–12:45 Location: HL 001

MM 73.1 Fri 10:30 HL 001

Ab initio photoluminescence in 2D materials — •Pedro Melo[1,4], Andrea Marini[2,4], Matthieu Verstraete[1,4], and Zeila Zanolli[3,4] — [1]NanoMat / CESAM, ULiege Belgium — [2]ISM CNR, Italy — [3]RWTH Aachen Germany — [4]ETSF

The theoretical study of photoluminescence (PL) has been hindered in the past due to lack of predictive ab initio numerical techniques [1,2,4]. We present a complete theoretical framework for the computation of PL where electrons, nuclei, and photons are quantised. The intrinsic non-equilibrium nature of the process is fully taken into account [3]. Starting from the Keldysh contour, we arrive at a set of equations for the Green's functions of electrons, phonons, and photons where the different kinds of interactions are treated on the same footing. These equations are then simplified by using the generalised Baym-Kadanoff ansatz and the completed collision approximation [3]. This reduces the problem to a set of decoupled equations for the density matrix that describe all kinds of static and dynamical correlations. We show how the micro-macro connection relates the observable spectrum with the time-dependent microscopic dynamics, via the Bethe-Salpeter equation. Finally, we present the results of our numerical studies on 2D materials, such as WS2, where we relate the evolution of the carrier populations in the Brillouin zone with the changes in the PL spectrum of the material, for a range of experimental setups. [1] M. F. Pereira and K. Henneberger, PRB 58, 2064 (1998). [2] K. Hannewald, et al, PRB 67, 233202 (2003). [3] P. M. M. C. de Melo and A. Marini, PRB 93, 155102 (2016). [4] S. W. Koch, et al, Nat Mat 5, 523 (2006).

MM 73.2 Fri 10:45 HL 001

Strain on molybdenum disulfide sheets with defects from first principles — •Mohammad Bahmani^1, Mahdi Faghihnasiri^2, and Thomas Frauenheim^1 — ^{1}BCCMS, Physics Department, Bremen University, Bremen, Germany — ^{2}Physics Department, Shahrood University of Technology, Shahrood, Iran

Single layer of transition metal dichalcogenides(TMDCs) are under intense investigations since the discovery of unique characteristics of 2D and Vann der Waals layered materials. They are predicted to be the most promising structure for various future nanoscale devices. They have also novel applications in spintronic and optoelectronic. As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which show significant effects on their electrical, optical, vibrational, magnetic, and chemical properties. Besides, mechanical strain has very much influence on the electronic properties of 2D materials, particularly TMDCs. For example, 0.5% biaxial strain force direct band gap in molybdenum disulfide(MoS2) to become indirect since it breaks the crystalline symmetry. Therefore, I study different types of point defects such as single and double sulfur(S), single molybdenum(Mo) vacancies, and removing a Mo with its three upper S neighbors. I also substitute a Mo vacancy with one and two S atoms. Furthermore, as the second aim of this study, I showed the modification of defect states under uniaxial and biaxial compression and tensile strain. For the case of one S vacancy, this moves shallow states into the valance band and importantly breaks the degeneracy of degenerate states.

MM 73.3 Fri 11:00 HL 001

Competion of magnetic interactions and in-field behavior of cycloidal Uranium compound UPtGe. — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Stimulated by recent high-field experiment [1] performed on unique actinide system with cycloidal magnetic structure, UPtGe, I performed a series of calculations aiming to understand the nature of the sequence of magnetic phase transitions caused by the applied magnetic field. The physics of the system is determined by the fine balance of the exchange interaction, magnetic anisotropy, and Dzyaloshinskii-Moriya interaction. This balance of interactions governs, in particular, the in-field behavior of the system. The physical consequences of the variation of the localization of the U 5f electrons is investigated.

[1] A. Miyake, A. Nakamura, Y. Shimura, Y. Honma, D. Li, F. Honda, M. Tokunaga, D. Aoki, doi.org/10.11316/jpsgaiyo.71.1.0_2062.

