MM 34: Poster session II

Time: Tuesday 18:30–20:30 Location: P4

MM 34.1 Tue 18:30 P4

The DFT (TB-mBJ) calculation of structural, electronic, elastic and vibrational properties of Mg2X(X=Si,Sn)

— •MARFOUA Brahim[1], LIDJICI Hamza[1,3], and LAGHOUN Brahim[2] — [1]Laboratoire étude et développement des matériaux semi-conducteurs et diélectriques, Université de Laghouat, Route de Ghardaïa B.P.37G. Laghouat. Algérie. — [2]Laboratoire de physique des matériaux, Université de Laghouat, Route de Ghardaia B.P.73G. Laghouat. Algérie. — [3]Laboratoire des Matériaux et Procédés, Université de Valenciennes et du Hainaut-Cambrésis, Z.I du Champ de Abbesse 59600 Maubeuge, France

The semiconductors with the formula Mg2X (X= Si and Sn), have attract attention as potential high-performance thermoelectric materials, and their electonic, vibrational and thermal properties have extensively investigated [1-4]. They are an indirect band gap semiconductor [5-6]. We carried in this work an ab initio study based on the density functional theory to calculate structural, electronic, elastic and vibrational properties of Mg2X(X=Si and Sn). The FP-LAPW method was used with different form of exchange-correlation potential (LDA, GGA, PBEsol and mbj). TB-mBJ give the best result for the lattice parameter, and the best estimation of the band gap energy. Our results are in good agreement with experiment data available and other theoretical results.

MM 34.2 Tue 18:30 P4

Synthesis and analysis of electrodeposited Ni-P nanoglass

— Farnaz Abdollahzadeh Davani, Stefan Ostendorp, •Martin Peterlechner, Daniel Gaertner, Sergiy Divinskiy, and Gerhard Wilde — Institute of Materials Physics, Universität Münster, Münster, Germany

Nanoglasses, i.e. glassy materials characterized by two different nanoscaled glassy structures have recently been discovered. As yet, their structure, dynamics and stability are a matter of controversy. In the present work, electrodeposited amorphous Ni-P thin films with a granular sub-structure were chosen as a model system and layered granular structures were grown by applying pulsed voltages. Due to the relatively simple synthesis route and cheap costs the system is an excellent candidate for future studies on the nanoglasses. Using transmission electron microscopy and energy-dispersive X-ray spectroscopy it is shown that phosphorous-rich layers are fully amorphous. The glass transition was investigated by means of differential-and fast-scanning calorimetries. The bimodal structure and the broad glass transition signal are indications that the pulse-deposited Ni-P thin film is a nanoglass, according to the definition given in the literature. Thus, multilayerd nanocrystalline-nanoglassy systems can be prepared by pulsed electrodeposition and subsequent aging. The results are discussed with respect to the structure and stability of Ni-P nanoglass.

MM 34.3 Tue 18:30 P4

Nucleation Kinetics of deeply undercooled Germanium melts

— •Manoel da Silva Pinto, Christian Simon, and Gerhard Wilde — Institut für Materialphysik - Wilhelm-Klemm Straße 10, 48149 Münster

In the classical nucleation theory the initial event of solidification is the stochastically formed metastable nuclei in the melt, which turn to be stable after exceeding the critical energy barrier. The statistical nature can be observed by the measurement of melting and solidification temperatures upon thermal cycling. By treating nucleation events as an inhomogeneous Poisson process, it is possible to estimate the nucleation rates from the undercooling values. Even an estimation of the interfacial energy applying classical nucleation theory is possible. The present work studies the nucleation of liquid germanium and estimates the nucleation rate and interface energy. We use differential thermal analysis to obtain sufficient big and accurate data sets. To avoid external nucleants and expel possible metal oxides from the sample, an inorganic glass is used as a fluxing agent and embedding medium.* A large undercooling is observed in pure germanium. The Gibbs free energy and the kinetic prefactor suggest a nucleation of heterogeneous nature. The geometric factor can be estimated and compared to the suggested value for this lattice system.

MM 34.4 Tue 18:30 P4

Friction under active control

— •Victor Pfahl[1], Walter Arnold[2], and Konrad Samwer[1] — [1]1. Physikalisches Institut, Universität Göttingen — [2]Department of Materials and Materials Technology, Saarland University

Dissipation of mechanical and kinetic energy at a sliding contact strongly depends on the topological structure and chemistry of the contact and on the dissipation mechanism of the underlying material. Instead of varying these mechanisms we are using external acoustic excitations and/or temperature variation to control friction actively.

Friction is measured with the lateral force microscopy (LFM) mode of an atomic force acoustic microscope (AFAM) and by studying microsliding in AFAM mode using acoustic excitation of the contact resonance frequency.

We investigated the reduction of friction of Si, amorphous PdCuSi and LaSrMnO as a function of amplitude of the cantilever at different temperatures. We can report a reduction of friction up to 100% on every system.

Due to a metal-metal transition near 350K temperature dependent measurements on LaSrMnO are interesting. The damping of the cantilever oscillations caused by micro-sliding of the cantilever tip on the surface decreases with temperature parallel to the increase in resistivity of the thin film. The behavior of the cantilever damping constant demonstrates that there is a direct coupling between mechanical friction and mobility of the electrons in the LSMO film.

We would like to thank the DFG for funding CRC 1073 Project A1.

MM 34.5 Tue 18:30 P4

Finite size corrections for periodic coupled cluster theory

— Ke Liao[1] and •Andreas Grüneis[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department Chemie, Technische Universität München (TUM) Lichtenbergstrasse 4, D-85747 Garching, Germany

We present a method to correct for finite size errors in periodic coupled cluster theory calculations of solids. The newly developed method shares similarities with electronic structure factor interpolation methods used in quantum Monte Carlo calculations [1]. However, in the case of coupled cluster theory no explicit calculation of density matrices is needed [2]. We discuss the asymptotic behaviour of the correlation energy with respect to the total number of k-points used to sample the first Brillouin zone. Furthermore we present results showing that chemical accuracy in the convergence of coupled cluster correlation energies per atom can be achieved using two atomic unit cells and 3 x 3 x 3 k-point meshes only.

