MM 12: Poster session I

Time: Monday 19:15–20:45 Location: Poster C

MM 12.1 Mon 19:15 Poster C

Amorphous interlayers in semiconductor metallization — •Dennis König, Efi Hadjixenophontos, Guido Schmitz, and Kevin Treder — Institute of Materials Sience, Chair of Material Physics, University of Stuttgart, Heisenbergstraße 3, 70569, Germany

Deposition of thin metallic films on monocrystalline silicon substrates has been extensively used in the past. An amorphous interlayer of few nm, between the silicon and the metallic coating is reported in such systems. During this work detailed investigation on this interlayer is done. Different parameters are studied such as: The cleaning time of the substrates, the power during deposition and the metallic element (Al, Au and Ag) in contact with the substrate. Samples are prepared by Ion beam sputtering with controlled thicknesses and are characterized by HRTEM after FIB cross sections. Further elemental analysis is done by EDX during microscopy. A clear dependency of the thickness of interlayer is observed on the cleaning time and power during deposition. Attempts to identify the composition of the amorphous interlayer are performed by Atom Probe Tomography.

MM 12.2 Mon 19:15 Poster C

Chemical bonding effects on the brittle-to-ductile transition in metallic glasses — •Franco Moitzi[1], Daniel Sopu[1,2], and Jürgen Eckert[1,3] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, 8700 Leoben, Austria — [2]Institut für Materialwissenschaft, Technische Universität Darmstadt, Otto-Berndt-Straße 3, 64287 Darmstadt, Germany — [3]Department Materials Physics, Montanuniversität Leoben, Jahnstraße 12, 8700, Leoben, Austria

By using molecular dynamics simulations we investigate the influences of composition and temperature on tensile deformation behavior of amorphous PdSi and CuZr alloys. While the plastic deformation in CuZr metallic glass occurs highly localized in one mature shear band, PdSi glass shows brittle cracking perpendicular to the loading direction. The crystal orbital hamilton population analysis based on electronic structure calculation from electronic structure calculation has revealed that the difference in the chemical bonding is responsible for the observed different deformation behaviors. The rigidity of the bonding impedes the strain and stress redistribution in PdSi metal-metalloid glasses and leads the brittle failure. Moreover, a brittle-to-ductile transition can be achieved upon increasing the temperature or/and decreasing the amount of silicon. The prevention of stress accumulation due to stress redistribution is identified to be the reason for the observed transition.

MM 12.3 Mon 19:15 Poster C

3D X-ray Diffraction Microscopy (3DXRD) using high resolution X-ray nanodiffraction — •Hergen Stieglitz[1], Christina Krywka[1], and Martin Müller[1,2] — [1]Helmholtz-Zentrum Geesthacht, Geesthacht, Deutschland — [2]Universität Kiel, Kiel, Deutschland

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

The planned experiment shall utilize a nano-focused synchrotron beam (e.g. Nanofocus Endstation of P03, PETRA III) to examine very fine-grained systems. The small beamsize allows detecting grains below the size limit of standard 3DXRD. With respect to the small beamsize of about 250 nm cross section, the precise positioning of the sample becomes more important to secure a constant scanned volume (the so called gauge volume). Otherwise some grains may be outside the gauge volume in some scans therefore they cannot be traced and produce mistakes while reconstructing.

To meet this challenge a stable and wobble-free rotary stage is planned to ensure a constant gauge volume. We are planning to use an interferomenter-based feedback loop to compensate the runout of the sample with a XY-stage.

MM 12.4 Mon 19:15 Poster C

Combining small-angle neutron scattering and analytical microscopy: An advanced method to characterize nano-precipitates in Ni-based superalloys — •Robert Lawitzki[1], Ralph Gilles[2], Michael Hofmann[2], Julia Wagner[1], and Guido Schmitz[1] — [1]Universität Stuttgart, IMW, Lehrstuhl für Materialphysik — [2]TU München, FRMII

We present an experimental method for the differentiation and quantification of the two strengthening phases, γ' and γ", in the Ni-based superalloy Inconel 718. For this alloy, an individual quantification of those phases is experimentally very difficult and was, by now, only achieved by nano-scaled characterization techniques. In this contribution, we were applying the technique small-angle neutron scattering (SANS) on differently heat-treated specimens to individually quantify the nanoprecipitates in bulk average. The interpretation of the SANS signal required a structural model that could only be set up by complementary information that were obtained mainly by transmission electron microscopy (TEM) and atom probe tomography (APT). The advantage of using bulk neutron diffraction for quantification is that several tens of cubic millimeters are analyzed and thus, significantly better statistics are obtained. The measured volume fractions of the γ"- precipitates are remarkably lower than stated in previous works, but now well fulfill the chemical mass balance. It will be further shown how this method can be adapted to other superalloys.

MM 12.5 Mon 19:15 Poster C

Real-time monitoring of laser powder bed fusion process using high-speed X-ray imaging — •Jan Rosigkeit[1], Dieter Lott[1], Marc-André Nielsen[1], Benjamin Wahlmann[2], Tao Sun[3], Marcus Rackel[1], Peter Staron[1], Florian Pyczak[1], and Martin Müller[1] — [1]Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Germany — [2]Department of Materials Science and Engineering, University of Erlangen-Nuremberg, Germany — [3]Advanced Photon Source, Argonne National Laboratory, USA

We employ the high-speed synchrotron hard X-ray imaging technique to monitor the laser powder bed fusion process of Ti-6Al-4V powder on a Ti-42Al-8.5Nb-0.2C base plate in situ and in real time. Many scientifically and technologically significant phenomena in laser powder bed fusion, including melt pool dynamics, powder ejection, rapid solidification and keyhole pore formation are experimentally revealed with high spatial and temporal resolutions. The data present here will facilitate the understanding of dynamics and kinetics in metal laser powder bed fusion process.