MM 73.4 Fri 11:15 HL 001

Electron correlation effects in the electronic structure of 4f-atoms adsorbed on metal and Graphene substrates — •Alexander B. Shick^1, Dmitry S. Shapiro^2, and Alexander I. Lichtenstein^3 — ^{1}Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — ^{2}nstitute of Radio Engineering and Electronics, Russian Academy of Sciences, Moscow — ^{3}Institute of Theoretical Physics, University of Hamburg, Germany

Surface supported single magnetic atoms, the so-called "single-atom magnets", open new opportunities in a quest for the ultimate size limit of magnetic information storage. Initially, the research mainly focused on 3d-atoms on surfaces. Recently, the attention was turned to the 4f-atoms, culminating in the experimental discovery of magnetically stable Ho atom on MgO(001) substrate [1], and Dy atom on graphene/Ir(111)[2]. We address the electronic and magnetic character of 4f-atoms on metal and Graphene substrate making use of a combination of the DFT with the exact diagonalization of Anderson impurity model (DFT+ED) [3]. The spin and orbital magnetic moments of Dy@Ir(111) and Dy/Graphene/Ir(111) are evaluated and compared with experimental XMCD data. The magnetic anisotropy energy is estimated, and the magnetic stability is discussed. The role of 5d-4f interorbital exchange polarization in modification of the 4f-shell energy spectrum is emphasized. [1] F. Donati et al., Science 352, 318 (2016). [2] R. Baltic et al., Nano Lett. 16, 7610 (2016). [3] A. B. Shick, D. S. Shapiro, J. Kolorenc, A. I. Lichtenstein, Sci. Rep. 7, 2751 (2017).

MM 73.5 Fri 11:30 HL 001

Interlayer trions in the MoS_2/WS_2 van der Waals heterostructure — •Thorsten Deilmann and Kristian Sommer Thygesen — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Electronic excitations in van der Waals heterostructures can have interlayer or intralayer character depending on the spatial localisation of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally. In contrast, studies of charged trions have so far been limited to the intralayer type.

Here we investigate the complete set of interlayer excitations in a MoS_2/WS_2 heterostructure using a novel ab-initio method, which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of 18/28 meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers.

MM 73.6 Fri 11:45 HL 001

The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining — •Miguel Marques^1 and Antonio Sanna^2 — ^{1}Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — ^{2}Max-Planck Institut für Microstrukture Physics, Weinberg 2, 06120 Halle, Germany

Starting from the experimental data contained in the inorganic crystal structure database, we use a statistical analysis to determine the likelihood that a chemical element A can be replaced by another B in a given structure. This information can be used to construct a matrix where each entry (A,B) is a measure of this likelihood. By ordering the rows and columns of this matrix in order to reduce its bandwidth, we construct a one-dimension ordering of the chemical elements, analogous to the famous Pettifor scale. The new scale shows large similarities with the one of Pettifor, but also striking differences, especially in what comes to the ordering of the non-metals.

MM 73.7 Fri 12:00 HL 001

Novel two-dimensional topological insulators from first principles materials screening — •Thomas Olsen and Kristian Thygesen — Technical University of Denmark

We have applied first principles calculations to find new stable two-dimensional materials with non-trivial band topology. The novel materials include more than 10 quantum spin Hall insulators, quantum anomalous Hall insulators and topological crystalline insulators protected by mirror symmetry. We also discuss the dual topological nature of the band structure in the presence of both time-reversal and mirror symmetry and show that odd mirror Chern numbers always imply a quantum spin Hall effect.

MM 73.8 Fri 12:15 HL 001

Nanoparticles Classification with Self-Organisation Map (SOM) on 3D Electrostatic Potential Surface (EPS) — •Baichuan Sun and Amanda Barnard — Molecular & Materials Modelling, Data61 CSIRO, Door 34 Goods Shed, Village St, Docklands, VIC 3008, Australia

State-of-the-art deep learning (DL) algorithms are having tremendous impact across all scientific fields, and Material Science (MS) is no exception. A combination of computational chemistry simulations and DL techniques requires a hybrid computation/data research workflow, which represents a revolutionary approach to MS studies. There is a gap between the ab initio characterisation of nanomaterials with electronic structure simulations and its analytics with DL frameworks which stems from difficulties in representing quantum mechanical properties in such a way that is suitable for artificial neural networks. To overcome this issue we are evaluating the efficiency of visualising the 3-D Electrostatic Potential Surface (EPS) with Self-organising Maps (SOM), and integrating them directly into reliable DL frameworks. A Self-organisation Map classifies high-dimensional data into low-dimensional (normally 2D) space without supervision, while retaining the intrinsic topological relationship of the data set. As we will show, it is possible to represent a 3D molecular EPS with a single 2D snapshot, or "fingerprint" of the particle, provided they are orientationally invariant. In this study we demonstrate how Ag nanoparticles 3-D EPS self-organising texture maps can be used to classify nanoparticles based on the energy of the Fermi level.

