MM 28: Poster Session II

Time: Tuesday 18:30–20:30 Location: Poster E

MM 28.1 Tue 18:30 Poster E

Molecular dynamics simulation of mechanical properties of dilute α-Fe-C alloys — •Jan Janssen, Nina Gunkelmann, and Herbert M. Urbassek — Physics Department and Research Center OPTIMAS, University Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany

Using molecular dynamics simulation, we study the influence of carbon interstitials on the mechanical properties of α-iron. With increasing carbon concentration we observe an increase of the tetragonal distortion and a decrease of the elastic moduli. Furthermore we analyze various available iron-carbon potentials and compare the results to ab-initio calculations and experimental data.

MM 28.2 Tue 18:30 Poster E

Fitting an Interatomic Potential for Accurate Description of the Iron-Chromium System — •Sebastian Eich, Daniel Beinke, and Guido Schmitz — Institute of Materials Science, University of Stuttgart, Heisenbergstraße 3, D-70569 Stuttgart, Germany

A new potential for the iron-chromium (Fe-Cr) system was developed using the formalism of the embedded-atom method (EAM) within the two-band model (TBM) extension. The key improvement of this potential in comparison to available ones from literature is the accurate description of the miscibility gap according to experimental data and a recent CALPHAD parametrization. Furthermore, the potential was fitted to obtain an enriched solubility of chromium atoms in an iron matrix at 0 K which is predicted by several ab-initio calculations. The potential was also benchmarked against phonon excess entropies at 300 K and 1600 K and shows good agreement with inelastic neutron scattering measurements.

The development was restricted to the metastable α/α' phase and for the fitting only the direct interaction between iron and chromium was taken into account while the potentials for pure elements were taken from literature (Ackland[1] (Fe) and Olsson[2] (Cr)).

[1] Ackland et al., J. Phys.: Condens. Matter 16, S2629 (2004)
[2] Olsson et al., Phys. Rev. B 72, 214119 (2005)

MM 28.3 Tue 18:30 Poster E

Calculation of Electronic Thermophysical Parameters for Steel Alloys based on Density Functional Theory — •Juergen Sotrop[1], Jan Winter[1], Heinz P. Huber[1], Stephan Borek[2], and Jan Minar[2,3] — [1]Munich University of Applied Sciences — [2]Ludwig-Maximilians Universit, Muenchen — [3]University of West Bohemia, Pilsen

The ablation mechanism of matter irradiated with ultra-short laser pulses has been widely investigated over the last two decades. At present there is still lack of theoretical understanding of the interaction of ultra-short laser pulses with a metal alloy. By irradiating material with ultra-short laser pulses initially strong electron-phonon nonequilibrium will occur. The resulting difference in electron and phonon temperatures can be calculated with the so called two-temperature model (TTM). An essential prerequisite for the application of the TTM is a determination of the temperature dependent thermophysical parameters such as electron heat capacity and electron-phonon coupling factor. We will present a general method for the calculation of the electronic thermophysical parameters for metal alloys, here performed exemplarily on stainless steel (AISI 304). The method is based on the calculation of the electronic density of states (DOS) using a fully relativistic implementation of the KKR-formalism in the framework of spin density functional theory. Precise knowledge of the DOS will enable the calculation of the electron-phonon-coupling factor and the electron heat capacity. The model is compared with the well-known parameters for iron to show the validity.

MM 28.4 Tue 18:30 Poster E

Exact models and numerics for the relativistic single-site scattering problem — •Matthias Geilhufe[1], Steven Achilles[2], Markus Arthur Koebis[3], Martin Arnold[3], Ingrid Mertig[2,1], Wolfram Hergert[2], and Arthur Ernst[4,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [3]Institut für Mathematik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [4]Wilhelm-Ostwald-Institut für Physikalishe und Theoretishe Chemie, Universität Leipzig, Leipzig, Germany

The Korringa-Kohn-Rostoker Green function method (KKR) based on density functional theory is a powerful tool for electronic structure calculations. For the discussion of spin-orbit coupling driven phenomena e.g. on surfaces a fully-relativistic treatment within the full-potential approximation [1] is necessary. The numerical solution of the fully relativistic single-site scattering will be discussed for the Coulomb and the Mathieu potential. In this context, the solution of the fully-relativistic full-potential single-site scattering problem using integral equations is compared with a direct solution of the differential equations via various methods. The advantages and disadvantages of the used methods will be discussed and proposals for accurate and efficient methods will be given.

[1] T. Huhne et al., PRB **58**, 16, 10236 (1998)

MM 28.5 Tue 18:30 Poster E

Correlation energy evaluation in extended systems beyond the RPA — •Emanuele Maggio and Georg Kresse — University of Vienna, Faculty of Physics and Centre for Computational Materials Science, Sensengasse 8/12, Vienna, Austria

The description of electronic correlations plays a pivotal role in the accurate modelling of structural and electronic properties of materials [1]. A range of well-developed methods has come into maturity in recent years [2, 3]; however a full scale assessment of the correlation energy remains restricted to systems with very few atoms per unit cell owing to the high computational demands.

To improve upon the Random Phase Approximation (RPA), we develop a computational scheme that exactly includes all second order contributions [4, 5] to the correlation energy and is also able to implicitly account for higher order diagrams. The inclusion of an effective screened interaction between electrons, alongside an improved description of the reference state at the GW_0 level of theory are key features of the method proposed, whose performance is assessed for a set of prototypical semiconducting materials and for the homogeneous electron gas.