The laser beam carrying various powers entered into the chamber straight down on the powder bed. The laser was operated in a spot-heating mode and in a line scanning mode. The X-ray beam impinged on the samples horizontally providing a side view of the powder bed.

All image series were taken with a frame rate of 50 kHz and an exposure time of 1 μs for each individual image. It can be observed that the process starts with the melting of theTi-6Al-4V powder around the laser spot and then the Ti-42Al-8.5Nb-0.2C base plate.

MM 12.6 Mon 19:15 Poster C

Status of the materials science x-ray scattering beamline BL9 of DELTA — •Michael Paulus, Christian Sternemann, and Metin Tolan — Fakultät Physik/DELTA, Technische Universität Dortmund, D-44221 Dortmund, Germany

Beamline BL9 is a multi-purpose x-ray scattering beamline at the synchrotron radiation facility DELTA located at the TU Dortmund, Dortmund, Germany. The beamline is dedicated to x-ray reflectivity, x-ray diffraction, small-angle x-ray scattering and fluorescence experiments using hard x-rays predominantly in the energy range between 10 keV and 30 keV. The current experimental setup will be presented and selected examples of prototype experiments will be given, ranging from investigations of biological to solid state samples as well as applications in cultural heritage. Future experimental perspectives will be discussed in light of the implementation of a new superconducting wiggler.

MM 12.7 Mon 19:15 Poster C

Deoxidation of copper surfaces by a dilectric barrier discharge plasma — •Aaron Arendt[1], Sebastian Dahle[1], and Wolfgang Maus-Friedrichs[1,2] — [1]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 9, 38678 Clausthal-Zellerfeld, Germany

— [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The production in the metalworking industry takes place in the presence of oxygen. Although, attempts are made to keep the concentration of oxygen low with the aid of technical high vacuum and inert gases, there is still an oxide layer on the metal surfaces, which can form immediately under these conditions. This oxide layer could be advantageous for applications, for example in joining processes. State of the art is to reduce the surface by heat treatment with the help of high temperatures in order to make connections possible. Here, we present an alternative process in form of a DBE plasma in an argon/hydrogen atmosphere using the example of an oxidized copper sample. This plasma is used to reduce the copper oxide surface at room temperature. To reduce also deeper layers, the copper is additionally heated to allow diffusion processes to take place. X-ray photoelectron spectroscopy (XPS) is used to investigate the surface stoichiometry and depth profiling is done with a combination of sputtering and auger electron spectroscopy (AES). We show that 60 s of plasma treatment leads to an appreciable deoxidation of the copper surface.

MM 12.8 Mon 19:15 Poster C

The inline branch of the Swedish Materials Science Beamline P21.2 at PETRA III — •Timo Müller, Zoltan Hegedüs, Sven Gutschmidt, Thomas Bäcker, and Ulrich Lienert — Deutsches Elektronen-Synchrotron DESY, Photon Science, Hamburg, Germany

The high-energy beamline P21 at the third generation synchrotron source PETRA III is dedicated to materials science and is funded by Sweden. The instrumentation of the inline branch, P21.2, is designed to combine complementary experimental techniques (WAXS/SAXS/imaging) for the investigation of bulk samples and interfaces. The photon energy can be chosen in the range from 40 to 150 keV. The beam size can be varied from millimeters down to (sub-) microns by focusing with compound refractive lenses. This is the basis for the in-situ characterization of microstructures and phase transformations using various techniques, particularly during thermo-mechanical processing. The beamline has seen first light in September 2018 and is currently in its commissioning phase. First results will be presented and discussed. The goal is to give a comprehensive overview of the possibilities for future user experiments, since the beamline will start user operation in the second half of 2019.

MM 12.9 Mon 19:15 Poster C

the structural, thermodynamics, nonlinear properties and vibrational analysis of 4',5'-dibromo-2',7'-dinitro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3',6'-diolate — •Jean Baptiste Famkam Fankam[1], Jean Mari Bienvevu Ndjaka[1], and Jeh Wilson Geh[2] — [1]University of Yaounde I, Yaounde, Cameroon — [2]National Higher Polytechnic Institute, University of Bamenda, Bamenda, Cameroon

This review gives an overview concerning the structural, thermodynamics, nonlinear properties and Vibrational analysis of 4',5'-dibromo-2',7'-dinitro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3',6'-diolate which has been theoretically studied. We used the RHF and DFT (PBE1PBE, MPW1PW91, B3PW91 and B3LYP) approach to calculate the optimized parameters, Dipole moment **, average polarizability *α*, anisotropy ***, first hyperpolarizabilitiesβ, the zero-point vibrational energy ZPVE, sum of electronic energy without zero-point correction Eelec, with zero-point correction E0, with thermal energy E, with enthalpies H, with free energies G, contribution of thermal energy correction Ethermal, molar heat capacity at constant volume Cv and entropy S with cc-pVDZ basis set. In addition, we also computed IR and Raman activity spectrum. Our results suggest that this molecule have potential applications as linear and nonlinear optical materials. In spite of the large hyperpolarizability of this molecule, we are optimistic that this molecule has a potential application in the *eld of optoelectronic and medicine. This can be a promising material for optical limiting applications.

MM 12.10 Mon 19:15 Poster C

Analysis of the phase transition processes of sodium borohydride and first tests about its rehydration by means of cold dielectric barrier discharge plasmas — •Maik Szafarska[1,2], Georgia Sourkouni-Argirusi[1], and Wolfgang Maus-Friedrichs[1,2] — [1]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

In the last decade, sodium borohydride has attracted attention in energy storage research, caused by its high hydrogen density and relatively low cost, making it a potentially better hydrogen (and energy) storage unit compared to compressed hydrogen gas tanks and liquid hydrogen. Therefore it would be an innovation for fuel cell economy and energy storage. To make it economically viable, its dehydration temperature has to be lowered and a new rehydration method has to be found. The phase transition mechanisms are a key for understanding the behavior of the material during these two processes. To investigate the phase transition and the rehydration of the material further, Thermogravimetric- and Multi Gas-Analysis were performed. The experimental results show that released hydrogen and the decomposition of the material occur during different phase transitions. Additionally first tests about the rehydration via dielectric barrier discharge plasmas show optimistic results.