MM 73.9 Fri 12:30 HL 001

Regulation of structure and high thermoelectric performance of 1D SnTe via encapsulation within single-walled carbon nanotube — Andrij Vasylenko[1], •Jamie Wynn[2], Sam Marks[1], Paulo V. C. Medeiros[3], Quentin M. Ramasse[4], Andrew J. Morris[4], Jeremy Sloan[1], and David Quigley[1] — [1]University of Warwick, Coventry, UK — [2]University of Cambridge, Cambridge, UK — [3]Daresbury Campus, Darsbury, UK — [4]University of Birmingham, Birmingham, UK

We present the extreme case of nanostructuring, exploiting capillarity of single-walled carbon nanotubes (SWCNTs) for synthesis of the smallest possible thermoelectric SnTe nanowires with cross sections as small as a single atom. By adapting high-throughput ab initio random structure searching, we discover several structures of SnTe that can be formed within SWCNT and compare results with experimentally obtained encapsulated SnTe nanowires. From first principles, we demonstrate that by choosing the appropriate diameter of a template SWCNT, we can manipulate the structure of 1D SnTe and its thermoelectric performance. The demonstrated technique opens a practical route towards nanostructural manipulation of electrical and thermoelectric properties of the 1D materials. The best candidate 1D SnTe structures demonstrate strongly enhanced ZT over a unprecedentedly broad temperature range with a maximum value of 3.25.

MM 74: Structural Materials (Steels, light-weight materials, high-temperature materials)

Structural Materials II

Time: Friday 11:15–12:15 Location: H 0106

MM 74.1 Fri 11:15 H 0106

Structure and Properties of Al Alloys Produced by Friction Stir Processing — •Maximilian Gnedel[1], Amanda Zens[2], Ferdinand Haider[1], and Michael Friedrich Zaeh[2] — [1]Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 2, 86159 Augsburg, Germany — [2]Institute for Machine Tools and Industrial Management, Technical University of Munich, Boltzmannstraße 15, 85748 Garching, Germany

Friction Stir Processing (FSP) can be used to locally modify properties in materials such as aluminum. Furthermore, the composition of the alloy can be changed by this technique. Intermixing specific micrometer-sized metal powders helps to optimize both the microstructural stability during subsequent heat treatment, as well as the mechanical properties in general. This work provides insights into the properties of an AA1050 aluminum matrix with dispersed copper and iron particles added through FSP. The characteristics examined include the grain structure, the microhardness and the formation of intermetallic phases. Suitable processing parameters were found to produce homogenous aluminium samples containing spherical particles with an average diameter of several micrometers. X-Ray computed tomography examination confirmed a consistent distribution in the welding direction. Etching and electron microscopy investigation revealed a unique grain structure and intermetallic layers formed during the process, which yielded a remarkable change in microhardness in comparison to FSPed aluminium without additive particles. Future studies will help to understand the properties of such non-equilibrium alloys.

MM 74.2 Fri 11:30 H 0106

Impact of Microstructure and Geometric Length Scales on Miniaturized Tensile Tests of Advanced Steels — •Jonas Finn Kutschmann[1], Thomas Pretorius[2], Andreas Offergeld[2], Friederike Emeis[1], Niklas Nollmann[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Westfälischen Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster — [2]thyssenkrupp Steel Europe AG, Kaiser-Wilhelm-Straße 100, D-47166 Duisburg

In this work the mechanical properties of advanced steels are characterized by a miniaturized tensile test and compared to the results of other mechanical testing methods. The eleven steel raw materials were provided by thyssenkrupp and the miniaturized specimens were cut with a dog-bone shape contour. For one type of steel the dimensions were severely changed to verify an occurring specimen size effect. The influences of the geometric length scales were investigated by microstructural analysis using EBSD.