[1] Harl, J.; Schimka, L.; Kresse, G. *Phys. Rev. B* **2010**, 81, 115126. [2] Shepherd, J. J.; Booth, G. H.; Alavi, A. *J. Chem. Phys.* **2012**, 136, 244101. [3] Booth, G. H.; Grüneis, A.; Kresse, G.; Alavi, A. *Nature* **2013**, 493, 365-370. [4] Bates, J. E.; Furche, F. *J. Chem. Phys.* **2013**, 139, 171103. [5] Grüneis, A.; Marsman, M.; Harl, J.; Schimka, L.; Kresse, G. *J. Chem. Phys.* **2009**, 131, 154115.

MM 28.6 Tue 18:30 Poster E

Gutzwiller Density Functional Theory — •Tobias Schickling, Jörg Bünemann, and Florian Gebhard — FB Physik, Philipps Universität Marburg, D-35032 Marburg, Germany

Density Functional Theory (DFT) is the workhorse of electron structure theory. It reduces the genuine many-body problem to an effective single-particle theory that is readily evaluated numerically. However, electrons in narrow bands, e.g., 3*d*-electrons in transition metals and their compounds, require a more sophisticated treatment. Unfortunately, model Hamiltonians for correlated electrons often oversimplify the problem while, at the same time, they reintroduce the full complexity of the many-body problem. I present the Gutzwiller DFT that combines the advantages of both schemes: it retains the computational efficiency of existing DFT codes and it treats electronic correlations on the basis of Gutzwiller's variational many-body approach for multiband Hubbard models. A first application to fcc nickel resolves all of the DFT shortcomings regarding lattice spacing, magnetic moment, bulk modulus, and Fermi-surface topology. Moreover, I will show results of the bcc-hcp transition of iron.

MM 28.7 Tue 18:30 Poster E

Automatically generated MEAM potentials from DFT for simulation of Li_xSi_y battery materials — •Sebastian Schwalbe and Jens Kortus — TU Freiberg, Institute of Theoretical Physics

We implemented an optimization procedure using the so called particle swarm optimization (PSO [1]) to automatically optimize modified embedded atom method (MEAM [2,3]) parameters. In detail physical properties (elastic constants, bulk modulus, total energy) calculated with density functional theory (DFT) will be used as constraints for

the PSO algorithm leading to a DFT like accuracy MEAM potential. We generated these optimized MEAM potentials for Li and Si to be used for large scale simulations of Li_xSi_y battery materials.

[1] J. Kennedy, R. Eberhart, IEEE Vol. 4 (1995), pp. 1942-1948
[2] Murray S. Daw, and M. I. Baskes, Phys. Rev. B 29(12), 1984.
[3] B. Jelinek, S. Groh et al., Phys. Rev. B 85(24), 2012.

MM 28.8 Tue 18:30 Poster E

Efficient numerical treatment of irregular coupled radial scattering solutions — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The numerical determination of the coupled radial scattering solutions of the stationary Schrödinger equation for a general non-spherical potential is particularly difficult if one needs not only the regular but also the irregular solutions. These are, for instance, necessary in the complex energy formulation of the Korringa-Kohn-Rostoker (KKR) Green-function (GF) method. The difficulty for the irregular solutions arises from their divergent behaviour near the origin where functions of very different magnitudes are coupled. A technique will be presented which overcomes this problem by use of an analytical decoupling scheme and a subinterval procedure with Chebyshev interpolations in each subinterval. It will be shown that accurate irregular solutions can be obtained and that this is important for the calculation of precise forces in the KKR-GF method.

MM 28.9 Tue 18:30 Poster E

Computational Study of Cu Doped Ag Nano Alloy Clusters. — •Prabhat Ranjan — MANIPAL UNIVERSITY JAIPUR, JAIPUR, INDIA.

There is a number of reports available in favour of Bi-metallic nano alloy clusters for a wide range of applications. As the bi-metallic nano alloy clusters have diverse physico-chemical properties, among such nano clusters, the compounds formed between Cu-Ag have gained a considerable interest because they possess unique optical, electronic and magnetic and mechanical properties, which have extensive applications in the field of optoelectronics, optics and nanoscience. Density Functional Theory (DFT) is one of the most popular techniques of quantum mechanics to study the electronic properties of materials. Recently, conceptual DFT based descriptors have been turned to be indispensable tools for studying the experimental properties of compounds. In this work we reported a theoretical analysis on the stabilities, electronic properties and geometries of Cu-Agn; (n=1-10) system using B3LYP with basis set LanL2DZ. The electronic properties of Cu-Agn Viz. HOMO-LUMO gap (eV), Global Hardness (η), Global Softness (S), Electronegativity(χ), Electrophilicity Index(ω), Dipole Moment and Bond length are successfully computed and compared in terms of DFT based global descriptors. This study is probably the first attempt to explore the electronic properties of Cu-Agn Nanoalloy cluster in terms of DFT based descriptors.

MM 28.10 Tue 18:30 Poster E

Calculated Mechanical and Thermal Properties of $CePt_3Si$ and $CePt_3B$ above their Magnetic-Ordering Temperatures by an LDA-Based Ab-Initio Theory — •Rudolf Sykora[1], Dominik Legut[2], Gerda Rogl[3,4,5], Peter Müller[4], Herbert Müller[4], Ernst Bauer[4], Stephan Puchegger[5], and Peter Rogl[3] — [1]Nanotechnology Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [2]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [3]Institute of Physical Chemistry, University of Vienna, Wien, Austria — [4]Institute of Solid State Physics, University of Technology, Wien, Austria — [5]Faculty of Physics, University of Vienna, Wien, Austria

Adopting the plane-wave pseudopotential VASP[1] DFT package, using a simple local density approximation for electronic exchange and correlation effects, and disregarding spin-orbit interaction we calculate (a necessarily naive) electronic structure of $CePt_3Si$ and $CePt_3B$ materials (the former being known as a heavy-fermion superconductor with no inversion centre) under several discrete values of stress and strain. For each such configuration we calculate its phonon spectrum with a direct (supercell) method as supplied by the Phonopy program. Combining the results we obtain materials' thermal and mechanical properties within the quasi-harmonic approximation, presumably applicable to temperatures above magnetic-ordering temperatures. Results are compared to experimental data.