MM 12.11 Mon 19:15 Poster C

Ab-initio Phase Stabilities of Ce-based Hard Magnetic Materials — •Halil ibrahim Sözen, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany

Due to the developments in e-mobility and renewable energies, hard magnets composed of rare earths have gained increasing importance in the last decades. Recently, there is a growing interest in developing alternative hard magnetic materials, that reduce or even remove the need to use their expensive RE elements. The strategy is to use 3d elements with high magnetic anisotropy such as e.g. Fe-Co-B alloys. In order to support these efforts, we performed ab initio calculations of finite temperature phase stabilities of Ce-based alloys. The Helmholtz free energy F(T, V) is calculated for all relevant competing phases using a sophisticated set of methods capturing vibrational, electronic, magnetic and configurational entropy contributions. The study includes unary Ce, binaries of Ce-Fe and Fe-Ti phases, and ternary Ce-Fe-Ti phases. In a first step, we test the performance of our approach and find good agreement with experimental data. In a second step, we calculate the finite temperature phase formation diagram. This diagram shows that the presence of the CeFe2 phase prevents any formation of the targeted hard magnetic Ce-Fe-Ti alloys. This observation is supported by recent EDS experiments. In a third step, we, therefore, extend our study to quaternary alloys. Specifically, we study the effects of Cu and Ga substitution by introducing a screening scheme that allows testing all 3d and 4d elements.

MM 12.12 Mon 19:15 Poster C

Beyond the typical use of symmetry in Crystal structure prediction — •James Darby — TCM, Cavendish lab, University of Cambridge, UK

First-principles crystal structure prediction (CSP) is a well established technique which is routinely used to predict crystal structure in a diverse range of systems such as periodic solids, interfaces, encapsulated nanowires etc. However, one downside of CSP is that the number of minima in the potential energy surface scales exponentially with system size. As such, it rapidly becomes computationally unfeasible to search for more complex structures with larger unit cells. Here we discuss how going beyond the normal use of symmetry in CSP can be used to overcome this difficulty and work with more complex systems. In particular we focus on the generation of symmetric trial structures and how the distribution of these can lead to very biased searching if not done carefully. Results from structure searching using a modified version of the ab initio random search technique, and the CASTEP density functional theory code, will also be presented. In particular Magnesium Sulfide compounds will be discussed with reference to their use as anode materials in Magnesium ion batteries.

MM 12.13 Mon 19:15 Poster C

icet - A Pythonic approach to cluster expansions — •Mattias Ångqvist[1], William A. Muñoz[1], J. Magnus Rahm[1], Erik Fransson[1], Paul Erhart[1], Céline Durniak[2], Piotr Rozyczko[2], and Thomas Holm Rod[2] — [1]Chalmers University of Technology, Department of Physics, Gothenburg, Sweden — [2]Data Management and Software Centre, European Spallation Source, Copenhagen, Denmark

Many materials exhibit some form of chemical ordering, which can have a crucial impact on their macroscopic properties. Here, atomic scale modeling based on the so-called alloy cluster expansion (CE) technique can yield very valuable information. In this contribution, we present the open-source icet package that provides an efficient implementation of this methodology. It takes advantage of state-of-the-art ma-

chine learning techniques to generate accurate and predictive models based on quantum mechanical calculations. The ICET package features a Python interface that enables seamless integration with other Python libraries including for example SciPy or scikit-learn. Yet, all computationally demanding parts are written in C++ providing performance while maintaining portability. We demonstrate the application of ICET by (1) studying chemical ordering and associated properties in a series of intermetallic clathrates as a function of composition and temperature and (2) by predicting the phase diagrams of bulk and surface alloys.

MM 12.14 Mon 19:15 Poster C

Atomistic Simulation of Incipient Plasticity in Compressed Au Nanowires — •Aviral Vaid[1], Subin Lee[2], Julien Guenole[1], Arun Prakash[1], Sang Ho Oh[2], and Erik Bitzek[1] — [1]Materials Science and Engineering, Institute I, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Department of Energy Science, Sungkyunkwan University (SKKU), Suwon, Republic of Korea

Modern in-situ TEM experiments offer a unique possibility of imaging the nucleation of dislocations and the resulting plasticity in metallic nanowires. But the time resolution of these experiments is often too limited to study the details of dislocation-based deformation processes. Here, we present our results on recent atomistic simulations addressing the mechanisms and conditions under which prismatic dislocation loops can form during uniaxial compression tests of [110] oriented Au nanowires as reported by Lee et. al (Nat. Comm., 2014, 5, 3033). Such dislocations with Burgers vector parallel to the compression axis were unexpected, as they experience no resolved shear stress during uniaxial compression. Molecular dynamics simulations using an EAM potential and different indenter types and radii as well as nanowire geometries and sizes allowed to reproduce the observed prismatic dislocation loops and identify their formation mechanism. Building a model based on the geometry of the nanowire cap and the indenter radius, we derived a criterion under which conditions prismatic loops could form. Furthermore, we deduced the size range of asperities on the nominally flat punch indenter necessary for the formation the prismatic dislocation loops observed in experiments.