The tensile test results were correlated to Vickers hardness measurements, average grain size and thyssenkrupp database values for the ultimate tensile strength. Some steels reproduce the macro-scale results well in miniaturized testing whereas others show a significant drop in the performance. The overall performance of the miniaturized tensile tests were evaluated by the ultimate tensile strength and the fracture strain for one type of steel by varying the geometrical dimensions. The results suggest the inclusion of the standard deviation of the grain size distribution for a more independent evaluation of the specimen size effect.

MM 74.3 Fri 11:45 H 0106

Advanced microstructural characterization of nanoprecipitates in nickel-based superalloys — Robert Lawitzki[1], Salman Ul-Hassan[1], Lukas Karge[2], Julia Wagner[1], Michael Hofmann[2], •Ralph Gilles[2], and Guido Schmitz[1] — [1]Universität Stuttgart, Institut für Materialwissenschaft — [2]TU München, FRMII

Nickel-based superalloys are high performance alloys that can be found in high temperature structural applications like aero and land-based gas turbine engines. Most important for the mechanical properties of these alloys is the presence of nanoprecipitates. The addition of elements like Al, Ti or Nb and a suited heat treatment are the requirement for their controlled precipitation. Finding the optimum heat treatment depends on the solubility of the nanoprecipitates and often requires associated studies by electron microscopy of small samples in the micrometer scale.

In this contribution, we present results of the microstructural characterization of differently heat treated nickel-based superalloys Inconel 718, which were further characterized by small angle neutron scattering (SANS). Information about the morphology - obtained by electron microscopy - and about the composition - obtained by atom probe tomography - of nanoprecipitates, are used as input parameters to simulate the SANS data. The obtained models give information about the volume fraction and size of precipitates in the mm-scale and can be further used for in situ neutron experiments during heat treatment or plastic deformation on bulk samples.

MM 74.4 Fri 12:00 H 0106

Defect Imaging Using the Positron-Microbeam of the CDB Spectrometer at NEPOMUC — •Thomas Gigl, Lukas Beddrich, Marcel Dickmann, Benjamin Rienäcker, Mathias Thalmayr, Sebastian Vohburger, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The Coincidence Doppler Broadening Spectrometer (CDBS) at the positron beam facility NEPOMUC was upgraded with a beam brightness enhancement system in order to enable CDB spectroscopy with improved spatial resolution. The positron is transported in a newly designed μ-metal shielded optically column comprising several electrostatic lenses, magnetic compensation coils, and beam monitors. The new brightness enhancing device is integrated in the electrostatic beam guiding system and basically comprises a beam focusing unit and a Ni(100) foil of 100 nm thickness working as transmission remoderator. For high resolution measurements the positron beam is first focused onto the Ni remoderation foil before it is accelerated up to 25 keV onto the sample. In order to estimate the beam diameter at the sample position spatially resolved DB measurements have been performed. Without remoderator a lateral resolution of 200 μm is obtained. Using the brightness enhancement system the beam spot could be reduced to 33 μm. Benefiting from the improved resolution of the CDBS *upgrade*, defect spectroscopy on various light metal alloys has been performed recently.

MM 75: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data VII

Time: Friday 11:15–12:45 Location: H 0107

Topical Talk MM 75.1 Fri 11:15 H 0107

Higher-dimensional synchrotron-based tomography for nanostructure characterization — •Manuel Guizar-Sicairos — Paul Scherrer Institut, Villigen PSI, Switzerland

High-energy X-rays can probe the nanostructure of a broad range of biological and synthetic materials, based on electron-density heterogeneity. Currently, the high photon flux employed to carry out synchrotron experiments has increased the acquisition speed in measurements and enabled multidimensional characterization of materials. Alongside from direct structure imaging via tomography, scanning small-angle X-ray scattering (sSAXS) can be used to gather statistical information about the local nanostructure, in the range from 1 to 100 nm, on macroscopic samples of a few millimeters in size. Thus, sSAXS is very well suited to study correlation between heterogeneous nanostructure and macroscopic sample characteristics.

After a brief introduction I will describe our efforts towards automatic classification and segmentation of the large volumes of data generated by sSAXS and some of its applications. Furthermore I will discuss the combination of sSAXS with computed tomography, a technique we term small-angle-scattering tensor tomography (SASTT), which allows probing 3D nanostructure anisotropy, within subvolumes (voxels) of a sample. Some emphasis will be given on the measurement and algorithms used for reconstruction of the 6D spatially-resolved reciprocal-space map.