References:

1.G. Kresse, J. Furthmueller, J. Comput. Mater. Sci. **6**, 15 (1996).

MM 28.11 Tue 18:30 Poster E

Simulation of the elastic properties of nanomechanical beam and membrane resonators — •Kristian Scholz, Ananta Kälberer, Tobias Kemmer, Thomas Möller, Daniel Mutter, Markus Ring, Ralf Schmid, Martin Vögele, and Peter Nielaba — University of Konstanz, Germany

The oscillation behavior of nanomechanical resonators in the form of doubly clamped beams and clamped membranes is investigated by Molecular Dynamics simulations. After setting up the initial structure, the end points of the beams or the outer border of the membranes, respectively, are fixed and a constant force is applied over all atoms in order to achieve a transverse deflection. The force is then turned off resulting in a free oscillation of the structures. Besides varying the size of the structures, the effects of temperature, external stretching fields, cavities and crystal faults are explored. The results show a decrease of the oscillation frequencies and an increase of the damping coefficient with rising temperature, a strong increase of the frequencies with external stress (stretching), a decrease of frequencies with size and an increase of the damping coefficient when adding cavities to the structures. It is also possible to observe the dissipation of energy from the collective oscillation of the structures into thermal energy of the degrees of freedom of the constituting atoms.
Different materials (e.g. Si, Si_3N_4 and NiTi memory alloys) are explored as well. In order to explore quantum effects in the low temperature regime Path Integral Monte Carlo simulations are performed.

MM 28.12 Tue 18:30 Poster E

Nanoporous Germanium-Silicon alloys by ion irradiation at low energies — •Fritz Lehnert[1] and Stefan G. Mayr[1,2,3] — [1]Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM) — [2]ranslationszentrum für regenerative Medizin (TRM) Leipzig — [3]Fakultät für Physik und Geowissenschaften, Universität Leipzig

Nanoporous materials exhibit a very large surface area compared to their volume and are therefore an interesting material class for all surface active processes such as catalysis membranes or gas adsorption storage applications. While the influence of ion radiation on single-crystal germanium as a semiconductor material, has been studied in the past decades, the effects on their alloys remains yet uninvestigated. Therefore the development of a nanoporous surface layer during ion bombardment of germanium-silicon-alloys was studied in detail experimentally. Amorphous germanium-silicon thin films produced by electron beam evaporation were irradiated with low energy 30 keV Ga-ions using a focued ion beam. The surface morphology and topography was investigated by SEM and AFM measurements. The nano-structure development was found to depend strongly on the silicon-to-germanium ratio. The investigation of semiconductor alloys is expected to lead to a better understanding of the processes involved in the development of a nanoporous structure by ion bombardment.

[1] S. G. Mayr and R. S. Averback, Phys. Rev. B 71 (2005) 134102.

MM 28.13 Tue 18:30 Poster E

Absolute Photoluminescence Quantum Yields and Lifetimes of in Toluene Dispersed Hexagonal β-$NaYF_4$: x % Tm^{3+}, 20 % Yb^{3+} Upconversion Nanoparticles — •Marco Kraft[1], Martin Kaiser[1], Christian Würth[1], Tero Soukka[2], and Ute Resch-Genger[1] — [1]BAM Bundesanstalt für Materialforschung und -prüfung, Richard-Willstaetter-Str. 11, 12489 Berlin — [2]Department of Biotechnology, University of Turku, Tykistoekatu 6A, FI-20520 Turku, Finland

Hexagonal β-$NaYF_4$ doped with Yb^{3+} and Tm^{3+} is an efficient upconversion (UC) phosphor for the conversion of 976 nm to 800 nm and 450 nm light. The emission behavior of this material is strongly influenced by the doping concentration, particle size, and surface chemistry. The design of nm-sized UC particles requires reliable spectroscopic tools for the characterization of the optical properties of these materials like the UC quantum yield (QY_{UC}). This UC emission originates from multi-photonic absorption processes, rendering the QY_{UC} excitation power density (P) dependent. The absolute measurement of QY_{UC} presents a considerable challenge due to the low absorption coefficient and the P-dependence of these materials, which can introduce a dependence of QY_{UC} on illumination geometry. Here, we present the P-dependent QY_{UC} of 30 nm-sized $NaYF_4$ UC particles with systematically varied dopant concentrations of 20 % Yb^{3+} and x % Tm^{3+} (x = 0.2, 0.5, 0.8, 1.1, 2). In addition to QY_{UC}, the emission intensities and lifetimes of the different UC bands are studied as function of excitation power density to gain a better insight of their photonic nature.

MM 28.14 Tue 18:30 Poster E

Structural and electronic properties of amorphous graphene — •Soumyajyoti Haldar[1], Basu Oli[2], Parthapratim Biswas[2], and Biplab Sanyal[1] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]Department of Physics and Astronomy, University of Southern Mississippi, USA

Non-crystalline graphene structures have interesting structural and electronic aspects, which may be explored for various applications. In our work, amorphous graphene in various number densities (lower and higher compared to crystalline graphene) and system sizes (∼ 500-2048/supercell) have been simulated using density functional based molecular dynamics and Monte Carlo techniques. The resulting structures have a variety of networks of disordered small and large carbon rings, which have been analyzed by ring and Mermin statistics. Interestingly, linear chains of carbon atoms are also observed for certain densities. Comparisons have been made with recent experimental and theoretical studies[1,2]. Our calculations of densities of states show finite contributions at the Fermi level. The analysis of inverse participation ratio confirms that the states near the Fermi energy are delocalized.

