MM 20: Computational Materials Modelling: HEA, Alloys & Nanostructures

Time: Wednesday 10:15–13:00 Location: H44

MM 20.1 Wed 10:15 H44

Microstructural evolution of severely deformed nanocomposite high entropy alloys irradiated by swift heavy ions — •Shabnam Taheriniya[1], Christian Gadelmeier[2], Harald Rösner[1], Martin Peterlechner[1], Christoph Gammer[3], Marilena Tomut[1,4], Sergiy V. Divinski[1], Uwe Glatzel[2], and Gerhard Wilde[1] — [1]Institute of Materials Physiks, University of Münster, Germany — [2]Metals and Alloys, University of Bayreuth, Bayreuth, Germany — [3]Erich Schmid Institute of materials Science, Austrian Academy of Science, Leoben, Austria — [4]GSI Helmholtz Center for Heavy Ion Research, Darmstadt, Germany

Structural modifications induced by the processing of high entropy alloys (HEAs) under non-equilibrium conditions are investigated to shed light into the stability of such advanced materials. The nanocomposite HEAs are produced by the room-temperature high pressure torsion (HPT) of stacked single-phase equiatomic FCC CoCrFeMnNi (Cantor) and BCC HfNbTaTiZr (Senkov) alloys. Solely Cantor and Senkov alloys were HPT-processed under the similar conditions, too. Cross-sections of the HPT-processed disks were subjected to high fluences of Au swift-heavy-ion irradiation at ambient and cryogenic temperatures. Deformation and irradiation-induced microstructural changes were examined in detail applying scanning and transmission electron microscopies with respect to evolution of chemical composition and local microstructure. A combination of nano-beam diffraction with angular correlation was utilized to provide information about the resolved crystal structures and strain fields in the different HEA phases.

MM 20.2 Wed 10:30 H44

Impact of high-pressure torsion and post-deformation annealing on CoCrFeMnNi high-entropy alloy with carbon content — •Sandra Hecht, Sergiy V. Divinski, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Münster, Germany

The well-known Cantor alloy CoCrFeMnNi provides attractive mechanical properties and strength-ductility combinations, which can be improved by further alloying of small amounts of carbon.

In the present work, the impact of high-pressure torsion (HPT) and post-deformation annealing on equiatomic Cantor alloy and nearly-equiatomic (C alloyed (4.4 at.%)) Cantor alloy, produced via arc-melting and subsequent homogenization at 1373 K for 3 days under pure Ar, is examined. The thermal, mechanical and microstructural properties of the initially coarse-grained samples were investigated before and after deformation at room temperature (5 rotations at 8 GPa) and afterwards post-deformation annealing treatments using differential-scanning calorimetry (DSC), X-ray diffraction (XRD), scanning and transmission-electron microscopy (SEM & TEM) as well as micro-hardness measurements. Impact of the interstitial carbon and in particular the carbides $Cr_{23}C_6$ on the mechanical response and microstructure evolution is examined.

MM 20.3 Wed 10:45 H44

Phase Stability and Ordering in Ta-Mo-Cr-Ti-Al Refractory High Entropy Alloys — •Yilun Gong[1], Alexander Shapeev[2], Fritz Koermann[1,3], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Germany — [2]Skolkovo — [3]Delft University of Technology, The Netherlands

Predictive capabilities of phase stability and ordering in multi-component systems are critical to designing better alloys. This is particularly important for properties which are difficult to be quantified by traditional experimental techniques.

In the present work, a class of body-centered-cubic (bcc) refractory high entropy alloys was studied. In contrast to its superior high-temperature behaviour, it shows less-satisfying ductility below 600 °C. As origin of the poor mechanical performance long-range B2-ordering at low temperatures has been proposed but is still controversially discussed due to contradicting experimental findings. To predict and to quantify the temperature-dependent stable structure, we employed on-lattice machine-learning interatomic potentials (namely low-rank potentials). This type of potentials is capable of accurately describing chemical interactions in multi-component systems used in subsequent Monte Carlo simulations. Systematic studies of training qualities, statistical uncertainties and impact of local lattice distortions were conducted. Computed ordering sequence, site occupancies, short-range order parameters and alloying with interstitial O will be discussed.