[1] M. Holzmann, R. C. Clay, M. A. Morales, N. M. Tubmann, D. M. Ceperley, and C. Pierleoni, Phys. Rev. B 94, 035126 (2016).

[2] K. Liao, and A. Grüneis, J. Chem. Phys. 145, 141102 (2016).

MM 34.6 Tue 18:30 P4

The Mg(111)/H_2O interface studied by empirical potentials and density functional theory using automated tools

— •Sudarsan Surendralal, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

Modern supercomputers have made efficient electronic structure and atomistic simulation methods commonplace. Integrated computational materials design involves the combination of computational data associated with different length and/or time scales to aid materials discovery and the understanding of materials properties. However, the combination of different methods is often tedious in practice, since input and output of the employed methods have usually different formats. Our in-house python based computational materials library PyIron, handles this problem with the use of a database backend and the hierarchical HDF5 data storage format, which provides a user friendly interface to popular simulation packages. The capabilities of PyIron will be demonstrated using the Mg(111)/water interface, which is of interest for electrochemical applications. Water structures obtained by molecular dynamic simulations performed using an empirical TIP3P potential are easily integrated to provide a good starting configuration for the water structure used within the ab-initio calculations of the Mg(111)/H_2O interface. The then computed electronic structure provides insight into bonding and interactions at the metal water interface.

MM 34.7 Tue 18:30 P4

Spatially resolved in-situ defect spectroscopy with a positron beam during tensile tests — •Matthias Thalmayr, Thomas Gigl, Marcel Dickmann, Benjamin Rienäcker, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The positron beam facility NEPOMUC at the Research Neutron Source FRM II provides the worlds most intense mono-energetic positron beam with an intensity of 10^9 moderated positrons per second. The CDB spectrometer at NEPOMUC enables depth dependent and spatially resolved defect studies by using Doppler broadening spectroscopy (DBS), and measurements with coincident DBS. Among the numerous techniques applied for characterizing solids, (C)DBS is nondestructive and has an outstanding sensitivity on open volume defects like vacancies, dislocations and nano-voids. A novel device is presented that enables both, in-situ tensile tests and simultaneously spatially resolved high resolution defect spectroscopy of the specimen in the sample chamber of the upgraded CDB spectrometer. While recording the stress-strain curve of the specimen being deformed during conventional tensile tests, the changes of the lattice and in particular the formation of lattice defects and the increase of the defect concentration can be studied by analyzing the observables of the electron-positron annihilation process. With the new setup it will be possible to image the distribution of lattice defects at the annihilation site with an anticipated resolution in the micrometer range.

MM 34.8 Tue 18:30 P4

Comparing interatomic potentials for Si and Mo — •Yury Lysogorskiy, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Interatomic interaction potentials are widely used in computational materials science for simulations at the atomistic level. Nowadays a large number of interatomic potentials is available for a wide range of chemical elements and their mixtures [1,2]. We compare the most prominent interatomic potentials that are available for two prototypical elements, Si and Mo, with respect to predictions from density functional theory calculations. The comparison of the potentials is done at two levels. First, a number of properties of the potentials are evaluated. This includes the cohesive energy, atomic volume, elastic coefficients, vibrational properties, thermodynamic potentials, and defect formation energies for relevant crystal structures. From this a fingerprint characterisitic of the performance of the potential is derived. Second, the data is used to qualify a given potential for situations that were not explicitly tested at the first step, i.e. to assess the transferabilty and predictive capability of a potential. We illustrate the very different behaviour of the potentials and relate this to the functional form of the potential as well as the purpose for which the potential was originally fitted.

[1] E. B. Tadmor, R. S. Elliott, J. P. Sethna et al. Knowledgebase of Interatomic Models (KIM). https://openkim.org, 2011

[2] C.A. Becker, et al. Curr. Opin. Solid State Mater. Sci., 17, 277-283 (2013).http://www.ctcms.nist.gov/potentials

MM 34.9 Tue 18:30 P4

Ab initio study of planar defects in Ni and Co based superalloys — •Aparna P. A. Subramanyam, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr University-Bochum, Bochum, Germany

Single-crystal Ni-based and Co-based superalloys are used in high temperature applications in land-based turbines and jet engines. These alloys exhibit resistance to deformation at high temperatures due to precipitates of $L1_2$-Ni_3Al type. One important deformation mechanism of plastic deformation is dislocation shearing of the precipitates by the formation of planar defects.

In this study, we investigate the structural stability of superlattice intrinsic and extrinsic stacking faults (SISF, SESF), anti-phase boundaries and complex stacking faults in the $L1_2$ phase of Ni_3Al and $(Co/Ni)_3Al$ using density functional theory calculations. The segregation of alloying elements to the stacking faults is analysed for the technologically important alloying elements Re, W and Cr. These results are compared to the segregation to twin boundaries in Ni_3Al and $Co_3(Al/W)$.

MM 34.10 Tue 18:30 P4

Effect of Al alloying on the martensitic temperature in Ti-Ta shape memory alloys — •Alberto Ferrari, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44780 Bochum, Germany

Ti-Ta-based alloys are promising candidates as high temperature shape memory alloys (HTSMAs) for actuators and superelastic applications. The shape memory mechanism involves a martensitic transformation between the low-temperature α'' phase (orthorhombic) and the high-temperature β phase (body-centered cubic). In order to prevent the degradation of the shape memory effect, Ti-Ta needs to be alloyed with further elements. However, this often reduces the martensitic temperature M_s, which is usually strongly composition dependent. The aim of this work is to analyze how the addition of a third element to Ti-Ta alloys affects M_s by means of electronic structure calculations. In particular, it will be investigated how alloying Al to Ti-Ta alters the relative stability of the α'' and β phases. This understanding will help to identify new alloy compositions featuring both a stable shape memory effect and elevated transformation temperatures.