Reference:

1. E. Holmström, J. Fransson, O. Eriksson et. al. Phys. Rev. B 84, 205414 (2011)
2. F. Eder, J. Kotakoski, U. Kaiser et. al. Scientific Reports 4, 4060 (2014)

MM 28.15 Tue 18:30 Poster E

Plasticity at the low end of the nanoscale - a crossover to glass-like behavior? — •Christian Braun, Manuel Grewer, and Rainer Birringer — Universität des Saarlandes, FR 7.2 Experimentalphysik, Campus D2.2, 66123 Saarbrücken

Polycrystalline metals at the low end of the nanoscale with grain sizes of 10 nm or less are characterized by a grain boundary volume fraction of at least 30%. Grain boundary deformation modes similar to shear transformations (STs) in bulk metallic glasses (BMGs) may therefore play a non-negligible role in the mechanical behavior of nanocrystalline (nc) metals. In fact, a couple of similarities between this two material classes have been observed, e.g. comparable values for the shear activation volume, activation energy or Mohr-Coulomb friction coefficient. However, in BMGs increasing load involves percolation of STs followed by shear band formation manifesting stick-slip behavior that eventually leads to catastrophic failure. In contrast, for nc Pd90Au10 we observe absence of stick-slip behavior implying that shear banding is missing. In fact, the operation of STs at/along grain boundaries in conjunction with the network constraints of the nanoscale microstructure avoids pronounced shear band propagation. We present results of mechanical testing of nc Pd90Au10 samples synthesized by inert gas condensation and deformed in shear compression geometry under different loading conditions. These results are analyzed in terms of activation parameters and pressure or normal-stress dependence of plasticity. Furthermore, the interplay and the succession of active deformation mechanisms are investigated using in situ X-ray diffraction.

MM 28.16 Tue 18:30 Poster E

Investigation of the magnetic phase transition in iron-rhodium thin films by ferromagnetic resonance — •Alirerza Heidarian[1], Jürgen Lindner[1], Rantej Bali[1], Kay Potzger[1], Jörg Grenzer[1], Sven Hoffmann[1], Michael Farle[2], and Florian Römer[2] — [1]HZDR Institute of Ion-Beam Physics and Materials Research, Dresden, Germany — [2]Faculty of Physics and Center for Nanointegration, University of Duisburg-Essen, Duisburg, Germany

Due to the first-order phase transition from an antiferromagnetic (AF) to a ferromagnetic (F) state at 370 K, the equiatomic FeRh alloy has raised growing interest. In our study, the phase transition of FeRh thin films was analyzed by means of ferromagnetic resonance (FMR). $Fe_{50}Rh_{50}$ films are obtained by molecular beam epitaxy on MgO single-crystal substrates. The films are 37 nm and 6 nm thick and were co-deposited from separate Fe and Rh sources. FMR was observed in an X-band cavity set-up, with variable temperature. As the temperature crosses 370 K, resonance lines associated with the F phase appear. Furthermore, resonance lines due to possible acoustic- and optical-resonance modes are observed. Our measurements show that temperature dependent FMR can be used to determine the relative volumes of AFM and FM regions across phase transition. The transition from AF to F coupling can therefore be tracked using FMR measurements. Moreover, the phase transition temperature for 6 nm thick film is 285 K which resonance lines of F phase emerge. Therefore FMR can be an effective tool in unraveling coupling phenomena in FeRh.

MM 28.17 Tue 18:30 Poster E

Laser assisted fabrication of chalcogenide nanostructures with tailored morphology — •Thomas Vasileiadis[1,2] and Spyros N. Yannopoulos[1] — [1]Foundation for Research and Technology Hellas, Institute of Chemical Engineering Sciences (FROTH/ICE-HT), P.O. Box 1414, GR-26504, Rio-Patras, Greece — [2]Fritz Haber Institut der Max Planck Gesellschaft, Faradayweg 4 - 6, D - 14195 Berlin, Germany

Low dimensional nanostructures of chalcogens and chalcogenides have attracted considerable attention over the last years. Here we present a simple and cost effective laser-assisted method for the growth of low dimensional nanostructures based on functional chalcogenides. Te nanotubes can be easily prepared via cw laser ablation in a one-step method. By changing the irradiation conditions different morphologies arise in a controllable way, such as t-Te nanospheres. Differences in the morphology control are observed for elemental Se, a good glass-former. This synthetic strategy can be readily applied in many other functional chalcogenides e.g. As2S3 and phase-change materials, e.g. GeTe. Since chalcogenides are mostly famous for their sensitivity to external stimuli such as light, post-treatment of the resulting nanostructures with low light fluence is also investigated. A series of light-driven phase transition is employed to controllably transform Te nanotubes to core-Te/sheath-TeO2 and/or even neat TeO2 nanowires.

MM 28.18 Tue 18:30 Poster E

metallic nanoparticles and nanoalloys fabricated via solid state deweting — •Dong Wang, Andreas Herz, and Peter Schaaf — TU Ilmenau, FG Werkstoffe der Elektrotechnik, Ilmenau, Germany

metallic an alloy nanoparticles are paid increased attention due to their potential applications in catalysis, magnet memories, sensors, and plasmonics. Here, nanoparticles, nanoporous nanoparticles and bi-metallic nanoparticles were fabricated by using solid-state dewetting. By using pre-patterned substrate, ordered arrays of nanoparticles can be realized due to the curvature driven diffusion through the modulation of the chemical potential by substrate local curvature. By combining the solid state dewetting of Ag/Au bilayer with a subsequent dealloying process, nanoporous gold nanoparticles were fabricated, and possess a different plasmonic property comparing to the solid gold nanoparticles. In addition, the alloying behavior in the microscale can be well studied through the solid state dewetting of metallic bilayer. Different Ni-Au nanoparticles were realized by controling the process parameters.