MM 20.4 Wed 11:00 H44

Stabilities and Mechanical Properties of Mg-based Light Metal Multi-Principal Alloys — •Wernfried Mayr-Schmölzer[1], Johannes Kirschner[2], Clemens Simson[4], Christoph Eisenmenger-Sittner[2], Johannes Bernardi[3], and Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, TU Hamburg — [2]Institute of Solid State Physics, TU Vienna — [3]USTEM, TU Vienna — [4]LKR, Austrian Institute of Technology GmbH

Compositionally Complex Alloys (CCAs) consist of four or more elements alloyed in approximately equal fractions and often crystallize in a simple crystal lattice. In many cases, their mechanical properties like structural stability or ductility exceed that of common modern alloys. Usually, they mainly contain heavy d-Orbital metals, and investigations into low density light metal CCAs have been rare due to the complex binding modes of their constituents.

We use both a Cluster Expansion approach with stochastic prescreening steps and neural network based pair potentials to scan the large configuration space of the Mg-Al-Cu-Zn system for stable phases. Training data was generated using DFT calculations implemented in the VASP code. In conjunction with experiments, we find that addition of Cu into the Al-Mg-Zn system inhibits phase separation by formation of a stable cubic phase, reflected in an increase of the calculated bulk modulus. Furthermore, we evaluate the predictive power of these screening methods and their ability to provide insights into simulation of physical properties of these complex multicomponent alloys.

MM 20.5 Wed 11:15 H44

In-situ Nanoalloying by Laser Powder Bed Fusion: Molecular Dynamics Simulations of Cantor-Alloy Formation in a Powder Blend — •Yulia Klunnikova[1], Arne J. Klomp[2], and Karsten Albe[3] — [1]klunnikova@mm.tu-darmstadt.de — [2]klomp@mm.tu-darmstadt.de — [3]albe@mm.tu-darmstadt.de

Laser powder bed fusion (LPBF) is an additive manufacturing technology involving a gradual build-on of layers to form a complete component typically starting with prealloyed particles. Alternatively, one can also start with a power blend and initiate in-situ alloying by the laser beam. In this context, multi-component systems, including high entropy alloys, are of particular interest. In this contribution we show results of molecular dynamics simulations of high-entropy nanoalloys formed by LBPF. We use the Cantor alloy as model system and explore the possibility to create the FeCrCoMnNi alloy from powder blends under far-from-equilibrium conditions and compare to the case of prealloyed nanopowders. By varying parameters (temperature field, melt pool, substrate type, etc.) we explore the correlation to microstructural features. In the case of the powder blend the elemental components mix in the liquid phase and solidify partially in crystalline and glassy states. Depending on the parameters of the laser (irradiation temperature, laser spot size) we see varying amounts of crystal defect, such as stacking faults, twinning, and vacancies. The results show that the resulting structures are delicately depending on the interplay of laser parameters, heat transport, interdiffusion and geometric factors. We acknowledge the NHR4CES for the computing time.

15 min. break

MM 20.6 Wed 11:45 H44

Phase stability and formation energies of stacking faults in intermetallic $Mg_xAl_{2-x}Ca$ Laves phases — •Ali Tehranchi, Tilmann Hickel, and Jörg Neugebauer — Max Planck institute for Iron research, Max Planck Straße 1, 40237 Düsseldorf

The intermetallic Laves phases that form in Mg-based alloys at higher alloying concentrations have a significant impact on their mechanical properties. For example, they can enhance the creep resistance of the alloys and extend their application to higher temperature domains. However, the mechanisms of deformation of these phases are not fully understood. In this work, at first the formation energies of the different realizations of C14, C15, and C36 Laves phases in the composition domain, Mg_xAl_{2-x} with $0<x<2$, using the ab initio simulations is

calculated. Using these formation energies, the phase diagram of the phases of interest is constructed. The effect of the strain fields on the relative stability of these phases is included. In addition, using the analytic Axial Next-Nearest Neighbor Ising (ANNNI) type model, the basal stacking faults in each phase and composition are calculated. The results of the analytic models are in good accordance with the results of the direct DFT simulations of the stoichiometric stacking faults. The gamma surface of certain realizations of the C36 phase is also investigated and explain the experimentally observed planar defects in the C36 phase.