MM 12.15 Mon 19:15 Poster C

Tuning the electronic structure of organometallic Kagome systems — •Marius Fuchs, Domenico Di Sante, and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg

We investigate organometallic Kagome systems consisting of 2 metal ions coordinated by DCA organic groups. The system was predicted to exhibit characteristic Kagome bands close the the Fermi level as a result of tight binding-like interaction of 'superatomic' p-orbitals originating in the organic system[1]. Our investigation focuses on tuning the electronic structure of synthesizable[2] thin films along with constituent metal ions and possible doping. In that we give special attention to the Fermi surface and its potential instabilities at van-Hove filling.

[1] L. Z. Zhang et al. 2016, Intrinsic Two-Dimensional Organic Topological Insulators in Metal - Dicyanoanthracene Lattices, NanoLetters, 16, 2072 - 2075

[2] G. Pawin et al. 2008, A Surface Coordination Network Based on Substrate-Derived Metal Adatoms with Local Charge Excess, Angew. Chem. Int. Ed. 2008, 47, 8442 - 8445

MM 12.16 Mon 19:15 Poster C

Atomistic investigation of non-stoichiometric stacking faults in Fe-Nb alloys — •Ali Zendegani[1], Michaela Šlapáková Poková[1,2], Christian Liebscher[1], Frank Stein[1], Sharvan Kumar[3], Thomas Hammerschmidt[4], Fritz Körmann[1], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Charles University, Prague, Czech Republic — [3]Brown University, Providence, USA — [4]Ruhr-Universität Bochum, Bochum, Germany

In Fe-Nb alloys a hardening via tetrahedrally close-packed (TCP) phases (e.g. Laves Fe_2Nb and μ Fe_7Nb_6) can be achieved. At the same time, various types of stacking faults occur during deformation. To investigate the correlation of both features in a Nb-rich Laves phase, *ab initio* calculations are combined with thermodynamics concepts.

By performing gamma surface calculations we resolve the atomic structure of these planar faults and show that they have a surprising geometrical complexity. Introducing a new thermodynamic framework allows us to compare the stability of planar faults (2D) with bulk phases (3D) in a convex hull diagram. The resulting diagram reveals that Nb-rich crystal structures next to basal and pyramidal stacking faults can become energetically more favorable than the nucleation of an epitaxially constrained μ phase. Excess Nb results thus in an enhanced formation of 2D stacking faults rather than forming 3D Nb rich precipitates in form of the μ phase. This unexpected finding allows a direct interpretation of recent HR-TEM studies on this materials system.

MM 12.17 Mon 19:15 Poster C

A first-principle self-consistent phonon approach for studying the vibrational properties of the high-temperature phases of pervoskites. — •Sohaib Ehsan, Marco Arrigoni, Georg Madsen, and Peter Blaha — Institute of Materials Chemistry, Vienna University of Technology, Vienna, Austria

In this study we investigate the phonon properties of perovskites in their high-temperature phases by first- principle methods. We use BaTiO3 , which shows a stable cubic phase above 120 C, as a model material. Due to the presence of unstable phonon modes in the harmonic approximation, we include an-harmonicity by calculating self-consistently temperature-dependent interatomic force constants. We show that in this way we are able to reproduce the experimentally observed phonon dispersion relations. Such approach allows to predict other vibrational properties of these compounds, such as the transition temperature between the low- and high-symmetry phases and the lattice thermal conductivity.

MM 12.18 Mon 19:15 Poster C

The AiiDA-KKR plugin for high-throughput ab-initio impurity embedding — •Fabian Bertoldo, Philipp Rüssmann, Jens Bröder, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present the AiiDA-KKR package [1,2] which enables users to conveniently perform complex tasks with the JuKKR package through AiiDA [3] (Automated interactive infrastructure and database for material science). Therefore, the plugin and its respective workflows are introduced. They significantly reduce the workload of the user by automating most of the trivial steps of large-scale scientific calculations. Especially, results will be stored in a database and the provenance of all conducted steps (inputs, checkpoints, results) can be tracked and accessed at any desired point. The workflows and calculation can be launched with simple python scripts. Using this framework, we calculate the behavior of impurities in different host systems. Due to the high-throughput design of AiiDA and the AiiDA-KKR package we are now able to investigate multiple of those impurities in an easy manner which was not possible before by just using the plain KKR code.

[1] https://github.com/JuDFTteam/aiida-kkr

[2] https://aiida-kkr.readthedocs.io

[3] G. Pizzi, et al. Comp. Mat. Sci. 111, 218-230 (2016)

MM 12.19 Mon 19:15 Poster C

Mixing thermodynamics of MoO_3–WO_3 solid solutions from first-principles calculations — •Jongmin Yun[1], Ricardo Grau-Crespo[2], and Aloysius Soon[1] — [1]Department of Materials Science & Engineering, Yonsei University, Seoul 03722, Korea — [2]Department of Chemistry, University of Reading, Reading RG6 6AD, United Kingdom

To date, solid solutions of high work-function transition metal oxides, e.g., MoO_3 and WO_3 are still poorly understood due to the complexity of site-occupancy disorder in these solid solution systems. Having a deeper understanding of these oxide solid solution systems will greatly benefit the engineering of new oxide heterojunction devices. Here, we perform first-principles density-functional theory calculations for the $(MoO_3)_x(WO_3)_{1-x}$ solid solution and multi–configurational supercell analysis for the reliable mixing thermodynamics. Namely, we aim to report the relative thermodynamic stability of these solid solutions as a function of mixing ratios with regards to the parent polymorphic phases. Moreover, we examine the trends in the electronic structure of the energetically favored configurations.

