MM 7: Mechanical Properties and Alloy Design II

Time: Monday 15:45–18:30 Location: SCH/A215

MM 7.1 Mon 15:45 SCH/A215

On-the-Fly Machine Learning of Interatomic Potentials for Elastic Property Modeling in Al-Mg-Zr Solid Solutions — •Lukas Volkmer[1], Leonardo Medrano Sandonas[1], Philip Grimm[2,3], Julia Kristin Hufenbach[2,3], and Gianaurelio Cuniberti[1,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials,TUD Dresden University of Technology — [2]Institute of Materials Science, Technische Universität Bergakademie Freiberg — [3]Leibniz Institute for Solid State and Materials Research Dresden — [4]Dresden Center for Computational Materials Science, TUD Dresden University of Technology

Aluminum-based alloys offer exceptional mechanical performance due to their low density, high specific strength, and strong resistance to oxidation and corrosion. In this work, we develop a scalable and transferable machine-learning interatomic potential (MLIP) capable of accurately predicting thermodynamic, mechanical, and microstructural properties across a broad concentration space of Al-Mg-Zr alloys. The MLIP is trained using an active-learning workflow that combines ab initio molecular dynamics, Bayesian uncertainty quantification, and kernel ridge regression, enabling efficient exploration of diverse atomic environments. Additionally, we model an Al/Al3Zr grain-boundary system using experimentally observed orientation relationships and calculate the stress-strain behavior. This framework provides a computationally efficient strategy for exploring the phase space of Al-based alloys and guiding the design of materials with optimized mechanical properties.

MM 7.2 Mon 16:00 SCH/A215

Atomistic modelling of Ni-based superalloys at real chemical complexity — •Aditya Vishwakarma, Sarath Menon, Thomas Hammerschmidt, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Germany

Ni-based superalloys are critical high-temperature high-load materials for jet-engine turbine blades. While *ab-initio* computation has been essential for fundamental understanding (e.g., in binary NiAl), simulating the full chemical complexity of commercial superalloys has remained computationally infeasible. In this work, we demonstrate how Graph Atomic Cluster Expansion (GRACE) foundational models overcome this limitation to investigate the complex phase stability of the γ and γ' phases in industrially relevant Ni-based superalloys. We compute the binary NiAl phase diagram, successfully reproducing the critical γ-γ' phase coexistence. We then extend these phase stability calculations to a CMSX-4 type multi-component composition using hybrid Molecular Dynamics/Monte Carlo simulations. Our results reveal the short-range order (SRO) in the γ phase and quantify long-range order (LRO) in the γ' phase. We specifically find that refractory alloying elements (Ta, W, Ti) exhibit strong LRO alongside Al across the operational temperature range. These findings validate that foundational machine learning interatomic potentials are now capable of calculating complex phase diagrams and capturing subtle ordering and clustering phenomena in multi-component alloys. This capability marks a crucial step toward realizing faster, computationally-driven design of next-generation, single-crystal Ni-based superalloys.

MM 7.3 Mon 16:15 SCH/A215

A machine-learning approach to investigate deformation mechanisms in Mo-Si-based alloys — •Julie Hammoud and Karsten Albe — Technische Universität Darmstadt, Darmstadt, Germany

Mo-Si-X alloys have gained significant attention for high-temperature applications such as turbine blades, due to their outstanding creep resistance, thermal stability and corrosion resistance. In general, Mo-Si-X alloys include three phases: two intermetallic phases (Mo_3Si and Mo_5SiX_2) and a Mo solid solution phase Mo_{ss}. Despite its limited oxidation resistance, the solid solution phase enhances the room temperature fracture toughness of the system. However, the Mo solid solution also incorporates Si-rich subphases with a complex microstructure that leads to an unconventional and still insufficiently understood solid solution strengthening behaviour. Previous studies indicate that small additions of Si (0.1 wt.%) soften Mo, motivating a closer examination of this effect. In this study, we employ a machine-learning interatomic potential (MLIP) based on the Atomic Cluster Expansion (ACE) formalism for the Mo-Si binary system. MLIPs have demonstrated their capability to combine first principles calculations accuracy with the scalability characteristic of empirical potentials. To investigate how Si affects the mechanical response of Mo, we examine two aspects: (i) the concentration dependence of Si on the elastic moduli, analyzed within the framework of the Fleischer model, and (ii) the influence of Si on the behaviour of screw dislocations activity under external loading.