MM 34.11 Tue 18:30 P4

Deformation Mechanisms in Magnetron Sputtered Thin Film Metallic Glasses — •Marlene Mühlbacher[1], Christoph Gammer[2], Ruth Konetschnik[1], Thomas Schöberl[2], Christian Mitterer[1], and Jürgen Eckert[1,2] — [1]Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [2]Erich Schmid Institute for Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, 8700 Leoben, Austria

Amorphous metallic coatings have recently emerged as promising thin film materials due to their excellent chemical stability, good wear resistance and exceptionally high strength. Their mechanical behavior, however, is fundamentally different from their crystalline counterparts, due to the disordered structure lacking dislocations as carriers of plastic deformation. To investigate the different deformation mechanisms, we have synthesized Pd-based crystalline/amorphous multilayer systems by unbalanced dc magnetron sputtering. Hardness and Young's modulus of the multilayer systems are assessed by nanoindentation. Indents are evaluated by atomic force microscopy and scanning electron microscopy for a quick estimation of the coatings' response to plastic deformation. Micromechanical samples of selected systems are prepared in a focused ion beam instrument. Deformation mechanisms and their dependence on layer arrangement are then investigated with a particular emphasis on in-situ tensile testing and bending in the electron microscope. This approach allows for a direct comparison of plastic deformation through the movement of dislocations and shear bands in the crystalline and glassy layers, respectively.

MM 34.12 Tue 18:30 P4

Ab initio investigation of Re-Re interactions in Ni-base superalloys — •Maximilian Grabowski, Jutta Rogal, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Deutschland

Ni-base superalloys are widely used in high-temperature applications e.g. in turbine blades for jet engines of aeroplanes. In these applications, the materials have to perform at high temperature and high stress. Ni-base superalloys have a complex composition where one of the key ingredients is Re, which significantly improves the mechanical behaviour.

Using density functional theory (DFT) calculations we investigate the Re-Re interaction in Ni with a particular focus on the role of magnetism. The nearest neighbour Re-Re interaction in the nonmagnetic and in the ferromagnetic configuration exhibit a qualitatively different behaviour from strongly repulsive to weakly attractive. We show that this is mainly due to a decrease of the Ni magnetic moment in the vicinity of Re and discuss possible consquences for the clustering of Re in Ni-based superalloys. In a next step we investigate the mobility of Re in Ni in concentrated Ni-Re alloys. As a basis for our dynamical simulations, we use a cluster expansion (CE) to evaluate the energies of the binary Ni-Re and the ternary Ni-Re-Vacancy system. DFT calculations are used to determine the effective cluster interactions (ECI) for the CE. We will also report on our progress of a CE for the diffusion barriers, which -when converged- enables us to predict diffusion in concentrated Ni-Re alloys from first-principles calculations.

MM 34.13 Tue 18:30 P4

Implementation of nonlocal van der Waals functionals into the LAPW method — •Fabien Tran, Julia Stelzl, and Peter Blaha — Vienna University of Technology, Institute of Materials Chemistry, A-1060 Vienna, Austria

The so-called van der Waals density functionals (vdW-DF) [1], which are much more reliable than the traditional semilocal functionals for systems where the dispersion forces play a major role, are nonlocal in the sense that they consist of a double integration over the space. Therefore, the implementation of vdW-DF is much more involved and the computational time is higher compared to semilocal functionals. For plane-wave pseudopotential methods, an efficient algorithm proposed by Román-Pérez and Soler [2] based on fast Fourier transform was proposed, such that the vdW-DF are nowadays widely used in the pseudopotential community. However, for all-electron densities, the scheme of Román-Pérez and Soler can not be applied efficiently, since a plane-wave expansion of the all-electron density would require an extremely huge number of terms. In this work, a smoothing procedure of the all-electron density in a region around the nucleus is applied, such that the scheme of Román-Pérez and Soler can be applied efficiently. This is done in the framework of the all-electron linearized augmented plane-wave (LAPW) basis set as embodied in the WIEN2k code. The obtained results are compared with results from the literature.
[1] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).
[2] G. Román-Pérez and J. M. Soler, Phys. Rev. Lett. **103**, 096102 (2009).

MM 34.14 Tue 18:30 P4

Impact of magnetism on the stability of Laves phases in Fe-Nb alloys — •Ali Zendegani[1], Alvin N. Ladines[2], Thomas Hammerschmidt[2], Ralf Drautz[2], Fritz Körmann[1], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

Ferritic steels containing Fe-Nb Laves phases have a number of industrially relevant high-temperature applications, e.g., for automotive industry. The Laves phases play a decisive role for the high-temperature strength of these materials. To tailor their mechanical characteristics, e.g., via heat treatments, a precise knowledge of the Laves phase thermodynamic stability is essential.

We have investigated the phase stability of the three different Laves phases in Fe-Nb alloys, i.e. hexagonal C14 and C36, and cubic C15, combining density functional theory and thermodynamic concepts. The ground state energy as well as finite temperature entropy contributions of these structures are evaluated for various magnetic configurations, ranging from non-magnetic simulations over selected ferro/ferrimagnetic ones to fully paramagnetic calculations. We discuss the challenges and methodological advances developed for such computations.

MM 34.15 Tue 18:30 P4

Properties of mechanically intermixed Cu-Ta alloys — •Regina Post, Nazar Ibrahim, Sergiy Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Germany

Copper and tantalum are known to be fully immiscible and do not form an alloy by cooling from the liquid state. They can however be forced to mix by severe plastic deformation methods, such as high pressure torsion (HPT). Using HPT on a stack of alternating Cu and Ta thin foils, different mixing states can be created.

The present study is focused on the evolution of the microstructure with increasing number of revolutions of the HPT process by comparison of the cross section and plain view structures via orientation imaging microscopy applying the EBSD analysis. The microstructure of copper-rich grains is found to be remarkably stable even after annealing at high temperatures of about 95% of the copper melting point. The appearance of the Cu-Ta solid solution is investigated by TEM analyses and the results are discussed in terms of the mixing mechanism.