MM 12.20 Mon 19:15 Poster C

pyiron - an integrated development environment (IDE) for computational material science — •Jan Janssen[1], Sudarsan Surendralal[1], Osamu Waseda[1], Liam Huber[1], Yury Lysogorskiy[2], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany — [2]Interdisciplinary Centre

for Advanced Materials Simulation (ICAMS), Bochum, Germany

The past years witnessed tremendous progress in computational materials science both with respect to predictive power and scalability (e.g. high-throughput computations). These advances are not only related to the large gain in computer power but often to the development of advanced and computationally highly efficient algorithms and methods. A challenge in this respect is that the resulting simulation protocols are getting ever more complex: They often require the combination of high performance codes implemented in low-level programming languages with incompatible input/output formats, the implementation of flexible interfaces to dynamically adjust the order of the tasks in the simulation protocol, and the distribution of tasks on highly heterogeneous computing platforms. To foster the development of these novel techniques and their dissemination and use in our department we started several years ago with the development of the pyiron integrated development environment (http://pyiron.org). This framework allows to automatise routine tasks, to automatically store input/output data of all the individual jobs in a generic format together with the simulation protocols and the parent-child relationship of the tasks.

MM 12.21 Mon 19:15 Poster C

Computational study of the electronic properties of electrode materials — •Janis K. Eckhardt[1,2], Markus S. Friedrich[1,2], Simon Burkhardt[1,2], Michael Czerner[2,4], Matthias T. Elm[1,2,3], Christian Heiliger[2,4], and Peter J. Klar[1,2] — [1]Institut of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Center for Materials Research (LaMa), Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen, Germany — [4]Institute for Theoretical Physics, Heinrich-Buff-Ring 16, 35392 Giessen

Lithium ion batteries are widely used as power sources in portable electrical applications. In particular with regard to the optimization of existing applications or the development of new technologies, it is necessary to understand the fundamentals of ionic and electronic transport inside the active cathode material. Most scientists are examining cathode materials by using composite electrodes which also contain additives influencing their electrochemical properties. In order to avoid such influences, it is desirable to investigate the electrochemical properties of the pure active material. By performing density functional theory calculations, especially, with focus on equimolar lithium nickel cobalt manganese oxide (NCM-111), it was possible to gather additional information about its electronic structure. The screened Korringa-Kohn-Rostoker method has been employed in these calculations. Density of states calculations with reference to $Li_{1-x}[Ni_{1/3}Co_{1/3}Mn_{1/3}]O_2$ for different amounts of lithium within the crystal structure imply changes of the magnetic moment of the transition metals.

MM 12.22 Mon 19:15 Poster C

Smart-data machine learning for surface polymorph search — •Andreas Jeindl, Lukas Hörmann, Alexander T. Egger, and Oliver T. Hofmann — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

The major challenge of surface structure search is the large number of possible polymorphs. The SAMPLE approach [1,2] can help circumvent this problem. It combines a coarse-grained potential energy surface with Bayesian linear regression to efficiently predict the adsorption energies of an exhaustive set of commensurate organic monolayers.

In this contribution we present the SAMPLE approach. The first step is finding all local minima for a single molecule on the surface. We then create all possible combinations of these local minima up to a certain unit cell size. With the help of 'experimental design' theory, we select a subset of maximally diverse structures. This subset is evaluated with dispersion-corrected density functional theory and used as training set for a Bayesian linear regression model. The linear regression uses an energy model based on the assumption that the main interactions on the surface are governed by molecule-substrate interactions and pairwise molecule-molecule interactions. Thus, we can not only predict the adsorption energies of millions of possible polymorphs, but also gain meaningful physical insight.

We use three complementary molecules on coinage metals to showcase the capabilities of our approach.

[1] Scherbela et al., Phys. Rev. Materials 2, 043803
[2] Hörmann et al., arXiv:1811.11702

MM 12.23 Mon 19:15 Poster C

DFT study of the charge density wave metal LuNiC2 — •Soner Steiner[1,2,3], Herwig Michor[2], and Dominik Legut[1] — [1]IT4Innovations, VSB - Technical University of Ostrava, Ostrava, Czech Republic — [2]Institute of Solid State Physics, TU Wien, 1040 Wien, Austria — [3]University of Applied Sciences Wiener Neustadt, Austria

We have investigated the charge density wave (CDW) metal LuNiC2 by means of density functional theory (DFT) . We report on the electronic structure, fermi surface and the CDW transition. The formation of a significant gap due to the CDW transition is seen in the density of states at the Fermi level, which reduces the electronic density of states from N(Ef)=1.03 states/eV f.u. without CDW to N(Ef)=0.4 states/eV f.u. . The Sommerfeld value corresponding to the CDW density of states at the Fermi level is in reasonable agreement with the experimental value. The formation of the CDW modulated structure is causing a fragmentation of the Fermi surface into several isolated electron and hole pockets.

MM 12.24 Mon 19:15 Poster C

A first-principles study of the phase diagram of solid hydrogen — •Alice Shipley, John Trail, and Richard Needs — Cavendish Laboratory, University of Cambridge, UK

Hydrogen is the most abundant element in the universe and the simplest atom. However, the behaviour of dense hydrogen is far from simple. Solid hydrogen possesses a rich phase diagram and, as a substance predicted to exhibit room-temperature superconductivity at high pressures [PRL 21, 1748 (1968)], has been of experimental and theoretical interest for decades. In computational studies, density functional theory (DFT) traditionally offers an attractive balance between accuracy and cost; a consideration which is essential here as there are many candidate structures separated by static-lattice enthalpy differences on the order of meV/atom. It is therefore also essential to consider vibrational effects in order to determine phase stability. Unfortunately, the solid hydrogen phase diagrams produced using different standard exchange-correlation functionals do not qualitatively agree with one another. With this in mind, our work explores the accuracy of purpose-built exchange-correlation functionals for high-pressure hydrogen [PRB 95, 115116 (2017)]. The new pressure-temperature phase diagrams obtained will be presented alongside a discussion of the vibrational self-consistent field (VSCF) approach [PRB 87, 144302 (2013)] used to incorporate vibrational effects, including anharmonicity.

