MM 36: Mechanical Properties

Nanomaterials and Alloys

Time: Friday 10:15–13:00 Location: H23

MM 36.1 Fri 10:15 H23

STEM investigation of early precipitation reactions in Al-Cu alloys — •Johannes Berlin and Ferdinand Haider — Chair for Experimental Physics I, University of Augsburg, Universitätsstraße 1, 86159 Augsbur

Due to their excellent strength-to-weight ratio, heat-treatable Al-Cu alloys have been widely used since their invention. Although the occurring precipitates in naturally aging aluminium alloys are well known, the very early stages of formation mechanisms still are a topic of ongoing research. Scanning transmission electron microscopy is used to investigate the influence of different parameters, such as thermal history and effects of microalloying, on early-stage precipitate formation and transformation in Al. Due to their strong binding potential to quenched in vacancies even a few hundred ppm of trace elements such as tin and indium can alter the natural aging process drastically. Even after prolonged natural ageing, a slight increase in temperature can lead to drastic changes in precipitation size and densitiy inthese materials. This proves a long-lasting supersaturation of the material with vacancies. Additionally, these results are compared to the measurements of hardness, DSC and electrical resistance.

MM 36.2 Fri 10:30 H23

Surface structure and reactivity of Aluminium alloys studied by DFT — •Zhengqing Wei[1], Inna V. Plyushchay[2], Nebahat Bulut[1], Florian Lehmann[3], Maik Gude[3], Julia Hufenbach[4,5], and Sibylle Gemming[1,6] — [1]Inst. Physics, TU Chemnitz, Germany — [2]Natl. Taras Shevchenko University of Kyiv, Ukraine — [3]ILK, TU Dresden, Germany — [4]IFW Dresden, Germany — [5]Inst. Materials Science, TU-BA Freiberg, Germany — [6]MAIN Center, TU Chemnitz, Germany.

Classically, the mechanical properties of alloys are attributed to the action of stress fields around defect sites and to their combined influence on the overall elastic moduli. The present study employs first-principles modeling to include also changes of the electronic structure and investigate the bonding, stability, and reactivity changes around impurities in the bulk and at surfaces. We focus on Al alloys with low amounts of substitutional Mg, Zr, and Si atoms. The results indicate that the electron density changes mostly within the first coordination sphere around the impurity, the bond lengths vary locally within few percent, and there exists a thermodynamic driving force for most elements to diffuse to or near surfaces or interfaces. Stable 2D surface alloy compositions in part differ from the bulk phase and exhibit an element-specific reactivity with air and polymer coatings. Modeling the adsorption of oxygen, nitrogen and the PEEK polymer from first principles gives access to modified local potentials for the classical modeling of large-scale surface and interface areas (tu-dresden.de/ing/forschung/Graduiertenkollegs/grk2868#intro).

MM 36.3 Fri 10:45 H23

Active learning-based interatomic potential for investigating mechanical properties of Al-Mg-Zr alloys — •Lukas Volkmer, Leonardo M. Sandonas, Gianaurelio Cuniberti, and Markus Kästner — Technische Universität Dresden

The unique properties of aluminum-based alloys, such as low density, high specific strength, and excellent resistance to oxidation and corrosion, enable the design of advanced metamaterials. In this work, we theoretically investigate the effect of alloying aluminum with magnesium and zirconium on its thermodynamic and mechanical properties. Since exploring the vast chemical compound space of these alloys through Density Functional Theory (DFT) calculations is computationally prohibitive, we developed a scalable and transferable machine learning interatomic potential (MLIP) capable of accurately calculating diverse properties of Al-Mg-Zr alloys. The MLIP was trained using an active learning technique based on ab initio molecular dynamics simulations, Bayesian statistics, and kernel ridge regression. This methodology ensures that the MLIP captures the effects of alloying concentration and atomic configurations up to the solubility limit, providing access to highly accurate physicochemical properties of a wide range of Al-based alloys at a reasonable computational cost. We expect this approach to enable efficient phase space exploration, offering a robust tool for designing advanced Al-based alloys with optimized properties.