MM 7.4 Mon 16:30 SCH/A215

Jog-Pair Formation and Climb Mechanisms of Dissociated Dislocations in FCC Metals — •Erik Bitzek[1], Sergei Starikov[2], and Daria Smirnova[1,2] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]ICAMS, Ruhr-Universität Bochum, Germany

Jogs on dislocations are preferred sites for vacancy segregation and thus play a critical role in dislocation climb. Under conditions of high point-defect supersaturation – such as after quenching or irradiation – the availability of jogs along the dislocation line can become the rate-limiting factor for climb. Understanding jog-pair nucleation is therefore essential for modeling the kinetics of dislocation creep. Jog pair formation on split edge dislocations in fcc metals was first investigated by Thomson and Balluffi [J. Appl. Phys. 1962] and atomistic simulations [Sarkar et al., PRB 2012] confirmed the suggested mechanism. However, both studies assumed a certain vacancy configuration at the dislocation as the initial nucleus.

Using high-temperature molecular dynamics simulations of dislocations in vacancy supersaturated nickel, we identify an alternative pathway that takes place without predefined nuclei. We demonstrate the role of $\langle 110 \rangle$-oriented vacancy tubes in the climb of edge and 60° dislocations and propose a new climb mechanism for 30° dislocations involving double cross-slip of the screw partial dislocation. These findings highlight how atomistic simulations can inform mesoscale models of creep and annealing.

MM 7.5 Mon 16:45 SCH/A215

Seeking descriptors for predicting mechanical properties of transition-metal light-element compounds — •Rui Zhang[1,2], Xinlei Gu[1], Kan Zhang[1], Chang Liu[3], and David Holec[2] — [1]Department of Materials Science, Jilin University, Changchun 130012, China — [2]Department of Materials Science, Montanuniversity Leoben, Franz Josef-Straße 18, 8700 Leoben, Austria — [3]College of Physics, Jilin University, Changchun 130012, China

Mechanical strength and durability are key properties that dictate service life. To meet requirements of modern technological and industrial applications, it is essential to screen, sort and predict targeted mechanical properties via finding descriptors that can effectively identify materials with specific application needs. Transition-metal light-element (TMLE) compounds show superb mechanical, chemical and thermal properties. We focus on the analysis of the intrinsic physical/chemical parameters of the component elements and structure factors to identify the key factors affecting the mechanical properties of TMLE. In this presentation, we will introduce two research works: (1) Core electron count as a versatile and accurate new descriptor for sorting mechanical properties of diverse transition metal compounds; and (2) Nitrogen vacancy regulated lattice distortion improvement of mechanical properties and wear resistance of (NbMoTaW)Nx thin films. Ultimately, our work yielded a universal descriptor incorporating core electron count and established nitrogen-vacancy-driven lattice distortion as a key structural factor, offering two distinct pathways to guide the design of high-performance materials.

15 min. break

MM 7.6 Mon 17:15 SCH/A215

Atomistic-to-Mesoscale Computational and Experimental Analysis of the Interactions between Dislocations, Precipitates, Grain and Phase Boundaries in Complex Alloys — •Liming Xiong — NC State University, Raleigh, NC, USA

In this talk, we will present multiscale computational and experimental analysis on the deformation behavior of complex alloys. In experiments, polycrystalline nickel, alloy 709, and Ni3Al-NiCr (γ/γ') alloys are deformed in a transmission electron microscope (TEM). Mi-

crostructure evolution is imaged through in-situ TEM. Local stress build up at the slip-GB/PBs are measured by electron backscattering diffraction (EBSD). Meanwhile, concurrent atomistic-continuum (CAC) simulations are performed to understand how a queue of dislocations interacts with the atomically structured precipitates, coherent twin boundaries (CTBs), GB, and γ/γ' PB. One unique feature of CAC is to accommodate the microscale slip containing a large population of dislocations together with the atomistic structure nearby the precipitates/GB/PBs all within one model. Our several findings are: (i) the sequential dislocation-precipitates differs from the single dislocation-precipitates. It is history dependent and has a mechanism cross-over from Orowan bowing out to cross-slip; (ii) the CTBs don't block dislocations. They can accommodate incoming dislocations by allowing them to migrate and form a pileup on the CTB; (iii) dislocation motion is smooth in γ phase but jerky in γ' phase. Such insight will support the design of high-performance alloys by configuring the precipitates, CTBs, GBs, and PBs in them appropriately.

