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.

References [1] T. Sourmail, Prog. Mater. Sci. 50, 816 (2005).

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.

[1] K. Trepte et al., PCCP, vol. 17, pp. 17122-17129, 2015
[2] S. Schwalbe et al., PCCP, vol. 18, pp. 8075-8080, 2016
[3] K. Trepte et al., PCCP, vol. 19, pp. 10020-10027, 2017

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.

[1] I. Mirebeau and G. Parette, Phys. Rev. B 82, 104203 (2010).

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_3Al 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_3Al 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 $E\omega > E\alpha' > E\alpha'' > E\beta$ 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 $E\beta$ 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 $0.35 J/m^2$. 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 $C_xSi_yGe_{1-x-y}$ 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.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26** (2014) 363202
[2] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184** 1861 (2013)

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 $Al_xNa_{1-x}/Al(100)$, to highly complex structures, as e.g. the thermoelectric clathrates $Ba_8Al_xSi_{46-x}$ [2] and $Ba_8Ni_xGe_{46-x-y}\square_y$ 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.
[2] M. Troppenz, S. Rigamonti, and C. Draxl, *Chem. Mater.* **29**, 2414 (2017).

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 appli-

cation 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 antiferro-

magnetic 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 Bepi-Colombo 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.

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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.

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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 non-destructive - used to recover the erased markings in metals or poly-

mers: 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).