MM 36.4 Fri 11:00 H23

Phase identification by Raman Spectroscopy on pre-oxidized AISI 316L-MgO composite produced by Spark Plasma Sintering — •Julia Richter[1], Mahnaz Mehdizadehlima[2], Cameliu Himcinschi[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Straße 23, D-09599 Freiberg — [2]TU Bergakademie Freiberg, Institut für Werkstoffwissenschaft, Gustav-Zeuner-Straße 5, D-09599 Freiberg

Re-usage, recycling and upcycling of MgO-C refractories as they are widely used in the steel industry are crucial for resource efficiency. Our upcycling concept is aimed at steel-MgO composite anodes for application in the extraction of aluminum by fused-salt electrolysis. The composite anode material is produced by Spark Plasma Sintering based on 60 vol.% AISI 316L steel powder and 40 vol.% MgO. In this stage of development, the raw material is fused fresh MgO instead of recyclate as a proof of concept. Pre-oxidation treatment of the developed composite is intended to enhance the material's corrosion resistance in the aggressive environment of molten cryolite during application. In order to gain a better understanding of the oxidation behavior at different temperatures, phase identification is required. For this purpose, Raman spectroscopy as a sensitive, non-destructive, non-contact method is employed complementary to other investigative techniques; e.g., Scanning Electron Microscopy.

MM 36.5 Fri 11:15 H23

Atomic Cluster Expansion for Ag-Au-Pd alloys — •Yanyan Liang, Matous Mrovec, Yury Lysoroskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germay

Ternary alloys of Ag-Au-Pd are of technological importance in catalysis and electrical applications. However, the system lacks reliable and efficient interatomic potentials capable of accurately describing structural and thermodynamic properties, particularly for investigating complex segregation and ordering phenomena in bulk systems and nanoclusters. In this work, we present an atomic cluster expansion (ACE) model parameterized for the Ag-Au-Pd system with quantum-level accuracy. We demonstrate that the ACE model provides an accurate description of fundamental properties, including structural stability and thermodynamics, not only for the elemental metals but also for their binary and ternary compounds. Furthermore, we highlight the wide applicability of the ACE model for large-scale atomistic simulations, enabling predictive modeling of complex phenomena.

15 min. break

MM 36.6 Fri 11:45 H23

Scalable fabrication and mechanical behavior of hierarchical nanoscale network nickel — •Ulrike Dette[1,2], Lukas Lührs[2], and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

The recent fabrication of mechanically robust two-level hierarchical nanoporous gold by two-step electrochemical dealloying has enabled the demonstration of enhanced mechanical properties and reduced density attributed to the structural hierarchy in the nanoscale network materials. This work aims to develop a new method for the scalable fabrication of low-cost hierarchical nanoscale network metals. Here, two- and three-level hierarchical network (HN) Ni samples are successfully prepared from Ni foams by a novel and simple alloying-dealloying method. Bulk three-level HN Ni samples are characterized by three well-defined strut/ligament sizes (160 μm, $<$10 μm and $<$10 nm) and a low density down to 0.06. In addition, we systematically perform mechanical studies on both two- and three-level HN Ni via macroscopic compression tests. We propose general scaling equations between mechanical properties and relative density for HN materials.

MM 36.7 Fri 12:00 H23

Transferable machine learning interatomic potential for Au nanoparticles — •Jovana Vlahović, Cem Sevik, and Milorad V. Milošević — University of Antwerp, Groenenborgerlaan 171, Antwerp, Belgium

Effective molecular dynamics and Monte Carlo simulations fundamentally depend on the accuracy of interatomic potentials, which define the potential energy surface as a function of atomic positions. This precision is essential for metallic nanoparticles (NPs), whose small size and diverse morphologies demand robust modelling. While classical empirical potentials offer computational efficiency, they often lack the necessary accuracy and density functional theory (DFT) calculations, though highly accurate, are computationally prohibitive for NPs with thousands of atoms. This work introduces a machine learning-based interatomic potential for Au NPs, trained on a compact dataset of bulk structures, surface slabs and NPs containing up to 55 atoms. Our training dataset includes a diverse set of atomic configurations with corresponding properties obtained from ab initio molecular dynamics calculations, which we use to train a Gaussian Approximation Potential (GAP) via Gaussian Process Regression. Parameter optimization was performed to maximize model accuracy, and LAMMPS validation tests demonstrated GAP performance against DFT benchmarks. In addition, transferability tests on larger NPs of various shapes reveal our GAP's robustness beyond the training set. Comparisons with an existing GAP model and the universal MACE potential underscore our model's improved accuracy and generalizability for Au NPs.