MM 34.16 Tue 18:30 P4

Quantitative High-resolution TEM Imaging of Perovskite Interfaces — •Tobias Meyer[1], Patrick Peretzki[1], Benedikt Ifland[2], Birte Kressdorf[2], Christian Jooss[2], and Michael Seibt[1] — [1]IV. Physical Institute, University of Göttingen, Germany — [2]Institute for Materials Science, University of Göttingen, Germany

The Shockley-Queisser limit for single junction solar cell efficiencies is based on energy losses due to the transmission of low energy photons with energies below the band gap and the thermalization of hot charge carriers. In strongly correlated perovskite materials, which exhibit polaronic charge carriers, these losses can be reduced at the same time by harvesting long-living intraband excitations. Indeed, during the last decade the efficiency of halide perovskite based solar cells has been increased from 2 % to 20 %. However, the underlying materials are relatively instable – particularly under light illumination. In contrast to halide perovskites, transition-metal oxides are rather stable but their junctions exhibit lower photovoltaic energy conversion efficiencies. Since the electrical transport properties of these materials are highly dependent on the structure, a thorough understanding of the latter close to the interface is exceedingly desirable in order to tune perovskite junctions for photovoltaic applications. We investigated the structure of transition-metal oxide heterojunctions, i.e. the oxygen positions, in an image corrected high-resolution TEM. In order to enhance the contrast of the light oxygen columns, we used optimized conditions for the spherical aberration.

MM 34.17 Tue 18:30 P4

In-situ Electron Microscopy Studies of Electric Field Assisted Sintering of Oxide Ceramics — •Danny Schwarzbach, Max Steinbrück, and Cynthia A. Volkert — Institut für Materialphysik, Georg-August-Universität Göttingen

A wide range of studies show a dramatic effect of applied electric fields or currents on the sintering behavior of oxide ceramic powders. However, the mechanisms accounting for these strong effects remain elusive despite the wide application potential.

By using in-situ scanning and transmission electron microscopy, material changes during sintering of model oxide ceramics (e.g. ZnO) will be directly observed. The evolution of microstructure and morphology, including grain/void morphology, segregation, and precipitation, will be tracked, both with and without applied fields and currents. The results will be compared to models to determine the dominant driving forces and mechanisms for sintering, and how these are affected by fields and currents. In addition, in-situ high resolution and electron holography studies, EELS, and in-situ studies under oxidizing and reducing atmospheres will be used to gain insight into the atomic origins of sintering behavior, as well as of high conductivity states that occur in conjunction with flash events during field-assisted sintering.

Due to the fact that this project has just started, the focus of this poster is to present the above-mentioned methods and to provide an overview of the current state of research. Nevertheless, some initial results are already expected.

Support of SPP 1959 by the DFG is gratefully acknowledged.

MM 34.18 Tue 18:30 P4

Mechanical Analysis of Metallic Glasses in the Non-Linear Regime — •Clemens Garve, Birte Riechers, and Konrad Samwer — Georg-August-Universität Göttingen

Amorphous metals are used in various applications, however the strongly temperature dependent viscoelastic behavior under deformation is not fully explained yet. To gain more understanding we deform a Palladium-based metallic glass using oscillatory stresses with amplitudes sufficiently high to drive the system beyond the Hookian regime of linear response.

Following experimental approaches used in dielectric spectroscopy [1] an oscillating mechanical stress was applied, which was switched from a low to high stress amplitude and back using a dynamical mechanical analyzer. By using Fourier analysis, we were able to separate our data into nonlinear contributions at fundamental and higher harmonic frequencies. While deforming with high stresses and in the following low stress section, the nonlinear contributions show time-dependent behavior, which was characterized to extract the time-scale of structural recovery [2]. The temperature and stress dependence of nonlinear contributions regarding amplitude and timescale were investigated.

We acknowledge support by DFG Research Unit FOR1394.

Citations: [1] Huang and Richert. "Dynamics of glass-forming liquids..." J. Phys. Chem. 124.16 (2006) [2] Riechers, Samwer, and Richert. "Structural recovery in plastic crystals by time-resolved nonlinear dielectric spectroscopy." J. Phys. Chem. 142.15 (2015)

MM 34.19 Tue 18:30 P4

system identification for nanodevices based on anodic alumina oxide (AAO) templates — •Jesus Alan Calderon Chavarri[1], Min Zhou[2], and Yong Lei[3] — [1]TU Ilmenau, Ilmenau, Germany — [2]TU Ilmenau, Ilmenau, Germany — [3]TU Ilmenau, Ilmenau, Germany

Nanodevices based on AAO templates (like nanotubes, nanorods, and nanowires) have interesting properties which can be described by a mathematical analysis in order to propose mathematical modelings based on linear behavior. In this scenery, it can be demonstrated mathematically, some of their characteristics which are controllability and stabillity. Therefore, as it is shown in this work, it is proposed correlations among characteristics of nanodevices based on AAO templates with mathematical operations to identify physical properties of them through linear range of work. Furthermore, it can be tested different System Identification methodologies in order to get physical parameters, or to identify response of these nanodevices in front of input excitation signals. As a consequence, it is possible to design different algorithms to get optimization and predictions of physical properties, because of this system identification based on correlations proposed.

MM 34.20 Tue 18:30 P4

Mechanically tuned stress state of palladium thin films on rutile titanium dioxide — •Maximilian Litschauer[1], Marian David Bongers[1], Daniel Harding[2], Alec Wodtke[2], and Astrid Pundt[1] — [1]Institut für Materialphysik, Univ. Göttingen — [2]Institut für Physikalische Chemie, Univ. Göttingen

The mechanical stress state of epitaxially grown palladium (Pd) thin films on Al_2O_3 single crystals can be varied by the film thickness [1]. This stress state may also affect the surface conditions, for example by modifying the distance between the Pd surface atoms. This should result in a modified surface reactivity as suggested for example by the d-band model of Mavrikakis et al. [2]. In this study the stress states of differently prepared Pd films on titanium dioxide (TiO_2) is presented and the binding energies (BE) of carbon monoxide (CO) on these surfaces is determined. Therefore, the deposition temperature and film thickness of Pd thin films are varied. The films are deposited by magnetron sputtering on pretreated TiO_2(110) substrates. The stress state is characterized by X-ray diffraction via the Pd(111) peak shift. The related BE are addressed by using a novel ion imaging technique to directly measure the microsecond lifetime of CO on the surface [3]. The results are discussed with respect to the mechanical stress states.