MM 20.7 Wed 12:00 H44

Rational design of bimetallic nanoparticles — •Samuel Baltazar[1,2], Javier Rojas[1,2], Pamela Sepulveda[2], and Rafael Freire[2] — [1]Physics Department, Universidad de Santiago de Chile, Chile — [2]Center for the development of Nanoscience and Nanotechnology, Universidad de Santiago de Chile, Chile

The study of bimetallic nanoparticles (BNP) has recently attracted increasing attention from researchers worldwide due to their potential for technological applications in the electronic and environment fields. This study will be carried out through a theoretical framework to identify the fundamental atomic-scale mechanisms for BNP such as FeCu, AgCu, and FeNi. It is therefore necessary to determine the structural, electronic, and magnetic properties of the nanostructures with two or more elements, where the interplay between both metallic elements can be used to limit the oxidation of iron or the electron transfer between elemnts. This can be done based on some of the characteristics of these systems, such as (i) the surface-volume ratio, (ii) the shape of nanoparticles as an interesting aspect due to the physico-chemical properties at their surface, (iii) Concentration and (iv) distribution of elements. We performed molecular dynamics simulations under the NVT canonical ensemble to further deepen our study. The results pointed out that AgCu and FeNi BNP with a core shell and janus like morphologies are some of the most stable configurations, with a competition between them for FeCu as a function of the concentration and size of each element. These results were compared with experimental data for BNP, evidencing a good agreement among these approaches.

MM 20.8 Wed 12:15 H44

Atomic cluster expansion for the Ag-Pd system — •Yanyan Liang, Matous Mrovec, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Alloys of noble metals, such as silver and palladium, have been regaining attention in recent years due to their importance in nanotechnology and catalysis. However, for the binary Ag-Pd system reliable and efficient interatomic potentials that provide an accurate description of structural and thermodynamic properties are lacking. In this work, we developed a new atomic cluster expansion (ACE) parametrization for both elements Ag and Pd as well as their binary compounds by fitting to a large training set of ab initio data. The resulting ACE potential provides an accurate description for a wide range of fundamental properties, including the equations of states of various phases, elastic moduli, phonon frequencies, transformation paths, and defect energies. The excellent computer efficiency and linear scaling of ACE enable to carry out large-scale molecular dynamics and Monte Carlo simulations to evaluate complex phenomena, such as thermal expansion, melting, diffusion and phase diagrams. Examples of these simulations will be provided to demonstrate the outstanding predictive power of ACE.

MM 20.9 Wed 12:30 H44

Atomistic modelling of hybrid organic-inorganic nanocomposites — Kai Sellschopp[1], Wernfried Mayr-Schmölzer[1], Robert Meissner[2], and •Gregor Vonbun-Feldbauer[1] — [1]Institute of Advanced Ceramics, TU Hamburg, Germany — [2]Institute of Polymers and Composites, TU Hamburg, Germany

Novel hybrid materials like supercrystalline nanocomposites from nano-building blocks promise excellent properties and functions for diverse applications. One realization are inorganic nanoparticles (NP) from transition-metal oxides which are functionalized with organic ligands and then assembled on different levels of hierarchy. In this contribution atomistic modelling based on density functional theory (DFT) calculations is used to shed light on the first level of hierarchy. Particularly, the interfacial properties of different ligands and effects in the interphase between the NP are addressed. For modelling interfaces, the configuration space is a challenge and here the program CodeRed (Configuration space determination and Reduction) is presented which allows to sample the adsorption configuration space and to select configurations as input for DFT calculations using unsupervised machine learning approaches. The results are further facilitated to obtain mechanical properties using DFT, and as input for molecular dynamics simulations as a first step towards multi-scale modelling to allow for an accurate description of larger and more complex systems.

MM 20.10 Wed 12:45 H44

Ab initio investigation of Mg alloy corrosion in water — •Jing Yang, Mira Todorova, and Jörg Neugebauer — Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany

Magnesium alloys have great potential as structural materials for the automotive and aerospace industries, as well as bio-implants due to their low density and non-toxic nature. However, intrinsically poor ductility and poor corrosion resistance limit their practical application. In this work, we focus on the solid solution of Al and Ca in Mg, an alloying system which has shown improved ductility and corrosion resistance. In particular, we elucidate the effect of Al and Ca alloying on the aqueous corrosion process of Mg metal by ab initio molecular dynamics simulation of the metal/water system. We analyze the segregation behavior of the alloying elements, their impact on the interfacial water structure and dynamics, and the subsequent implication on corrosion kinetics. By combining our DFT calculations with thermodynamics, we construct interface phase diagrams for the Mg-Al-Ca system to elucidate the influence of the environment on surface structure and composition. We consider both implicit and explicit water calculations, which allows us to analyze the impact the water-modelling approach has on the constructed interface phase diagrams. We show that such ab initio molecular dynamics studies strongly improve our understanding on microscopic corrosion processes at realistic conditions.