MM 36.8 Fri 12:15 H23

Scaling behavior of Poisson's ratio in hierarchical nanoporous materials — •Haonan Sun[1,2], Lukas Lührs[2], Wei-che Chang[3], and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

The recent fabrication of crack-free monolithic hierarchical nested network nanoporous gold allows the investigation of the benefits of hierarchy in the aspect of mechanical properties at the nanoscale. It has been demonstrated that hierarchical nanoporous gold (HNPG) can achieve a substantially reduced solid fraction and enhanced specific stiffness and strength compared with non-hierarchical nanoporous gold. However, the role of hierarchical structure on Poisson's ratio has not been investigated yet. In this work, mm-sized HNPG samples are made out of an Ag93Au7 master alloy by a dealloying-coarsening-dealloying method. We then explore the elastic and plastic Poisson*s ratios of HNPG by using digital image correlation during compression tests. Remarkably, a scaling law of the elastic Poisson's ratio in hierarchical nanoporous materials with respect to the solid volume fraction is proposed and excellently supported by our experiments. This work enriches the understanding on the relationship between mechanical properties and microstructure in hierarchical network materials at the nanometer scale.

MM 36.9 Fri 12:30 H23

Frenkel pair energetics in disordered solid solutions and implications for alkali feldspar diffusivity — •Alexander Gorfer, Rainer Abart, and Christoph Dellago — University of Vienna, Vienna, Austria

Predicting defect concentrations from the density of states (DOS) of formation energies in disordered materials has recently been formulated for vacancies in high entropy alloys. That methodology however does not translate to disordered ionic crystals as charged defects need to be paired up to ensure charge neutrality. Here, we present a general expression to predict the defect concentrations of Frenkel pairs in disordered ionic crystals out of the DOS of formation energies of both positively and negatively charged defects. To demonstrate its applicability we use a recently developed machine learning force field to calculate the DOS of formation energies for different states of (dis)ordering in alkali feldspar $(Na, K)AlSi_3O_8$, an abundant mineral in the Earth's crust. Applying our expression to these DOS reveals a significant increase in the concentration of point defects in disordered ionic crystals as pairs of low formation energy defect states between the positively and negatively charged DOS can be identified. Implications for the diffusivity that controls the exsolution of alkali feldspars which is an important phenomenon in the formation of magmatic and metamorphic rocks are discussed.

MM 36.10 Fri 12:45 H23

Ferromagnetism at ambient temperature in Cantor and nanocomposite high-entropy alloys induced by severe plastic deformation — •Shabnam Taheriniya, Harald Rösner, and Gerhard Wilde — Universität Münster, Institut für Materialphysik, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

In this study, single phase Cantor (CoCrFeMnNi) and nanocomposite high-entropy alloys (HEAs) (CoCrFeMnNi and HfNbTaTiZr) were processed using high-pressure torsion (HPT), subjecting the samples to a constant pressure of 9 GPa either as a single disk or stacked disks, with the top anvil rotating at 1 rpm at ambient temperature for up to 15 revolutions. Vibrating sample magnetometry (VSM) confirmed that HPT processing induces the development of ferromagnetic properties. The distribution and orientation of magnetic domains post-deformation were examined in detail using differential phase contrast scanning transmission electron microscopy (DPC STEM), analytical TEM and atom probe tomography (APT) analysis. Our study demonstrates that HPT processing of HEAs induces a transition from paramagnetic to ferromagnetic states at ambient conditions. This deformation-induced ferromagnetism can be explained by the cocktail effect in HEAs, where the formation of ferromagnetic particles is linked to deformation-induced element-selective atomic migration and local enrichment of ferromagnetic elements.