This study is supported by the Deutsche Forschungsgemeinschaft via SFB1073, project C06 and C04 as well via the Heisenberg grant PU131/9-2. [1] S. Wagner et al., Acta Materialia 114 (2016) 116; [2] M. Mavrikakiset al., Phys. Rev. Lett. 81 (1998) 2819; [3] D. J. Harding et al., J. Phys. Chem. A 119 (2015) 12255

MM 34.21 Tue 18:30 P4

AiiDA Workflows with FLEUR for X-ray Photoelectron Spectroscopy — •Jens Bröder[1,2], Gregor Michalicek[1], Daniel Wortmann[1], Rudi Koslowski[2], Christian Linsmeier[2], and Stefan Blügel[1] — [1]Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Energie- und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We present the plug-in of the all-electron DFT code FLEUR [1] to AiiDA [2] (Automated interactive Infrastructure and database for material science) and our first established workflows to calculate electron binding energies and core level shifts (CLS) of X-ray photoelectron spectroscopy (XPS) of pure materials for surface science.

One workflow calculates CLS in the initial state approximation of bulk and slab geometries. Another workflow uses super cell core-hole calculations to extract binding energies. Their first application will be on materials relevant for research on plasma wall interaction in fusion. First results of different methods are compared to recent experimental data.

We acknowledge partial support from the EU Centre of Excellence "MaX Materials Design at the Exascale" (Grant No. 676598).

[1] www.flapw.de
[2] G. Pizzi, et al. Comp. Mat. Sci. 111, 218-230 (2016)

MM 34.22 Tue 18:30 P4

Lateral H-Diffusion in Mg thin films — •Niklas Teichmann, Magnus Hamm, and Astrid Pundt — Univ. Göttingen, IMP, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Hydrogen in metals like Magnesium changes the physical properties of the host material, such as the optical properties.[1] The optical light transmission can be used to determine locally the Hydrogen content, or to differentiate between phases (Hydrogenography).[2] For the Mg-H system, two phases are relevant at 300 K: the metallic α-phase and the transparent MgH_2-phase.

In this presentation, the hydrogen-induced optical change of thin Mg-films is investigated using electrochemical loading via a Pd-gate.[3] By this, the lateral diffusion and the MgH_2 formation can be directly seen and the formation kinetics can be studied. The influence of grain boundaries is discussed.

Financial support by the DFG via projects PU131/9-2 and PU131/10-2 is gratefully acknowledged.

[1] T. Richardson et al. Applied Physics Letters 78.20 (2001): 3047-3049.
[2] R. Gremaud et al. Advanced Materials 19.19 (2007): 2813-2817.
[3] J. Kürschner et al. Journal of Alloys and Compounds 593 (2014): 87-92.

MM 34.23 Tue 18:30 P4

Computional study of Y NMR shielding in intermetallic yttrium compounds — •Leila Kalantari and Peter Blaha — Institute of Material Chemistry, Vienna University of Technology, Getreidemarke 9/165-TC, A-1060 Vienna, Austra

Density functional theory calculations of the magnetic shielding for solid state nuclear magnetic resonance (NMR) provide an important contribution for the understanding of the experimentally observed signals. In this work, we present calculation of the Y NMR shielding in intermetallic compounds. (YM, YMX, YM_2X, YM_2X_2, Y_2MB_6 and Y_2MSi_3 where M represents various transition metals and X refers to Si, Ge, Sn). The total shift σ of this selection varies by about 2500 ppm and correlates very well with the experimentally observed shielding except for YMg and YZn. These two simple compounds have a spike in the DOS at E_F and a corresponding huge spin susceptibility which lead to the disagreement. The diamagnetic contribution σ_o (chemical shift) is by no means constant as often assumed when interpreting experimental metallic shifts and varies up to 1700 ppm, but still the dominating term is the spin contact term σ_c. Although all compounds are metals, only half of them have a paramagnetic (negative) σ_c due to reoccupation of the valence Y-5s electrons, while for others the induced Y-4d magnetic moment induces diamagnetic core contributions. In all our cases the spin dipolar contribution σ_{sd} is fairly small and $|\sigma_{sd}|$ is less than 200 ppm and often even much smaller except in a few very asymmetric compounds like Y_2ReB_6 ($\sigma_{sd} \approx 450 ppm$)

MM 34.24 Tue 18:30 P4

AUXILIARY-MODE APPROACH TO TIME-DEPENDENT PHONON TRANSPORT — •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, we present a method to describe time-dependent phonon transport based on the time-dependent Green's function formalism. This allows us to study local vibrations which are driven by time-dependent temperature differences between heat reservoirs.

MM 34.25 Tue 18:30 P4

Effects of surface diffusion and surface roughness on plastic behavior of nanoporous gold — •Jie Li[1], Nadiia Mameka[1], and Jörg Weissmüller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Institut für Werkstoffforschung, Werkstoffmechanik, Geesthacht, Germany — [2]Technische Universität Hamburg-Harburg, Institut für Werkstoffphysik und -technologie, Hamburg, Germany

The microstructure of dealloying-derived nanoporous metals may be understood as a network of interconnected single nanowires (or nanoligaments). The availability of millimeter-size samples of these nanomaterials predestine them for fundamental studies of small-scale effects on the mechanical behavior. While recent experiments and simulations have acknowledged important effects of ligament size along with solid fraction and network connectivity on both elastic and plastic deformation, the role of surface effects and their precise origin remain to be clarified. Among relevant microscopic processes at the surface are impact of the *surface diffusion* and *atomic-scale surface roughness* on the plastic behavior of the high surface area materials are explored in this study. We probe the plastic response of nanoporous gold to changes of the surface diffusion constant and surface roughness or smoothness of the nanoligaments by deforming the material in situ in an electrochemical cell with various surface conditions. The relationships between different surface morphologies induced in our experiments by the exposure to the specific electrochemical environments and the plastic behavior are discussed.

