# KFM 14: Mechanical Properties and Alloy Design: e.g. Light-Weight, High-Temperature, Multicomponent Materials (joint session MM/KFM)

Time: Wednesday 11:45–13:00 Location: C 230

KFM 14.1 Wed 11:45 C 230

**Atomic cluster expansion for binary Ag-Pd alloys** — Yanyan Liang, •Matous Mrovec, Yury Lysogorskiy, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, 44801 Bochum, Germany

Binary alloys of silver and palladium have recently attracted increased attention due to their applications in catalysis and nanotechnology. However, the binary Ag-Pd system lacks reliable and efficient interatomic potentials that provide an accurate description of structural and thermodynamic properties, in particular for atomistic simulations of nanoparticles as well as large scale simulations of mechanical properties. In this work, we present an atomic cluster expansion (ACE) parameterized for Ag-Pd with ab-initio accuracy. We show that the ACE parametrization provides an accurate description of the elastic, structural and thermodynamic properties of both elements as well as their compounds. We demonstrate the computational efficiency and the applicability of the developed potential for atomistic simulations of complex phenomena in elemental as well as Ag-Pd systems.

KFM 14.2 Wed 12:00 C 230

**Training strategies for machine-learning potentials suitable to simulate mechanical response of ceramics** — •Shuyao Lin[1,2], Zhuo Chen[3], Luis Casillas-Trujillo[2], Ferenc Tasnadi[2], Zaoli Zhang[3], Lars Hultman[2], Paul H. Mayrhofer[1], Davide G. Sangiovanni[2], and Nikola Koutna[1,2] — [1]Institute of Materials Science and Technology, TU Wien, A-1060, Vienna, Austria — [2]Department of Physics, Chemistry, and Biology (IFM), Linköping University, SE-58183, Linköping, Sweden — [3]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, A-8700, Leoben, Austria

Machine-learning interatomic potentials (MLIPs) offer a powerful avenue for simulations beyond length and timescales of *ab initio* methods. In particular, MLIPs enable investigations of mechanical properties and fracture behaviour of materials with supercell sizes, loading geometries and temperatures relevant for real operation conditions. Using the example of hard $TiB_2$ ceramic, in this talk we propose a strategy for fitting MLIPs suitable to simulate mechanical response of monocrystals from atomic to nanoscale, including strains until fracture and deformation-induced phase transformations. After validation, the best-performing MLIP is employed to carry out molecular dynamics simulations of various loading conditions, with main focus on tensile and shear deformation. Consequently, we derive size-dependent trends in theoretical strength, toughness, and crack initiation patterns of $TiB_2$. To approach experimental observations, we additionally apply our MLIP to models containing a pre-crack and/or grain boundaries.

KFM 14.3 Wed 12:15 C 230

**Investigating the yield stress anomaly of $Ni_3Al$ with physically informed machine-learning potential** — •Xiang Xu, Xi Zhang, Siegfried Schmauder, and Blazej Grabowski — University of Stuttgart, Stuttgart, Germany

The anomalously increasing yield stress with temperature of some intermetallics is predominately controlled by the Kear-Wilsdorf lock (KWL), of which the formation and unlocking are closely related to a cross-slip process. Yet so far, knowledge of this cross-lip process is limited, leading to significant approximations in existing models for predicting the mechanical behavior of those materials. In this study, molecular dynamics simulations were conducted by using a physically informed machine-learning potential to replicate dislocation activities of $Ni_3Al$. For the first time, it is observed that the formation and unlocking of KWL occurs with a step-by-step cross-slip process, of which the distance varies between one or two atomic planes inside each step. Moreover, a strong temperature dependence of the necessary stress to unlock a KWL was discovered, differing from previous approximations. This study not only advances the understanding on the yield stress anomaly in $Ni_3Al$, and also establishes a systematic workflow for yielding multiscale atomistic simulations using machine-learning potentials.

KFM 14.4 Wed 12:30 C 230

**The Effect of Al Sublattice in Tuning Elastic Anisotropy in Fe-Ta-Al Laves Phases** — •Nisa Ulumuddin, Christina Gasper, Zhuocheng Xie, and Sandra Korte-Kerzel — RWTH Aachen Institut für Metallkunde und Materialphysik

As Laves phases found in alloys are often undesirable due to its brittleness, fundamental knowledge on tuning its mechanical properties can pave the pathway for the enhanced design of engineering alloys. The structural motifs arising from the substitutional mixing of Al into the $Fe_2Ta$ Laves phase at varying Al:Fe ratios were studied by first-principles. The presence of an Al sublattice was found to reduce elastic anisotropy, owing to changes within the bonding nature of the crystal. They induce a higher degree of metallic bonding within the crystal as Al is relatively less electronegative than Fe. The increased degree of non-directional bonding decreases the directional preference for elastic deformation. These results signify the possibility of adjusting the mechanical properties of intermetallics by considering the electronic properties of their individual components.

KFM 14.5 Wed 12:45 C 230

**Effect of the V-VIB groups ternary elements on the properties of Ti2AlM-type O-phases: A first-principles study** — •Zeinab Heidari Pebdani[1,2], Florian Pyczak[1,2], and Rebecca Janisch[3] — [1]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]BTU Cottbus-Senftenberg, Cottbus, Germany — [3]ICAMS, Ruhr-Universität Bochum, Germany

Despite the recent introduction of $\gamma$-TiAl-based alloys into service, the assessment of TiAl-alloys based on the ternary Ti2AlM orthorhombic O-phase, which are promising high-temperature structural materials, has not yet been completed. The focus of this contribution is on the impact of ternary alloying elements of the V-VIB groups of the periodic table on phase stability, structural, mechanical, thermal properties, and lattice dynamics of Ti2AlM (M= V, Nb, Ta, Mo, W) type O-phases. All Ti2AlM compounds satisfy the Born stability criteria, but their properties are largely affected by the ternary element M. According to the energy of formation, Ti2AlMo is the most stable type of O-phase. The bonding behavior of all compounds is investigated by analyzing the electronic density of state plots. It was found that stronger Ti-M bonding enhances while stronger Ti-Al bonding decreases the ductility in the Ti2AlM compounds. The thermodynamic stability of the intermetallic phases is key information to further develop these materials. To consider this we have used a set of comprehensive ab initio methods, in order to determine the temperature dependence of the properties of those intermetallic phases.