MM 8: Topical session (Symposium MM): High entropy and compositionally complex alloys

Sessions: Modelling I and II

Time: Monday 15:45–18:30 Location: H43

Topical Talk MM 8.1 Mon 15:45 H43

First principles modeling of high entropy alloys — •Levente Vitos — Royal Institute of Technology KTH, Stockholm, Sweden

Thanks to impressive developments within Density Functional Theory (DFT), electronic structure solvers and computational power during the last few decades, modern materials research receives increasing support from first-principles modeling. Such approach gives fundamental understanding, offers efficient pre-screening against various degrees of freedom and provides information where experimental assessments are not feasible. Today the ab initio theory aided materials assay finds its way in almost all areas of advanced materials design and characterization.

Due to the complexity of the problem, DFT modeling was practically missing within the field of High Entropy Alloys (HEAs) for almost one decade after their discovery. Starting from early 2010s, we made a series of attempts to fill this gap and extend the scope of ab initio modeling to HEAs. In the present contribution, I will briefly overview the pioneering applications of alloy theory in the case of magnetic and refractory HEAs, and point out the main known and hidden challenges associated with such efforts. I will present our recent theoretical predictions for the mechanical and magnetic properties of existing and hypothetical HEAs. Special emphasis will be places on the plastic deformation mechanism in HEAs with close packed crystal structure and the role of intrinsic energy barriers in the competing deformation mechanisms.

MM 8.2 Mon 16:15 H43

The elastic-strain energy stability criterion for complex concentrated alloys — •Angelo F Andreoli[1], Jiri Orava[1], Peter K Liaw[2], Hans Weber[1], Marcelo F de Oliveira[3], Kornelius Nielsch[4], and Ivan Kaban[1] — [1]IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Materials Science and Engineering Department, The University of Tennessee, 414 Ferris Hall, Knoxville, TN 37996, USA — [3]Materials Science and Engineering Department, University of São Paulo, Avenida João Dagnone 1100, CEP 13563-120, São Carlos, SP, Brazil — [4]IFW Dresden, Institute for Metallic Materials, Helmholtzstr. 20, 01069 Dresden, Germany

An empirical method is developed, based on the calculated theoretical elastic-strain energy, to predict the phase formation and its stability for complex concentrated alloys. The method prediction quality is compared with the traditional empirical rules based on atomic-size mismatch, enthalpy of mixing and valence electron concentration for a database of 235 different alloys. Considering the different available empirical methods used to date, the *elastic-strain energy vs. valence electron concentration* criterion shows an improved ability to distinguish between single-phase solid solutions, mixtures of solid solutions and intermetallic phases. The criterion is especially strong for alloys that precipitate the mu phase. The theoretical elastic-strain-energy parameter can be combined with other known parameters, such as those noted above, to establish new criteria which can help predicting the design of novel high-entropy alloys with on-demand combination of mechanical properties.

MM 8.3 Mon 16:30 H43

***Ab initio* vibrational free energies including anharmonicity for multicomponent alloys** — •Prashanth Srinivasan[1], Yuji Ikeda[2], Blazej Grabowski[2], Jan Janssen[2], Alexander Shapeev[3], Jörg Neugebauer[2], and Fritz Körmann[1,2] — [1]TU Delft — [2]MPIE Dusseldorf — [3]Skolkovo Institute of Science and Technology

High entropy alloys have gained widespread attention owing to their superior mechanical properties. *Ab inito* modeling is a powerful tool to analyze and predict their thermodynamic properties. In combination with statistical sampling techniques, free energy surfaces *F(T,V)* are accessible from which properties such as thermal expansion coefficient and heat capacity can be derived and compared to experiments. At higher temperatures, the vibrational free energy — including anharmonic contributions — is a major contributor. But as the number of components in the alloy increases, *ab initio* calculations to obtain accurate values of the free energy become expensive. In this work, we present an efficient approach to numerically calculate exact vibrational free energies. Firstly, a machine learnt potential (moment tensor potential [Shapeev, 2016]) is built based on *ab initio* data, the validity of which is tested by comparing its results to DFT, and secondly, the MTP is used as a part of a thermodynamic integration to get accurate vibrational free energies. The approach is applied to 12 refractory alloys having two to five components to study the impact of configurational entropy on the vibrational free energies. The workflow is implemented in pyiron (http://pyiron.org) to enhance its dissemination and reuse.