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Grain refinement in ball-milled nanocrystalline iron-boron — •Max Steinbrück — IMP Universität Göttingen

In this thesis, iron-boron alloys were produced and the influence of the concentration of boron on the grain size was investigated. In theory, the relatively small boron atoms should segregate to the grain boundaries of iron. This reduces the surface energy of the grains and therefore favors the formation of grain boundaries and reduces grain growth. To investigate this, Fe and FeB powder were ball-milled to produce alloys with different boron concentrations. The grain size was determined by transmission electron microscopy and x-ray diffraction. It could be shown that in the investigated interval up to 17,3 at.% the grain size decreases with increasing boron concentration. The thermal stability of the powder was examined by differential scanning calorimetry, where a phase transition while heating and the formation of a Fe2B phase were observed. The results were connected to previous works on iron-oxygen and iron-carbon systems.

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Mechanical stress upon hydrogen absorption in Nb-Fe Films — •Philipp Klose, Magnus Hamm, and Astrid Pundt — Universität Göttingen, Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

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 7 nm and mechanical stress of up to -10 GPa is achieved.[5] The yield stress can also be affected by alloying. In this presenation we study the stress-development upon hydrogen loading in niobium-iron (about Nb90-Fe10) films. Films of different thickness were prepared by argon-cathode beam sputtering. Hydrogen loading was performed from the electrolyte using constant current conditions. For these films, stress linearity is found up to at least 40 nm film thickness.

This work is financially supported by the DFG via project PU131/12-1. [1] J. Weissmuller and C. Lemier, Philos. Mag. Lett. 80:6 (2000), [2] S. Wagner and A. Pundt, Appl. Phys. Lett. 92.5 (2008), [3] U. Laudahn et al., JALCOM 1999 ,[4] A. Pundt, et al., Phys. Rev. B 61.15 (2000), [5] Hamm, M., et al. "Achieving reversibility of ultra-high mechanical stress by hydrogen loading of thin films." Applied Physics Letters 106.24 (2015): 243108.

MM 34.28 Tue 18:30 P4

Tuning the amorphous phase of the Phase change materials GeSbTe225 and Sb2Te by altering the quenching-rate from the liquid phase — •Christoph Persch, Thorben Frahm, and Matthias Wuttig — 1.Physikalisches Institut IA, RWTH Aachen University, 52074 Aachen, Germany

Phase-change materials (PCMs) constitute a class of materials characterized by a pronounced difference in physical properties between the crystalline and the amorphous phase. The crystalline state usually features a low electric resistance and a high reflectivity while the amorphous state features a high electric resistance and a low reflectivity. As phase transitions are inherently fast, phase-change materials are of great interest for non-volatile memory applications, such as solid state PC-RAM. To investigate the switching behavior of phase-change materials, a measurement setup comprised of a pulse-probe laser system and a detection unit has been established. To deposit a sufficient amount of thermal energy in the PCM sample under investigation, the PCM layer is situated in a layer stack constituted of dielectric materials. This allows for a fine tuning of the heat flow into the substrate material upon heating and upon melt-quenching, so by altering the thickness of the dielectric layers, different quenching rates (q.r.) could be obtained. A significant change of the temperature-dependent crystal growth velocities in the amorphous phase of PCMs quenched at different rates has been observed. Thus, tuning the amorphous phase of PCMs by altering the q.r. has been demonstrated, rendering the q.r. another important factor to consider in the process of device-design.

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Computational thermodynamics applied to battery materials — •Sebastian Schwalbe[1], Kai Trepte[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany — [2]Technische Universität Dresden, Theoretical Chemistry, Germany

From the computational point of view battery materials (e.g. $\mathrm{Li}_x\mathrm{Si}_y$, $\mathrm{Li}_x\mathrm{Sn}_y$ or FePO_4) are numerically very demanding, as they are described by large unit cells with up to hundreds of atoms. We present ab-initio thermodynamic data sets (e.g. isobaric heat capacities) calculated in the framework of density functional theory and the quasi-harmonic approximation. Further, we used force-field potentials to reproduce ab-initio thermodynamic data reducing computational time [1]. Our goal is the construction of the phase diagram based on calculation without the need of experimental input.

[1] Schwalbe et al., arXiv preprint arXiv:1610.08991

MM 34.30 Tue 18:30 P4

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

Grain boundary (GB) diffusion differs from bulk diffusion in crystals. For substitutional solvents in metals, GB diffusion is several orders of magnitude faster, for interstitial solvents it can be either slower or faster, depending on the solvent concentration [1,2]. In this work the diffusion of hydrogen gas in the magnesium-hydrogen system is used as a model system. To explore the dependence of the diffusion coefficient on grain boundaries, the sample grain size is varied, thereby achieving differing grain boundary volume fractions. Additionally, the difference between the metallic magnesium and the hydride phase is studied. Magnesium thin films and ECAP treated bulk magnesium samples are characterized using optical and electron microscopy. Purity and grain structure of the bulk samples are investigated by EDX and EBSD measurements. Hydrogen gas volumetry is used to determine the diffusion behaviour in the α-regime and the hydride phase and to calculate the related diffusion coefficients. Financial support provided by the Deutsche Forschungsgemeinschaft via the projects PU131/9-2 and PU131/10-1 is gratefully acknowledged. [1]I. Kaur und W. Gust, Fundamentals of grain and interphase boundary diffusion, Stuttgart: Ziegler Press, (1989) [2]T. Muetschele and R. Kirchheim, Scripta Metallurgica 21, 135-140 and 1101-1104, (1987)

MM 34.31 Tue 18:30 P4

Polypyrrole confined in porous silicon: From fundamentals to applications — •Manuel Brinker[1], Guido Dittrich[1], Philipp Timm[1], Thomas Keller[2,3], Pirmin Lakner[2], and Patrick Huber[1] — [1]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg (TUHH), Eißendorfer Straße 42, 21073 Hamburg — [2]DESY NanoLab FS-NL, Research Group X-ray Physics and Nanoscience, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg — [3]Departement Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg

We investigate the properties of the semi-conducting polymer polypyrrol (PPy) in parallel, tubular pores of monolithic micro- (pore diameter $D < 2$nm)-, meso- ($2 < D < 20$nm) and macroporous ($D > 50$ nm) silicon (PSi). On the one hand PPy offers the opportunity to modify the electrical conductivity of the PSi, while sensoric and actoric applications for the PPy/PSi hybrid system are possible as well. We investigate the electrochemical polymerisation process of PPy in PSi [1] with regards to the orientation of the molecules in the pores and the role of the pore surfaces. [1] F.A.Harraz, Electrochemical formation of a novel porous silicon/polypyrrole hybrid structure with enhanced electrical and optical characteristics, J. Electroanal. Chem. 729 (2014) 68*74.