MM 28.19 Tue 18:30 Poster E

In-situ and ex-situ HRTEM characterization of heated, supersaturated metal-carbide nanoparticles — •Michael Hering[1,2], Darius Pohl[1], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany — [2]TU Dresden, IFWW, D-01062 Dresden, Germany

The segregation of carbon from supersaturated metal-carbon compounds is a highly important step in the production of many novel materials. It is, e. g., an essential process during the growth of carbon nanotubes or in the formation of high-anisotropy granular magnetic FePt-X films. A detailed knowledge of this segregation is thus mandatory. Inert gas condensation is utilized to fabricate Fe-C and Ni-C nanoparticles, and much effort is made to determine the key parameters to tune the size, morphology and structure of the particles in order to generate single-crystalline or well faceted polycrystalline carbide particles with high carbon content. The characterization of these particles is then performed in an aberration-corrected FEI Titan^3 80-300 microscope. The poster presents in a first part the different types of Fe-C and Ni-C particles and correlates the observed structures to the applied process parameters. E.g., in case of Fe-C nanoparticles, the inert gas condensation process mostly results in the formation of particles with a distinct core-shell structure of an iron core surrounded by a carbide shell. The carbon segregation of these particles as induced by a thermal treatment is then presented in the second part. Therefore, a special TEM sample holder for in-situ heating experiments with silicon nitride window chips is used.

MM 28.20 Tue 18:30 Poster E

Highly ordered one-dimensional metal nanowire arrays for SERS — •yong-tae kim[1], stefan l. schweizer[1], jörg schilling[1], and ralf b. wehrspohn[1,2] — [1]Martin-Luther-University Halle-Wittenberg, Halle, Germany — [2]Fraunhofer Institute for Mechanics

of Materials, Halle, Germany

Recent progress in nanotechnology have created new insight about controlling various structures and properties of nanostructured materials that can support surface plasmons for specific applications. Especially metallic nanostructured materials made of noble metals show localized surface plasmon resonance (LSPR) phenomenon when the materials interact with incident light of correct frequency and polarization.

Surface-enhanced Raman spectroscopy (SERS) has been recognized as a useful tool for ultra-sensitive detection of trace amount of chemicals with fingerprint character. The SERS intensity depend strongly on the electromagnetic field enhancement induced from LSPR at nanogaps between plasmonic nanostructures, called hot spots. To obtain high sensitivity and good reproducibility of SERS signal, it is required to have a highly ordered nanostructures with well-controlled narrow gaps that induce hot spots.

Herein, highly ordered one-dimensional metal nanowire arrays with single- or multi-segmental structures composed of gold, silver, and nickel have been prepared via hard-template synthetic method as an active substrate for SERS. Those materials have been investigated to study the effect of dimension and composition of metal nanowire arrays on SERS enhancement factor.

MM 28.21 Tue 18:30 Poster E

Simulation of Nanocolumn Formation in a Plasma Environment — •Jan Willem Abraham[1], Thomas Strunskus[2], Franz Faupel[2], and Michael Bonitz[1] — [1]Institut für Theoretische Physik und Astrophysik, CAU Kiel — [2]Institut für Materialwissenschaft, CAU Kiel

Recent experiments and kinetic Monte Carlo (KMC) simulations [1,2] demonstrated that physical vapor co-deposition of a metal alloy (Fe-Ni-Co) and a polymer (Teflon AF) can lead to self-organized growth of magnetic nanocolumns. While these experiments have been carried out with thermal sources, we analyze the feasibility of this process for the case of a sputtering source. For that purpose, we extend our previous simulation model by including a process that takes into account the influence of ions impinging on the substrate [3]. The simulation results predict that metal nanocolumn formation should be possible. Furthermore we show that the effect of ions, which create trapping sites for the metal particles, is an increased number of nanocolumns.

[1] H. Greve et al., Appl. Phys. Lett. 88, 123103 (2006)
[2] L. Rosenthal et al., J. Appl. Phys. 114, 044305 (2013)
[3] J.W. Abraham et al., submitted to J. Appl. Phys. (2014)

MM 28.22 Tue 18:30 Poster E

Polar Catastrophy by Incremental Charge Differences — •Arwa Abdullah Albar — King Abdullah University of Science and Technology, Thuwal , Saudi Arabia

We report the creation of a two-dimensional electron gas at the SnO/SnO_2 heterointerface. To analyze the mechanism behind this observation, we study the electronic states as a function of the distance to the interface. A polar catastrophy scenario based on incremental charge differences due to covalency effects is developed to explain the creation of the electron gas. This scenario applies not only to polar/polar interfaces but also modifies the expected carrier density at polar/nonpolar interfaces of semiconducting perovsite oxides, in agreement with experimental results.

Authors: A. Albar, H. A. Tahini and U. Schwingenschlögl

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MM 28.23 Tue 18:30 Poster E

Atomistic simulations of interfaces and dislocations in Mg-Al alloys — •Tobias Klöffel[1,2], Bernd Meyer[2], and Erik Bitzek[1] — [1]Materials Science and Engineering, Institute I, FAU Erlangen-Nürnberg — [2]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Their low density and high strength make magnesium alloys key structural materials for lightweight constructions. The intermetallic $Mg_{17}Al_{12}$ phase is the dominant precipitate phase and influences to a large degree the mechanical properties of Mg alloys. Here we present a computational study of $Mg/Mg_{17}Al_{12}$ interphase boundaries (IPBs), combining density functional theory (DFT) calculations with large-scale atomistic simulations using a semi-empirical potential of the modified embedded atom method (MEAM) type. DFT calculations of the γ surfaces in $Mg_{17}Al_{12}$ are used to validate the MEAM potential. DFT and atomistic calculations were then performed to characterize the IPB structure and energy for different orientation relationships to the Mg matrix. The results are compared to both, theoretical and experimental findings. Additional atomistic simulations were performed to determine the core structure and Peierls stress of various dislocations in the $Mg_{17}Al_{12}$ phase.