MM 75.2 Fri 11:45 H 0107

40 years of material science at ISOLDE-CERN using TDPAC and MS — •Juliana Schell[1,2], Peter Schaaf[3], Hans-Christian Hofsäss[4], and Doru C. Lupascu[2] — [1]European Organization for Nuclear Research (CERN), Switzerland — [2]University of Duisburg-Essen, Germany — [3]TU Ilmenau, Germany — [4]Georg-August-Universität Göttingen, Germany

Since the late 70ies researchers at ISOLDE-CERN have been applying nuclear techniques to materials science research. A considerable infrastructure has been built up on-site to allow scientists to perform experiments using short-lived isotopes, especially using Time Differential Perturbed Angular Correlations (TDPAC) [1] and Mössbauer Spectroscopy (MS) [2, 3]. The online production of radioactive isotopes with high yield and elemental and isotopic purity allow the choice of the adequate probe to study the relevant solid state problem. In this context, TDPAC and emission MS are very powerful to characterize new materials and particularly atomic defects in them with very small concentrations of nuclear probes. Our facilities at ISOLDE-CERN are the world reference for these measurements. They are dedicated to many different purposes e.g. investigations of semiconductors oxides, photocatalytical materials, multiferroics, superconductors, metals, and alloys. In this presentation, we explore the multiple measurement possibilities.

References [1] J. Schell, P. Schaaf, and D. C. Lupascu, AIP Advances 7, 105017 (2017). [2] J. Schell, P. Schaaf et al. Not yet published. [3] MS Collaboration at ISOLDE-CERN: http://e-ms.web.cern.ch/

MM 75.3 Fri 12:00 H 0107

New Tolerance Factor to Predict Perovskite Oxide and Halide Stability — •Christopher J. Bartel[1], Christopher Sutton[2], Bryan R. Goldsmith[3], Runhai Ouyang[2], Charles B. Musgrave[1], Luca M. Ghiringhelli[2], and Matthias Scheffler[2] — [1]University of Colorado Boulder, Boulder, USA — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]University of Michigan, Ann Arbor, USA

Using the novel data analytics approach sure independence screening and sparsifying operator (SISSO) [1] an accurate one-dimensional tolerance factor (τ) is developed that correctly classifies 92% of compounds as perovskite or nonperovskite for an experimental dataset containing 576 ABX_3 materials. Importantly, τ has nearly a uniform performance across the five anion subsets: oxides (92%), fluorides (92%), chlorides (90%), bromides (93%), iodides (91%). In comparison, the widely used Goldschmidt tolerance factor (t) achieves a maximum accuracy of only 74% for the same set of materials, with a significantly lower accuracy for chlorides (52%), bromides (56%), and iodides (33%) than for oxides (83%) and fluorides (85%).The accuracy of τ combined with its simplicity, a continuous function of only the oxidation state of the A-site cation and Shannon ionic radii, allows for new physical insights into the stability of the perovskite structure and the prediction of more than 1,000 new stable inorganic and hybrid organic-inorganic double perovskite halides. [1] R. Ouyang, et al., arXiv:171003319 (2017).

MM 75.4 Fri 12:15 H 0107

Taming the Configurational Explosion - Statistical Learning for Structure Search — •Lukas Hörmann, Michael Scherbela, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Austria

Monolayers of organic molecules on inorganic substrates often show rich polymorphism with diverse structures in differently shaped unit cells. Determining the different commensurate structures from first principles is far from trivial due to the large number of possible polymorphs. We pursue the SAMPLE approach[1][2], which is based on coarse-graining the potential energy surface and applying Gaussian Process Regression to efficiently find the energy of all polymorphs. To that end, we first determine adsorption geometries of isolated molecules as well as all possible unique substrate supercells. Then we combine each adsorption geometry with every super cell to generate all configurations. For a subset of these configurations, adsorption energies are determined using DFT. This subset serves as training data for the machine learning algorithm, that allows us to predict the adsorption energies for all polymorphs. Finally, all configurations with an adsorption energy below predefined energy threshold are reranked using DFT.

We demonstrate the capability of our approach for Naphtalene on Cu(111). We determine the adsorption energies for a large number of polymorphs and compare the results to the experimentally obtained phase diagram.