MM 7.7 Mon 17:30 SCH/A215

The Effect of Rhenium on Irradiation Induced Defects in Tungsten-Rhenium Alloys Studied by Positron Annihilation Spectroscopy — •Lisa-Marie Krug[1], Danny R. Russell[1], Maximilian Suhr[1], Leon Chryssos[1], Lucian Mathes[1], Mikhail Zibrov[2], Thomas Schwarz-Selinger[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Garching, Germany — [2]Max Planck Institute for Plasma Physics, Garching, Germany

The plasma-facing components in a nuclear fusion reactor have to withstand irradiation by 14 MeV neutrons. Tungsten is considered to be the most suitable plasma-facing material, due to its high melting point, high thermal conductivity and low erosion under fusion reactor operating conditions. In addition to radiation damage, neutron irradiation of tungsten induces nuclear transmutation reactions, resulting in the formation of rhenium. We investigated the effect of Re on the defects produced during the irradiation of W. We provide bench-marking data at extremely high damage doses using ion-irradiation. Transmutation to Re is substituted by Re-ion irradiation or the use of W-Re alloys. Positrons provide a non-destructive, atomic scale resolution of defect analysis of the irradiation damage. Positron Annihilation Spectroscopy (PAS) is a suitable method to determine the defect type, concentration and chemical surrounding. We observe a positive effect of Re on the radiation damage after irradiation at both room temperature and 1350 K. We have found evidence that fewer vacancy clusters are present after irradiation of W-3%Re alloys.

MM 7.8 Mon 17:45 SCH/A215

Understanding the influence of residual elements on the toughness of martensitic steels towards recycled steels — •Eloho Okotete, Subin Lee, and Christoph Kirchlechner — Karlsruhe Institute of Technology, Karlsruhe, Germany

Martensitic steels are critical for many load-bearing applications due to their inherent microstructure, giving rise to unique mechanical properties. However, traditional steelmaking routes produce high greenhouse gas emissions, posing a long-term threat to our environment. Cleaner steel production alternatives aim to use recycled iron scrap as input to electric arc furnaces used in steelmaking. A significant concern for key stakeholders in the steel industry and academia is the presence of residual elements, including Cu, Sn, Sb, As, and P, in iron scrap. Hence, an in-depth analysis of the role of the residual elements on the local and global mechanical properties of martensitic steel would provide relevant insights for the development of environmentally friendly steelmaking alternatives. Small-scale mechanics using indentation-based techniques can help locally probe how the critical microstructural features of lath martensite, such as prior austenite grain boundaries, packets, blocks, and laths, are affected by residual elements.

In this talk, we use nanoindentation, micro-pillar compression, and micro-cantilever bending experiments to identify the residual element that has the most detrimental effect on the microstructure and properties of our lath martensite. Then, proceed to determine the most impacted microstructural feature of our microstructure as well as the predominant damage mechanism in the steel samples.

MM 7.9 Mon 18:00 SCH/A215

Martensitic phase transformation and anomalous hardening of CrMnFeCoNi high-entropy alloy deformed by high pressure torsion — Robert Chulist[1], Aurimas Pukenas[2], Anton Hohenwarter[3], Reinhard Pippan[3], and •Werner Skrotzki[2] — [1]AGH University of Science and Technology, Krakow, Poland — [2]Technische Universität, Dresden, Germany — [3]Montanuniversität, Leoben, Austria

Under hydrostatic pressure, the CrMnFeCoNi high-entropy alloy (HEA) undergoes a phase transformation from face-centered cubic to hexagonal close-packed. The onset pressure is strongly reduced by high pressure torsion (HPT): shear stress promotes partial dislocation slip. HPT of the low stacking fault energy HEA leads to a nanocrystalline microstructure. The hardness anomaly is due to the extreme nanostructuring, with grain boundary/interphase boundary sliding acting as predominant deformation mechanism: inverse Hall-Petch regime, in which hardness increases with increasing grain size. In submicrocrystalline materials, conventional Hall-Petch hardening dominates, i.e., hardness decreases with increasing grain size.

MM 7.10 Mon 18:15 SCH/A215

Insights into loading condition and microstructural evolution under tribological load — •Antje Dollmann, Robin Freville, Patric Gruber, Christoph Kirchlechner, and Christian Greiner — IAM, KIT, Karlsruhe, Germany

Tribological loading changes the microstructure of materials in contact, e.g. in coarse-grained metals, grain refinement occurs, followed by cracks formation and wear particles removal leading to component failure. This requires an adequate description of the stress field to understand the ongoing microstructural evolution. Due to the complexity of tribological loading, two approaches were explored, both on single-crystalline face-centred cubic metallic materials:

(1) The experiments on CoCrFeMnNi were designed in such a fashion that in some crystal orientations deformation twins were formed. These served as probes to validate various stress field models. General trends regarding the influence of different materials parameters can be identified. The most significant mismatch is between the experimentally observed deformation layer depth and the calculated depth by the stress field. (2) In copper, one deformation layer was analysed by *Laue. Based on its higher sensibility towards small deformations, the deformation layer thickness was greater than what had been detected previously. The combination of those approaches gives deep insight into the so far hidden stress field, which will support future efforts in designing materials to withstand tribological loading.