MM 12.25 Mon 19:15 Poster C

Hydrogen detection in high strength steels with Scanning Kelvin Probe Force Microscopy — •Ines Traxler[1,2], Gabriela Schimo-Aichhorn[1], Andreas Muhr[3], Gerald Luckeneder[3], Hubert Duchaczek[3], Karl-Heinz Stellnberger[3], Josef Faderl[3], Darya Rudomilova[4], Tomáš Prošek[4], and Sabine Hild[1,2] — [1]CEST Competence Center for Electrochemical Surface Technology, Viktor-Kaplan Str. 2, 2700 Wr. Neustadt and Stahlstr. 2-4, 4031 Linz, Austria — [2]Institute of Polymer Science, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria — [3]voestalpine Stahl GmbH, voestalpine-Str. 3, 4020 Linz, Austria — [4]UCT Prague, Zizkova 7, 27801 Kralupy, Czech Republic

Hydrogen embrittlement is a big problem in the automotive industry, as even small amounts of hydrogen have detrimental effects on steel properties. Scanning Kelvin Probe Force Microscopy (SKPFM) is a hopeful technique for the investigation of hydrogen in steel and the visualization in the individual steel phases with a very good spatial resolution. The impact of hydrogen diffusion on zinc coated high strength steels was investigated using SKPFM. Also, the hydrogen insertion at cut edges and coating defects was studied. To induce corrosion and to promote hydrogen entry into steel, various salt solutions were applied on the backside of uncoated and zinc coated dual phase steels. The hydrogen inserted into the sample is subsequently permeating through the steel until it reaches the other sample side,where the effect on the contact potential difference (CPD) and therefore the hydrogen permeation is monitored with SKPFM.

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AuCuNiPdPt as a benchmark for high entropy alloys — •Jens Freudenberger[1,2], Felix Thiel[1,3], Alexander Kauffmann[4], Martin Heilmaier[4], and Kornelius Nielsch[1,3] — [1]IFW Dresden — [2]TU Bergakademie Freiberg — [3]TU Dresden — [4]Karlsruhe Institut für Technologie

The high entropy alloy AuCuNiPdPt appears single-phase and with

the Cu-type structure. Additionally, non-stoichiometric alloys made from any of these elements with arbitary composition also crystallise single-phase with the Cu-type structure. Therefore, these alloys can be used to separate the material behaviour of the HEAs cleanly from that of single phase conventional alloys and to identify which issues are special for HEAs leading to their peculiar properties. The present study presents the mechanical behaviour and a microstructure analysis of AuCuNiPdPt.

MM 12.27 Mon 19:15 Poster C

Characterization of diffusive transport in polycrystalline tungsten trioxide thin films — •Jan L. Dornseifer[1,2], Alexander G. Strack[1,2], Simon Burkhardt[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-Universität, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-Universität, Germany

Tungsten trioxide (WO_3) is an electrochromic material, thus, it can change its optical properties through insertion of charge carriers. Its electrochromic properties depend on the deposition process and resulting morphology. Polycrystalline WO_3 thin films are prepared by electron-beam evaporation and a subsequent heat treatment at 450 °C. To investigate the diffusive transport of hydrogen in WO_3, the electrochemical properties are estimated by measurments using the galvanostatic intermittent titration technique (GITT) and electrochemical impedance spectroscopy (EIS). The impedance spectra obtained are fitted with a Randles circuit. The self-bleaching of WO_3 influences the experimental data in a significant way which has an impact on the evaluation of the data and the determination of the diffusion coefficients. In situ transmission measurements during the impedance spectroscopy reveals an oscillating behavior of the transmission at excitation signal frequencies below 91 mHz. This interesting behavior may yield additional information about the diffusive ion transport.

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Impact of Severe Plastic Deformation on Al_xCoCrFeNi High Entropy Alloys — •Lena Frommeyer[1], Mehdi Eizadjou[2], Anna Ceguerra[2], Peter K. Liaw[3], Harald Rösner[1], Sergiy Divinski[1], Simon Ringer[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Australian Center for Microscopy and Microanalysis, University of Sydney, Australia — [3]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, TN 37996, USA

During the last few years, a new class of materials called high entropy alloys has been extensively studied. The multi-principal element approach opens a wide compositional space with complex possibilities of combining 5 or more elements, each of them having originally equiatomic concentration. The main research focus was initially set to obtain single-phase alloys. However, secondary phases in alloys can lead to improved properties. In this study, the high entropy alloy AlCoCrFeNi was modified by adding Al in various amounts. Moreover, the arc melted and homogenized alloys have been severely deformed by high pressure torsion (HPT). Subsequently, the un-deformed as well as the severely deformed alloys were examined by X-ray diffraction, electron back-scatter diffraction/transmission Kikuchi diffraction, transmission electron microscopy, energy-dispersive X-ray spectroscopy and atom probe tomography. Transitions from pure fcc to fcc+B2 and to fcc+B2+A2 as well as severe grain refinement and high twin densities were observed and are discussed with respect to the variations of composition and strain.

MM 12.29 Mon 19:15 Poster C

Magnetic properties of the CoCrFeMnNi high entropy alloy — •Soner Steiner[1,2,3], Sergii Khmelevskyi[4], and Dominik Legut[1] — [1]IT4Innovations, VSB - Technical University of Ostrava, Ostrava, Czech Republic — [2]Institute of Solid State Physics, TU Wien, 1040 Wien, Austria — [3]University of Applied Sciences Wiener Neustadt, Austria — [4]Center for Computational Materials Science, Vienna University of Technology, Wiedner Hauptstrasse 8, 1040 Vienna, Austria

We investigated the elastic properties and magnetism of the high entropy alloy CoCrFeMnNi in the basis of first principles. We have calculated the elastic properties at elevated temperatures taking into account longitudinal spin fluctuations (LSF). We show that LSF essentially renormalize the elastic constants compared to those calculated for magnetically ordered state. With the use of calculated exchange constants in paramagnetic state we attempt to understand the kind of magnetic ordering in this system. We also employ the locally self-consistent Green's function (LSGF) within the exact muffin tin method (ELSGF) formalism to visualize the random spin glass like state by performing the first-principles calculations for large random supercells (up to 500 atoms).