MM 34.32 Tue 18:30 P4

Potential-strain coupling on electrocatalysis of nanoporous platinum — •Xinyan Wu[1], Shan Shi[1,2], Anastasia Strasser[1], Matthias Graf[1], and Jörg Weissmüller[1,2] — [1]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg, Hamburg — [2]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht

Nanoporous platinum derived from dealloying shows excellent electrocatalytic activity such as methanol electrooxidation due to their extremely high specific surface area. Elastic deformation is known to strongly impact many chemical reaction processes. So it is of great interest to detect and quantify the coupling of catalysis reaction to strain in nanoporous platinum. Here we fabricated nanoporous platinum thin films by dealloying cosputtered Pt-based alloys. Then we explored the influences of elastic strain on the methanol electrooxidation process (reaction potential, rate and efficiency, etc.) via dynamic electro-chemo-mechanical analysis (DECMA).

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in-situ TEM observations of motions of nanostructures entrapped in carbon nanotube — KECHENG CAO[1], JOHANNES BISKUPEK[1], THILO ZOBERBIER[1], THOMAS W. CHAMBERLAIN[2], ANDREI N. KHLOBYSTOV[2], and •UTE KAISER[1] — [1]Central Facility for Electron Microscopy, Ulm University, Ulm, Germany — [2]School of Chemistry, University of Nottingham, Nottingham, UK

Single-walled carbon nanotubes (SWNTs) are promising materials to realize the controllable transport of molecules due to their narrow cylindrical cavities. Time-resolved in-situ transmission electron microscopy (TEM) imaging with an atomic resolution enables direct visualization of molecular motion in SWNTs. The back and forth translations of a carbon capsule, LaC2 nanocrystal, C60 molecules in SWNTs have been subsequently reported. However, the driving mechanism of these motions is still unknown.

In this study we follow translational motion of different types of nanoparticles investigated by means of 30 and 80 kV time-resolved in-situ TEM in order to deduce the driving force of the motion. Prior to electron beam irradiation, the SWNTs were filled with Fe3(CO)12 molecules, which then converted into α-Fe nanoparticles and Fe compounds with amorphous carbon in the lumen of SWNTs.The reciprocating motions of Fe nanoparticles were observed and recorded. We demonstrated the electrostatic repulsion due to ionization of the nanoparticles by the electron beam as the most likely force propelling the nanoparticles in their translational motion.

MM 34.34 Tue 18:30 P4

Imaging and kinetics of MgH2 and TiH2 formation — •Efi Hadjixenophontos[1], Lukas Michalek[1], Manuel Roussel[1], Andreas Weigel[1], Toyoto Sato[2], Shin-ichi Orimo[2,3], and Guido Schmitz[1] — [1]Institut für Materialwissenschaft, (IMW) University of Stuttgart, Heisenbergastrasse 3, 70569 Stuttgart, GERMANY — [2]Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577 JAPAN — [3]WPI-Advanced Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577 JAPAN

Among the metal hydrides, Mg and its alloys show an excellent performance for the H-fuel based economy.In order to improve the system, it is first important,to understand the reason for the slow kinetics of hydride formation, which is surprisingly still an open field of research and the focus of this work. TM-metals,have shown to lower the activation energy, and therefore improve the kinetics.Here we study separately the two systems: MgH2 with Pd as catalyst, and TiH2 thin films and compare them to their bulk behaviour.The two metals show a different mechanism of hydrogenation, and the oxide layer in the case of Ti seems to have a great impact. Hydrogen diffuses in Ti faster and TiH2 is first formed closer to the substrate.In the case of Mg a microscopic imaging of the co-existence of the hydride and pure phases shows that MgH2 is immediately formed at the interface between the Pd catalyst coating and the Mg thin film and it grows in a layer-like reaction towards the substrate.XRD,SEM-FIB and TEM are the combined techniques used to discus the diffusion coefficients and mechanisms of hydrogenation.

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Single-spin hybridization expansion continuous-time Monte Carlo for time-dependent Anderson impurity model — •Patryk Kubiczek[1], Alexey Rubtsov[2], and Alexander Lichtenstein[1] — [1]Institute of Theoretical Physics, University of Hamburg, Germany — [2]Russian Quantum Center, Moscov, Russia

In this work we propose a modified version of the standard continuous-time hybridization expansion quantum Monte Carlo method (CT-HYB-QMC) in which the expansion is performed only for a single-spin channel. At the same time the effective single-particle Schrödinger equation for the other spin-channel is solved explicitly. We apply this method to the time-dependent Anderson impurity model and show that it leads to the sign problem alleviation, which makes it possible to find the exact solutions of the model for larger timescales.

MM 34.36 Tue 18:30 P4

Diffusion in intermetallic AlAu$_4$: MD study down to temperatures relevant to wire bonding — •Mohammed Guerdane — Karlsruhe Institute of Technology, IAM-CMS, Karlsruhe

We show the ability of long time ($\sim 1\mu$s) molecular dynamics modeling to provide quantitative diffusion coefficients for the compound AlAu$_4$ (β-Mn type), down to temperatures ($\sim$ 200 °C) that are relevant to Al-Au wire bonding. Concerning Au diffusion, our results agree quite well with DFT calculations of the vacancy-formation energy, the activation energy, and the diffusion mechanisms. The van Hove correlation-function analysis shows that Au diffusion takes place mainly on the Wyckoff **b** sublattice. Moreover, we shed light on the high-temperature region, as the stability limit $T^\star$ of AlAu$_4$ is approached and unfavorable jumps contribute to the diffusivity. This concerns, for instance, jumps generating antisites defects. The latter lead to a massive disorder which ends up in a phase change to a distorted fcc structure at $T^\star$. Including the melting temperature in the potential-fitting procedure seems to be an effective way to gauge the temperature scale and properly capture the order of magnitude of diffusion.