[1] Obersteiner, Hörmann, et. al., Nano Lett. 17 (7), pp 4453-4460

[2] Scherbela, Hörmann et. al., arXiv: 1709.05417

MM 75.5 Fri 12:30 H 0107

Machine learning the structure-energy-property landscapes of molecular crystals — •Felix Musil[1], Sandip De[1], Jack Yang[2], Joshua Campbell[2], Graeme Day[2], and Michele Ceriotti[1] — [1]COSMO, EPFL, Lausanne, Switzerland — [2]University of Southampton, Southampton, UK

Molecular crystals play an important role in several field of science and technology. They often crystallize in many different polymorphs with substantially different physical properties. To help prioritize the synthesis of candidate materials, atomic-scale modelling can be used to enumerate the stable polymorphs and to predict their properties, as well as to propose heuristic rules to rationalize the correlations between crystal structure and materials properties.

Here we show how a recently-developed machine-learning (ML) framework [1] can be used to achieve inexpensive and accurate predictions of the stability and properties of polymorphs, and a data-driven classification that is less biased and more flexible than typical heuristic rules. We discuss, as examples, the lattice energy landscapes and the automatic structural classification of pentacene and two azapentacene isomers that are of interest as organic semiconductor materials. We show that we can estimate lattice energies with sub-kJ/mol accuracy, using only a few hundred reference configurations, and provide a more detailed picture of molecular packing than that provided by conventional heuristics.

[1] De, S., Bartok, A. P., Csanyi, G., & Ceriotti, M. (2016). Phys. Chem. Chem. Phys., 18(20), 13754.

MM 76: Methods in Computational Materials Modelling (methodological aspecst, numerics)

Heat Transport

Time: Friday 11:15–12:30 Location: TC 006

MM 76.1 Fri 11:15 TC 006

Non-equilibrium dynamics of quantum heat transport in nanoscale devices — •Leonardo Medrano Sandonas[1,2], Alexander Croy[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1,3,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Dresden Center for Computational Materials Science, Dresden, Germany — [4]Center for Advancing Electronics Dresden, Dresden, Germany

Next to electrons, phonons play a major role for the behavior of nanoscale devices. Additionally, phononics and nano-mechanics offer the possibility to steer and manipulate phonons. Hence, a more detailed understanding of phonon dynamics is required. Using an auxiliary-mode approach, which has successfully been applied for the case of electrons [1], we present a method to describe time-dependent phonon transport based on the time evolution of the phonon density matrix. We compute the phonon density matrix by employing the non-equilibrium Green*s function formalism. This method allows us to gain insight into the behavior of local vibrations which are driven by time-dependent temperature differences between heat reservoirs [2,3]. In the present work, we apply this methodology to study the time dependence of the thermal current in molecular junctions. [1] B. S. Popescu and A. Croy, New J. Phys. 18, 093044, (2016). [2] R. Tuovinen et al., Phys. Rev. B 93, 214301, (2016). [3] Marcone I. Sena-Junior et al., J. Phys. A: Math. Theor. 50, 435202, (2017)

MM 76.2 Fri 11:30 TC 006

Anharmonic Effects in Solids: Putting Third-Order Expansion to the Test — •Florian Knoop, Hagen-Henrik Kowalski, Matthias Scheffler, and Christian Carbogno — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The standard *ab initio* formalism to compute thermal conductivities of solids relies on determining the second and third order force constants of the zero Kelvin potential-energy surface [1]. To understand the role of higher-order contributions not accounted for in such an approach, we investigate the thermal conductivities of a series of materials with increasing anharmonicity (e. g. Si, Ga_2O_3, CsCl, ZrO_2) using two advanced methodologies: Temperature-dependent effective potentials, in which higher-order anharmonicity is incorporated by a renormalization of lower-order force constants via statistical finite-temperature sampling [2] and the *ab initio* Green-Kubo formalism, in which all anharmonic effects are assessed non-perturbatively through *ab initio* molecular dynamics simulations [3]. We describe the computational challenges, e. g., finite time and size effects and the choice of the exchange-correlation functional. Eventually, we discuss how the obtained quantitative thermal conductivities allow for a qualitative understanding of high-order anharmonic nuclear dynamics and the implications for other vibrational properties of real materials.
[1] D. A. Broido, *et al.*, *Appl. Phys. Lett.* **91**, 231922 (2007).
[2] O. Hellman and I. A. Abrikosov, *Phys. Rev. B* **88**, 144301 (2013).
[3] C. Carbogno, R. Ramprasad, and M. Scheffler, *Phys. Rev. Lett.* **118**, 175901 (2017).