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Experimental Studies of Helium Diffusion and Trapping in Tungsten — •Vassily Vadimovitch Burwitz[1,2,3], Thomas Schwarz-Selinger[2], Thomas Dürbeck[2], Georg Holzner[2,4], Rodrigo Arrendo Parra[2,4], and Christoph Hugenschmidt[1,3] — [1]Physik Department E21, TU München — [2]Max-Planck-Institut für Plasmaphysik (IPP) — [3]Heinz Maier-Leibnitz Zentrum (MLZ) — [4]Lehrstuhl für Plasma-Material-Wechselwirkung, Fakultät für Maschinenwesen, Technische Universität München, 85748 Garching, Germany

Helium is insoluble and highly mobile in tungsten. However, bubbles and blisters are commonly found in helium ion exposed samples. While the bubble growth parameters are known, the bubble nucleation process is still unclear. A hypothesized explanation based on ab initio calculations is a combination of self-trapping and trap mutation. Three independent experimental methods are used to check these predictions: Temperature Programmed Desorption (TPD), Elastic Recoil Detection Analysis (ERDA) and Coincident Doppler Broadening Spectroscopy (CDBS). In combination, these techniques will yield trap concentration, trap energy, and helium distribution. A unique TPD setup that can reach a maximum temperature of 3000 K while preserving UHV conditions, a CDBS setup located at the worlds brightest positron source (NEPOMUC) and a foil-ERDA setup as well as first measurements of the system He in W will be presented.

MM 12.31 Mon 19:15 Poster C

Determination of the Vacancy Formation Enthalpy of La by Positron Annihilation Spectroscopy — •Lucian Mathes, Thomas Gigl, and Christoph Hugenschmidt — Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department E21, Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The coincident Doppler broadening (CDB) spectrometer at the positron beam facility NEPOMUC of the FRM II enables spatially resolved defect studies by using Doppler broadening spectroscopy (DBS) of the positron-electron annihilation line. In order to perform depth dependent measurements of the near-surface region and the bulk of a sample, the positron implantation energy can be set up to 30 keV. A heatable sample holder enables temperature dependent in-situ defect spectroscopy from room temperature up to 1000 K. By using temperature dependent DBS we succeeded in determining the vacancy formation enthalpy of La for the first time. First, the as-received samples were annealed in situ, i.e. the decrease of the so called S-parameter indicated the annealing of lattice defects. For comparison, Cu served as reference material. During a second heating cycle the increase of the vacancy concentration was clearly observed which allowed a calculation of the vacancy formation enthalpy. In addition, a temperature dependence of the vacancy formation enthalpy in La was observed. Financial support by BMBF (project no. 05K10WOB) is gratefully acknowledged.

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Grain-boundary diffusion in CoCrFeNi and CoCrFeMnNi high entropy alloy polycrystals — •Marcel Glienke[1], Mayur Vaidya[1], Lukasz Rogalc[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Westfälische-Wilhelms Universität, Institut für Materialphysik, Münster, Deutschland — [2]2Institute of Metallurgy and Materials Science, Polish Academy of Sciences, 30-059 Krakow, Poland

For the first time, grain boundary (GB) diffusion of Co, Cr, Fe and Mn have been measured in polycrystalline CoCrFeNi and CoCrFeMnNi high entropy alloys (HEAs) using the radiotracer technique. The alloys have been prepared using high frequency electromagnetic induction melting followed by homogenization at 1200°C for 50 h. X-ray diffraction confirms the single phase FCC structure of both the HEAs. Scanning electron microscopy along with electron back-scattered diffraction (EBSD) validates the equiatomic composition and coarse grained microstructures. Radioactive isotopes 57Co, 51Cr, 59Fe and 54Mn have been utilized to measure grain boundary self-diffusion in the temperature range of 800°C - 1000°C. The temperature and time of diffusion annealing are selected to ensure the B-type kinetics conditions for both the HEAs. The temperature dependence of the GB diffusion coefficients follows Arrhenius behavior for all the constituents in the HEAs. The obtained results are compared on the homologous temperature

scale with GB self-diffusivities in other FCC matrices.

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invar effects in FeNiCo medium entropy alloys: from an invar treasure map to alloy design — •ziyuan rao[1], dirk ponge[1], fritz körmann[1,2], yuji ikeda[1], oldřich schneeweiss[3], martin friak[3], jörg neugebauer[1], dierk raabe[1], and zhiming li[1] — [1]Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Materials Science and Engineering, Delft University of Technology, 2628 CD Delft, The Netherlands — [3]Institute of Physics of Materials, Academy of Sciences of the Czech Republic, v.v.i., žižkova 22, Brno CZ-616 62, Czech Republic

To facilitate the understanding and design of FeNiCo-base invar alloys characterized by low thermal expansion coefficient (TEC), we investigated the magnetic and thermal expansion behavior of an equiatomic prototype medium entropy alloy FeNiCo and a non-equiatomic (super invar) Fe63Ni32Co5 (at. %) reference alloy by means of experiments and ab initio calculations. Large spontaneous volume magnetostriction is observed in both alloys below their respective Curie temperatures. The invar effect in the non-equiatomic Fe63Ni32Co5 alloy is of step-type with nearly zero TEC over a wide temperature range (from room temperature to 120 oC) below its Curie temperature. The relationships among magnetic behavior, spontaneous volume magnetostriction and invar effects for a wider array of metallic alloys are discussed based on Masumoto*s rule and Wohlfarth*s itinerant electron theory. An invar alloy search map is constructed based on the present results and available literature data, which provides a design route for further developments of new invar alloys by tuning their magnetic properties.