MM 34.37 Tue 18:30 P4

Thermal Diffusivity Measurements with Single Particle Photothermal Microscopy — •André Heber and Frank Cichos — Universität Leipzig, Exp. Phys. I, Molecular Nano-Photonics Group, Leipzig, Germany

Photothermal single particle microscopy has proven to be a sensitive imaging technique for absorbing nanoparticles and molecules. Here, we discuss the extension of photothermal microscopy to the measurement of thermal diffusivities in the surroundings of an absorber. The photothermal contrast makes use of a heating induced refractive index change. As the refractive index change is small a modulated heating scheme is implemented in which the optical heating is harmonically modulated and the detection laser detects fluctuations at that particular modulation frequency. This configuration enables a high signal to noise ratio and adds a time scale for the measurement of thermal transport as the temperature profile is not instantly established. Here, we show how single particle microscopy can be used to sense anisotropies in the thermal transport and interfaces using single particle photothermal microscopy.

MM 34.38 Tue 18:30 P4

Electron transport in nanoparticle networks — •Michael Deffner[1], Florian Schulz[2], Carmen Herrmann[1], and Holger Lange[2] — [1]Institut für Anorganische und Angewandte Chemie, Universität Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Deutschland — [2]Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117 20146 Hamburg, Deutschland

Gold nanoparticles (AuNPs) are a stable and easy-to-functionalize platform for different purposes such as medical imaging or sensor applications. AuNPs can be functionalized by straightforward ligand exchange for example with thiols or amines, which bond easily to the surface of the nanoparticle and can induce aggregation processes.

In order to systematically study the transport properties of gold nanoparticle clusters, in a first step the formation of networks and clusters of AuNPs are studied using biphenyl-4,4'-dithiol, p-terphenyl-4,4"-dithiol and 1,9-nonane-dithiol as molecular linkers.

Electron transport properties of these networks are studied using terahertz spectroscopy as well as transport calculations for single gold–molecule–gold junctions following the Landauer–Büttiker formalism. Within this approach, electron transport is described as a tunneling problem which can be solved using quantum chemical software.

MM 34.39 Tue 18:30 P4

Effect of surface reconstruction on the exchange interactions in CaMnO3 — •Samara Keshavarz — Uppsala University, Uppsala, Sweden

The effects of geometrical relaxation at the surface as well as the change of crystal field are mostly able to influence the lower energy magnetic configuration. In particular, our analysis of CaMnO3 surface reveals that the exchange interaction between the Mn atoms belonging to the surface and the subsurface layers is very sensitive to the structural changes. An earlier study [A. Filippetti and W.E. Pickett, Phys. Rev. Lett. 83, 4184 (1999)] suggested that this coupling is ferromagnetic and gives rise to the spin flip process on the surface of CMO. In our work we confirm their finding for an unoptimised geometry, but once the structural relaxations are taken into account, this exchange coupling changes its sign and implies the surface of CMO to have the same G-type antiferromagnetic order as in the bulk. However, the suggested SF can be induced in the system by introducing an excess of electrons.

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Microstructure and Mechanical behavior of Copper-Iron Multilayers produced by Accumulative Roll Bonding

— •Maher Ghanem, Benoit Merle, Heinz Werner Höppel, and Mathias Göken — Department of Materials Science and Engineering, Institute I, University of Erlangen-Nürnberg (FAU), Germany

The accumulative roll bonding (ARB) process has been applied recently to produce multilayer composites with grain sizes in the range of submicron to nanometer. Such multilayer composites show a good ductility with reported tremendous increases in strength as the grain sizes are refined down to the submicron range.

Laminated Cu/Fe Nanocomposite with alternating layers of Oxygen-free copper (OFC) (>99.99% pure) and pure iron (99.85%) were produced by accumulative roll-bonding (ARB). The Nanocomposite was successfully roll bonded with 50% reduction through the addition of a heat treatment step at 150°C after each pass. The process was performed up to 8 passes (N8). Microstructure of the nanocomposites was evaluated using scanning electron microscope in the backscattered mode (BSE-SEM). Mechanical properties were investigated through tensile and nanoindentation tests. Nanoindentation and tensile tests were performed in order to observe the changes in the mechanical properties of samples both locally and globally as the number of ARB passes increased.

MM 34.41 Tue 18:30 P4

Current status and future prospectives of the multi-purpose x-ray scattering beamline BL9 of DELTA

— •Florian Otte, Jennifer Bolle, Michael Paulus, Christian Sternemann, and Metin Tolan — Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund

We present the current status of the multi-purpose beamline BL9 of the synchrotron radiation source DELTA located at the TU Dortmund. The beamline is dedicated to (surface) x-ray diffraction, x-ray reflectivity and small angle x- ray scattering experiments with focus on soft matter research and materials science. Examples for study of protein adsorption, protein-protein interaction and structure formation in alcohols will be given. The upgrade of the beamline with a new wiggler source in 2018 will be discussed along with the implications for future experiments.

MM 34.42 Tue 18:30 P4

Observation of the influence of hydrogen on the phase transformation and fracturing behaviour of steel samples during tensile tests using synchrotron radiation

— •Beate Pfretzschner, Axel Griesche, and Thomas Schaupp — Bundesanstalt für Materialforschung und -prüfung, Berlin, Deutschland

Hydrogen exhibits a detrimental influence on the mechanical properties of Fe-based alloys. The suggested mechanisms of hydrogen embrittlement are ambiguous and versatile. One of the effects of hydrogen in steels is its ability to change the phase transformation behaviour from austenite to martensite. In this work we present in-situ energy dispersive x-ray diffraction (ED-XRD) experiments performed on supermartensitic stainless steel samples with and without hydrogen during tensile tests. In order to perform ED-XRD scans, the path-controlled tensile test were paused every 0.25 mm. During these pauses spectra were acquired at seven positions on the sample along the tensile axis with a distance of 0.75 mm between each position. This procedure allows to follow the stress- or strain-induced phase transformation of the retained austenite to martensite in-situ. Simultaneous to the diffraction patterns, radioscopic images were acquired during the fracturing of the sample at a rate of 500 fps. Significant differences were observed in the phase transformation behaviour and the fracturing performance between hydrogenous samples and samples without hydrogen.