MM 28.24 Tue 18:30 Poster E

Measuring the Stress Distribution of Bio-Inspired Adhesives in Contact — •Jens W. Neubauer[1], Longjian Xue[2], Johann Erath[1], Dirk-Michael Drotlef[2], Aránzazu del Campo[2], and Andreas Fery[1] — [1]Physikalische Chemie II, Universität Bayreuth, Bayreuth, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany

The responsiveness and the strong restoring forces of polyelectrolyte brushes can be utilized to sense stresses on the microscale. Therefore, a polycationic brush was labeled with a fluorescent dye allowing to measure local pressures as low as 10 kPa from the mechano-response with a lateral resolution better than human skin (1 μm).

Applying a defined pressure with soft colloidal probe AFM, the fluorescence was observed with a confocal microscope. After calibration, the pressure distribution under bio-inspired microstructured adhesives in contact could be determined from the fluorescence of the polymer brush. The contact formation of the adhesives was controlled with a commercial setup (PVM-A, GeSiM).

Furthermore, the steric interactions of the polyelectrolyte brush were investigated. By force-mapping a pattern with brush-free areas, the separation on the polyelectrolyte brush could be defined without reaching the constant compliance regime.

MM 28.25 Tue 18:30 Poster E

Characterization of bioinspired hybrid materials by multi-scale analysis — •Britta Seidt[1], André Gjardy[1], Keith Gregorzyk[2], Mato Knez[2], Valeria Samsoninkova[3], Felix Hansske[3], Hans Börner[3], Peter Fratzl[1], and Wolfgang Wagermaier[1] — [1]Max Planck Institute of Colloids and Interfaces, Germany — [2]CIC nanoGune Consolider, Spain — [3]Humboldt-Universität zu Berlin, Germany

Specially designed hybrid materials can be used as a model system to compare its properties and structural design principles with those of biological materials such as bone. We aim to develop new combinations of multi scale analytic tools, to investigate the correlation between macroscopic material mechanics and microscopic structure of bioinspired hybrid materials. To understand deformation processes in two model systems, X-ray scattering techniques and tensile testing experiments were combined in a specially designed apparatus. The first model system is a composite material, composed of submicron metal fluoride particles embedded in a poly(ethylene oxide) matrix. First results allow us to follow crystal orientation effects during tensile testing, indicating a reorientation of crystalline domains in the material. The second model system is based on natural collagen extracted from turkey leg tendons as organic part infiltrated with different metals. We investigated the usability of these tendons as matrices for metal infiltration and compared untreated collagen with metal-infiltrated collagen. First results lead us to the assumption of a directional embedding of the metals into the collagen structure.

MM 28.26 Tue 18:30 Poster E

Characteristics of the artificial nanocrystalline calcium carbonate microlens arrays subjected to the amorphous/crystalline phase transformation — •Ingo Schmidt[1], Kyubock Lee[2], Emil Zolotoyabko[3], Peter Werner[4], Peter Fratzl[1], and Wolfgang Wagermaier[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Korea Institute of Energy Research, Daejeon, Korea — [3]Technion - Israel Institute of Technology, Haifa, Israel — [4]Max Planck Institute of Microstructure Physics, Halle, Germany

Natural biogenic materials with extraordinary properties, which often reveal a hierarchical arrangement of simple building blocks, serve as a comprehensive source for bio-inspired synthetic materials. Here we present structural aspects of nanocrystalline bioinspired calcite microlens arrays fabricated via an amorphous pre-phase. By the aid of polarized light microscopy we show that the calcite MLA crystallizes in spherulite-like patterns without changing the shape of individual microlenses. By mapping the local mean crystal orientations by microfocus X-ray diffraction, we find that the crystallization front propagates radially from the nucleation event, with the c-axis of calcite

being the crystal growth direction. TEM observations indicate an average calcite crystal size of about 15-20 nm. Such nanocrystallites minimize birefringent effects and inhibit undesirable light scattering at grain boundaries. The knowledge of the MLA crystallization pathways may give us new information on biomineralization processes in calcite-based bio-composites.

MM 28.27 Tue 18:30 Poster E

Hydrophobic interaction governs unspecific adhesion of staphylococci: a single cell force spectroscopy study — •Nicolas Thewes[1], Peter Loskill[1], Philipp Jung[2], Henrik Peisker[2], Markus Bischoff[2], Mathias Herrmann[2], and Karin Jacobs[1] — [1]Saarland University, Saarbrücken, Germany — [2]Saarland University Hospital, Homburg/Saar, Germany

Unspecific adhesion of bacteria is usually the first step of biofilm formation on abiotic surfaces, yet it is unclear up to now which forces are governing this process. Alongside long-ranged van der Waals and electrostatic forces, short-ranged hydrophobic interaction plays an important role. To characterize the forces involved during approach and retraction of an individual bacterium to and from a surface, single cell force spectroscopy is applied: A single cell of the apathogenic species S. carnosus isolate TM300 is used as bacterial probe. With the exact same bacterium, hydrophobic and hydrophilic surfaces can be probed and compared. We find that as far as 50 nm from the surface, attractive forces can already be recorded, an indication of the involvement of long-ranged forces. Yet, comparing the surfaces of different surface energy, our results corroborate the model that large, bacterial cell wall proteins are responsible for adhesion, and that their interplay with the short-ranged hydrophobic interaction of the involved surfaces is mainly responsible for adhesion. The ostensibly long range of the attraction is a result of the large size of the cell wall proteins, searching for contact via hydrophobic interaction. The model also explains the strong (weak) adhesion of S. carnosus to hydrophobic (hydrophilic) surfaces.