MM 76.3 Fri 11:45 TC 006

Generalized Langevin Thermostats for Tuning Dynamical Properties in Quantum Dynamics — •Mariana Rossi[1], Venkat Kapil[2], and Michele Ceriotti[2] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]EPFL, Switzerland

Generalized Langevin Equation (GLE) thermostats have been used very effectively as a tool to manipulate and optimize the sampling of thermodynamic ensembles and the associated static properties. Here [1] we show that a similar, exquisite level of control can be achieved for the dynamical properties computed from thermostatted trajectories. By developing quantitative measures of the disturbance induced by the GLE to the Hamiltonian dynamics of a harmonic oscillator, we show that these analytical results accurately predict the behavior of strongly anharmonic systems.We address the use of thermostats in the context of approximate path-integral-based models of quantum nuclear dynamics, demonstrating that a custom-tailored GLE can alleviate some of the artifacts associated with these techniques, improving the quality of results for the modelling of vibrational dynamics of molecules, liquids and solids. Finally we show the power of this technique by showing the importance of nuclear quantum effects in the close to full suppression of NH stretch signals in porphyrin derivatives.
[1] M. Rossi, V. Kapil, M. Ceriotti, JCP **148**, 102301 (2018)

MM 76.4 Fri 12:00 TC 006

Molecular Dynamics Simulation of Periodic Nanostructuring of Au due to UV Laser Pulse under Water Layer on the Experimental Scale — •Dmitry Ivanov[1,2], Andreas Blumenstein[2,3], Baerbel Rethfeld[2], Juergen Ihlemman[3], Peter Simon[3], and Martin Garcia[1] — [1]Physics Department, University of Kassel, 34132 Kassel, Germany — [2]Physics Department, Technical University of Kaiserslautern and OPTIMAS Research Centre, 67663 Kaiserslautern, Germany — [3]Laser-Laboratorium Göttingen e.V., 37033 Göttingen, Germany

The physical mechanism of materials surface restructuring involves a lot of fast, non-equilibrium, and interrelated processes while the solid is in a transient state. While the experimental investigation of the material restructuring mechanism can be limited to post-priory observations, the theoretical methods, working within a single computational approach with corresponding spatial and temporal scales, cannot address all physical aspects of the nanostructuring process. In this work we propose a combined atomistic-continuum approach suitable for the investigation of periodic nanostructuring mechanism due to a UV ultrashort laser pulse on the experimental scale. The combined model is applied to investigate the nanostructuring mechanism under conditions of vacuum ambient and in the regime of spatial confinement due to a thick water layer above the target. The obtained results, generated on the same temporal and spatial scales as they are in the experiment, allowed to extract the main mechanisms of nanostructuring process and the reasons for a higher quality of structures generated under water.

MM 76.5 Fri 12:15 TC 006

Resistor network simulation method for graphene-based conductive fibers — •Leo Rizzi[1,4], Andreas Zienert[2], Jörg Schuster[3], and Martin Köhne[4] — [1]Faculty of Electrical Engineering and Information Technology, Technische Universität Chemnitz, Chemnitz, Germany — [2]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [4]Robert Bosch GmbH, Stuttgart, Germany

In recent years, graphene fibers (GFs) have emerged as a new form of electrical conductors. They consist of an assembly of graphene sheets spun into a textile fiber. GFs are lightweight, mechanically strong, and corrosion resistant. Defect-engineering and doping strategies have continuously improved the electrical conductivity of fibers towards metallic levels. However, it still remains below the conductivities of silver or copper.

While several groups have presented experimental results on the production of GFs, theoretical descriptions predicting their electrical behavior are less advanced. We present a simulative approach to model the electrical conductivity of GFs, based on a three-dimensional random network of resistors. We investigate the influence of the raw material's properties on the fiber electrical conductivity and identify the main influence parameters. Our results offer a deeper understanding of GFs and can be helpful to further enhance their electrical performance.