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atomic mobilities of fcc Co-V-Mo alloys: measurement and modeling — •Jingfeng Zhang[1], Yong Du[2], Sergiy Divinski[1], and Gerhard Wilde[1] — [1]Institute of Materials Physics, Westfälische-Wilhelms University of Münster, Münster, Germany — [2]State Key Laboratory of Powder Metallurgy, Central South University, Changsha, China

Co is widely used as a matrix binder phase for cemented carbides. Certain addition of V and Mo in Co can minimize the grain size of cemented carbides, behaving as the grain growth inhibitors. Though diffusion plays a key role in material manufacturing process, there are no investigations of diffusion kinetics of this ternary system so far.

Based on 18 sets of diffusion couples, the composition-dependent interdiffusion coefficients in the fcc Co-rich Co-V-Mo alloys at 1273, 1373 and 1473 K were obtained from the intersection points of the diffusion couples by means of EPMA technique coupled with the Whittle and Green method. With the experimentally determined interdiffusion coefficients and the critically reviewed experimental diffusivities available in the literature, the atomic mobilities of fcc Co-V-Mo alloys were assessed using Diffusion Controlled Transformation (DICTRA) software. The quality of the assessed atomic mobilities was confirmed by the comprehensive comparisons between various DICTRA-calculated diffusion behaviors and the experimental ones, including concentration profiles and diffusion paths. The results will be critically examined against direct measurements of the tracer diffusivities by the radiotracer technique.

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Grain-boundary diffusion in CoCrFeNi and CoCrFeMnNi high entropy alloybi-crystals — •Alexandra Everwand[1], Daniel Gaertner[1], Bengü Tas[1], Yury Chumlyakov[2], Gerhard Wilde[1], and Sergiy V. Divinski[1] — [1]Institute of Materials Physics, University of Münster, Münster, Germany — [2]Department of Physics of Metals, Tomsk State University, Tomsk, Russia.

The diffusion kinetics in the equiatomic quaternary CoCrFeNi and quinary CoCrFeMnNi high entropy alloys, the so-called Cantor-alloys, were previously investigated using the radiotracer technique in single- and poly-crystalline materials. For the first time, diffusion of all constituent elements and additionally solute diffusion of Mn in the quaternary alloy is investigated in bi-crystalline HEAs with a defined grain-boundary. In order to define the microstructure, the chemical composition of the bi-crystals and the grain-boundary structure, scanning electron microscopy (SEM), electron back-scatter diffraction (EBSD), energy dispersive X-ray spectroscopy (EDX) and transmission electron microscopy (TEM) analyses are performed. Using the radiotracer technique, the grainboundary diffusion coefficients of ^{57}Co, ^{51}Cr, ^{59}Fe, ^{54}Mn and ^{63}Ni are determined at a temperature of 1373 K according to Harrison's B-type, and at a temperature of 923 K according to Harrisons's C-type. The components are characterized by significantly different diffusion rates, with Mn being the fastest element and Ni and Co being the slowest ones.

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Brute force composition scanning with a CALPHAD database to find low temperature bcc high entropy alloys — •Peter Klaver, Darko Simonovic, and Marcel Sluiter — Department of Materials Science and Engineering, Delft University of Technology, Mekelweg 2, 2628CD Delft, The Netherlands

We used Thermo-Calc CALPHAD calculations to determine the stable phases of AlCrMnNbTiV, AlCrMoNbTiV, AlCrFeTiV and AlCrMnMoTi alloys. A five- or six-dimensional grid is constructed, with stable phases calculated at each grid point. Three million compositions were calculated, resulting in ~20000 compositions consisting of a single disordered bcc phase down to 800 K. By filtering out compositions with a single disordered phase, composition islands of high entropy alloys are determined. The sizes and shapes of such islands provide information about which element combinations have good high entropy alloy forming qualities as well as about the role of individual elements within an alloy. We determined which compositions lie near the centers of these islands and thus remain high entropy islands under small composition changes. These compositions make good candidates for experimental verification. The search for high entropy islands can be conducted under constraints, e. g. requiring a minimum amount of Al and/or Cr to promote oxidation resistance. It is also possible to look for alloys consisting of two different disordered phases. The high entropy forming qualities of AlCrMnNbTiV and AlCrMoNbTiV are relatively good, those of AlCrFeTiV are poor, while those of AlCrMnMoTi are poor at 800 K but quickly become better with increasing temperature.

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Universal 1/f type current noise of Ag filaments in redox-based memristive nanojunctions — •Botond Sánta[1,2], Zoltán Balogh[1,2], Ágnes Gubicza[1,3], László Pósa[1,4], Dávid Krisztián[1], György Mihály[1,2], Miklós Csontos[1,3], and András Halbritter[1,2] — [1]Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary — [2]MTA-BME Condensed Matter Research Group, Budapest, Hungary — [3]Empa, Swiss Federal Laboratories for Materials Science and Technology, Transport at Nanoscale Interfaces Laboratory, Dübendorf, Switzerland — [4]Institute for Technical Physics and Materials Science, Centre for Energy Research, Hungarian Academy of Sciences, Budapest, Hungary

The microscopic origins and technological impact of 1/f type current fluctuations in Ag based, filamentary type resistive switching devices have been investigated. The analysis of the low-frequency current noise spectra revealed that the main electronic noise contribution arises from the resistance fluctuations due to internal dynamical defects of the Ag nanofilaments. The resulting 0.01-1% current noise ratio is found to be universal: it only depends on the total resistance of the device, irrespectively of the material aspects of the surrounding solid electrolyte as well as of the specific filament formation procedure. Moreover, the resistance dependence of the current noise ratio also displays the diffusive to ballistic crossover, confirming that stable resistive switching operation utilizing Ag nanofilaments is not compromised even in truly atomic scale junctions by technologically impeding noise levels.