MM 28.28 Tue 18:30 Poster E

The influence of the stacking fault energy on the microstructure evolution of severely deformed Cu-Ni alloys — •Friederike Emeis, Gerhard Wilde, Harald Rösner, and Matthias Wegner — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, D-48149

Copper and nickel are completely miscible in the liquid and solid state forming face-centered cubic alloys. The microstructure evolution of different compositions (10/90, 50/50 and 90/10) was investigated after severe plastic deformation using high pressure torsion (HPT) followed by annealing. The grain size is thus reduced and the hardness increases. This microstructure evolution is influenced by the stacking fault energy (SFE). The SFE indicates how easily dislocations can form, which are required to operate for an easy plastic flow of the material. Other factors, such as precipitation hardening, can be neglected due to the complete miscibility. The grain size distributions, twin densities, dislocation densities and hardness were characterized using electron backscatter diffraction (EBSD) and Vickers Hardness measurements. The SFEs of the different alloys were experimentally determined by the dissociation width of the present dislocations using transmission electron microscopy (TEM). The obtained results are discussed.

MM 28.29 Tue 18:30 Poster E

Hot Isostatic Pressed Tungsten Fiber-Reinforced Tungsten — •Bruno Jasper[1], Jan W. Coenen[1], Johann Riesch[2], Till Höschen[2], and Christian Linsmeier[1] — [1]Forschungszentrum Juelich GmbH, IEK4 - Plasmaphysik, 52425 Jülich, Germany — [2]Max-Planck-Institut für Plasmaphysik, 85748 Garching, Germany

Tungsten fiber-reinforced tungsten (W_f/W) is a composite material that addresses the brittleness of tungsten (W) at low temperatures and after operational embrittlement, through extrinsic toughening by introducing crack energy dissipation mechanisms. Existing W_f/W samples produced via chemical vapor infiltration indeed showed higher toughness in mechanical tests than pure W. In this contribution W_f/W material specimens produced via powder metallurgical (PM) methods, e.g. hot isostatic pressing (HIP), are shown. A variety of measurements, e.g. 3-point bending and push-out tests, are presented to verify the operation of the expected toughening mechanisms. Therefore the focus of the investigations lies on the interface deboning behavior. In particular, the stability and integrity of the interface is investigated, since high temperatures (up to 1900 °C) and pressures (200 MPa) are present during the composite preparation. First HIP single-fiber samples indicate a compact matrix with densities of 99+ % of the theoretical density of W and showed signs of recrystallization and grain growth. SEM analysis demonstrates an intact interface with indentations of powder particles at the interface-matrix boundary. Push-out test results indicate that the structure of the interface may be damaged by HIPing since push-out of matrix elements is observed.

MM 28.30 Tue 18:30 Poster E

Effect of Mg addition on the mechanical properties of a Zn-Al-Cu alloy — •Zhicheng Wu, Liang Wu, Weiping Hu, Günter Gottstein, and Sandra Korte-Kerzel — Institut für Metallkunde und Metallphysik, RWTH Aachen, Kopernikusstr. 14, D-52074 Aachen, GERMANY

Zinc alloys are liable to creep even at only moderately elevated temperatures due to their low melting point of around 380°C. In order to increase the strength and especially the creep resistance of a Zn-Al-Cu alloy by solid solution and precipitation strengthening, the effect of Mg addition was studied. On the basis of the composition of the commercial alloy Z410 (4wt% Al, 0.5wt% Cu), three laboratory alloys were produced with different amounts of Mg (0.04wt%, 0.2wt% and 0.3wt%) and characterized in terms of their mechanical properties and microstructure using tensile tests in conjunction with scanning and transmission electron microscopy. Tensile tests were performed at RT, 55°C and 85°C and strain rates of 5×10^{-4}, 5×10^{-5} and $6\times10^{-6}/s^{-1}$. The true stress - true stain curves revealed at low strain rates (5×10^{-5} and $6\times10^{-6}/s^{-1}$) a regime with a nearly constant work softening rate. Based on the low strain rate tests, the steady state creep rate of the investigated Zn alloys was approximated in order to estimate the creep activation energy and stress exponent of the studied Zn alloys. It was found that the Zn alloy with medium Mg content (0.2wt%) had the highest yield strength both at RT and elevated temperatures and also the highest activation energy for creep. The underlying physical mechanisms of the observed phenomena will be briefly discussed.

MM 28.31 Tue 18:30 Poster E

Flow curve simulations of aluminum binary alloys — •Volker Pankoke[1], Volker Mohles[1], Philipp Schumacher[2], and Benjamin Milkereit[2] — [1]RWTH Aachen Univerity, Institute of Physical Metallurgy and Metal Physics, Aachen, Germany — [2]University of Rostock, Chair of Materials Science, Rostock, Germany

A work hardening model based on four different types of dislocation densities is used to calculate flow curves of aluminum alloys in a temperature range from 30 to 500°C and strain rates of 0.1 and $0.001s^{-1}$. Experimental input comes from stress strain curve measurements on Al-Si alloys with different Si content and precipitates, depending on the cooling rate settings of the alloy. During cooling the precipitation behavior of the samples is investigated by Differential Scanning Calorimetry (DSC) to measure and control precipitation. To describe the plasticity of the alloys with the Four Internal Variable Model (4IVM), solute atoms must be taken into account. The corresponding formulation of the previous model 3IVM+ failed for the Al-Si alloys under consideration. Several approaches were tested in order to develop a new model for solid solution strengthening. Among them are the assumption of a short range order stress which depends on temperature but not on the different strain rates. Additionally the effect of Cottrell-clouds is implemented in the model, which leads to a range of abnormal thermal dependence of the flow stress and to jerky flow under certain conditions. The simulated flow curves and their serrations are compared to the measurements.

MM 28.32 Tue 18:30 Poster E

Strong correlation between acoustic and electromagnetic emissions during plastic deformation and destruction in solids — Dimitris Mastrogiannis[1], Tatiana Antsygina[2], •Konstantin Chishko[2], Claire Mavromatou[1], and Vassilios Hadjicontis[1] — [1]University of Athens, Panepistimiopolis, Zografos, TK 157 84, Athens, Greece — [2]B. Verkin Institute for Low Temperature Physics and Engineering, 47 Lenin Ave., 61103 Kharkov, Ukraine

Simultaneous acoustic (AE) and electromagnetic (EME) emissions during uniaxial compression of LiF monocrystals and polycrystalline natural rocks are studied experimentally and interpreted theoretically. It is proved the strong correlation between AE and EME in solids of different types. It means that both AE and EME have the same physical background in evolution of crystal lattice defects (dislocations, vacancies, cracks) during plastic deformation and destruction, despite the different ways to form acoustic or electromagnetic response from the same deformation act. Generation of EME is due to macroscopic polar-

ization currents generated by dynamic lattice defects. In ionic crystals the currents are produced through pinning-unpinning between charged vacancies and dislocation lines which can transport the vacancies on macroscopically long distances. Granites are piezoelectric composites where deformation is mainly due to microcracking acts. Electromagnetic signal in this case forms within two steps: first, a short pulse from free charge re-distribution at crack nucleation, and, second, an electromagnetic satellite of emitted acoustic wave. EME is prospective for practical applications in areas where the only AE was used before.

MM 28.33 Tue 18:30 Poster E

(Nano-)Mechanical properties of intermetallic phases in the Fe-Mo system at elevated temperatures — •Sebastian Schröders and Sandra Korte-Kerzel — Institut für Metallkunde und Metallphysik, RWTH Aachen University, Kopernikustrasse 14, 52056 Aachen, Deutschland

Topologically close packed (TCP) intermetallic phases which precipitate in nickel-base superalloys are suspected to cause a deterioration of the mechanical properties of the γ - γ* matrix. Although the existing intermetallics, namely Laves-, R-, sigma- and mue-phases are well understood in terms of their structure, their mechanical properties have still not been investigated in detail due to their size and pronounced brittleness. In order to investigate the plastic deformation behavior of these phases, but exclude the effect of complex phase composition in the first instance, the Fe-Mo system was chosen as a model system, where all phases are available as binary alloys. Using nanomechanical testing methods like nanoindentation and micropillar-compression, the experimental challenges of high brittleness and anisotropy encountered in conventional testing can be disregarded and plastic deformation can be achieved due to the confining pressure in nanoindentation and the reduction in specimen size in microcompression. This work aims to examine the mechanical properties such as elastic modulus, yield and flow stress of intermetallic Fe-Mo phases over a range of temperatures. To this end, tests were performed in vacuum. Based on this type of study it is envisaged to form a better understanding of the way hard TCP precipitates influence the performance of superalloys.

MM 28.34 Tue 18:30 Poster E

Influence of heterogeneities on the fracture behavior of NiAl — •Polina N. Baranova, Johannes J. Möller, and Erik Bitzek — Department of Material Sciences & Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany

The fracture of a brittle solid is crucially determined by material heterogeneities directly at the crack front where the stress field diverges. Here, the usual homogenization strategies of continuum mechanics are no longer applicable, and currently there exist no consistent theory that relates local fluctuations in elastic properties, cohesion, toughness, or stress fields to the local fracture behavior and macroscopic failure criteria. Here we present atomistic simulations of static and propagating cracks in the Ni-Al system to study the influence of heterogeneities on the fracture behavior. Heterogeneities on the atomic scale were introduced by varying the composition of B2 NiAl, whereas voids and Ni-precipitates served as mesoscale heterogeneities. The simulation results are compared to experiments and discussed in the framework of linear elastic fracture mechanics for heterogeneous media.

MM 28.35 Tue 18:30 Poster E

Applying the concept of gradient elastic tensors in the determination of dislocation densities in MAX phases — Christoph Brüsewitz[1], Ulrich Vetter[1], •Hans Hofsäss[1], and Michel W. Barsoum[2] — [1]II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [2]Dep. Mat. Sci. & Eng., Drexel University, Philadelphia, PA 19104, USA

MAX phases provide an unusual combination of both metallic and ceramic properties. Their remarkable mechanical properties, especially their damage tolerance, are still not fully understood and are subject of current debates. In this context, a way to *in-situ* determine dislocation densities under deformation would be most helpful.

We will present an attempt for this determination that is based on an hyperfine interaction method, the perturbed angular correlation spectroscopy, by using the sensitivity of the electric field gradient (EFG) at a nucleus on the strain field of defects. The relevant parameter is the broadening of the EFG tensor components. The coupling between EFG tensor and strain field is generally described by the gradient elastic tensor whose structure is determined by the point group of the corresponding nucleus. In case of the MAX phases, the tensor components are experimentally not determinable which is why density functional theory calculations implemented in Wien2k were used instead. Based on these calculations, a first estimation of deformation induced dislocation densities is given.