MM 8.4 Mon 16:45 H43

Atomistic Simulation of Dislocations in High Entropy Alloys — •Aviral Vaid[1], Michael Zaiser[2], and Erik Bitzek[1] — [1]Materials Science and Engineering, Institute I, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Institute of Materials Simulation, Department of Materials Science, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

Understanding dislocation mobility and dislocation-obstacle interactions is of fundamental importance for the development of alloys with improved mechanical properties. Single phase high entropy alloys (HEAs) are a class of chemically complex alloys that have shown exceptional mechanical properties. Due to the chemical complexity of these alloys, the characteristics of energy landscape that a dislocation experiences in these alloys still needs to be investigated. Through atomistic simulations, we perform a comprehensive characterization of the segment-length-dependent dislocation properties such as Peierls barrier, Larkin length, dislocation line energy, and dislocation structure for both edge and screw dislocations. The dislocations are studied in model HEA systems using different potential formalisms to assess the robustness of the atomistic simulation results. The random nature of the pinning field, where in a sense every atom is a solute, leads to a complex situation as the dislocation adjusts its shape to the fluctuating energy landscape. The results are discussed in the context of parametrizing discrete dislocation dynamics models.

30 min. break

Topical Talk MM 8.5 Mon 17:30 H43

Machine-learning interatomic potentials for multicomponent alloys — •Alexander Shapeev — Skolkovo Institute of Science and Technology, Skolkovo Innovation Center, Moscow 143026, Russia

Multicomponent alloys are a challenge to materials design. It is time- and resource-consuming to exhaust the space of possible compositions experimentally, and equally time- and resource-consuming to do it via ab initio modeling. Moreover, many empirical and data-driven approximants to ab initio models also fail because the configurational space is huge and it is hard to avoid extrapolation when using such approximants for modeling multicomponent alloys.

In my talk I will present a machine-learning framework for the discovery of stable phases of multicomponent alloys and computation of their free energy and derivative properties including thermodynamic stability of phases. The framework is based on (1) machine-learning interatomic potentials capable of very accurately approximating ab initio models, and (2) an active-learning algorithm capable of detecting extrapolation in configurational space attempted when predicting interatomic interaction, and through additional fitting ensure reliability of the predictions.

MM 8.6 Mon 18:00 H43

Tuning magnetic properties of high entropy alloys: A combined theoretical and experimental study — •Biswanath Dutta[1], Ziyuan Rao[2], Lukas Schäfer[3], Zhiming Li[2], Oliver Gutfleisch[3], Fritz Körmann[1,2], and Dierk Raabe[2] — [1]Materials Science and Engineering, TU Delft, Delft, Netherlands — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [3]Institut für Materialwissenschaft, TU Darmstadt, Germany

Magnetic properties of high entropy alloys (HEAs) have been a topic of growing research in the last years. Of particular interest are subtle changes in magnetic features due to the substitution of non-magnetic

elements in magnetic HEAs. Using ab initio calculations, we investigate the impact of Cu on magnetic properties of FCC FeCoNiMn alloys. The coherent potential approximation is employed to address the chemical disorder while the high temperature paramagnetic state is treated within the disordered local moment approach. Among the considered magnetic states, our calculations reveal an antiferromagnetic order for Mn atoms in the lowest energy state. The impact of this on the prediction of Curie temperatures is subsequently discussed. We show that both the Curie temperature and the saturation magnetization increase due to Cu substitution. The obtained compositional trends are discussed in terms of varying concentration of magnetic elements and volume changes. Our predicted trends of the magnetic properties also show excellent agreement with the corresponding experimental results. Based on the achieved results we identify Cu as a promising element to tune and improve magnetic properties of FeCoNiMn-based HEAs.

MM 8.7 Mon 18:15 H43

Investigation of phase stability in high-entropy alloys with the use of machine-learning interatomic potentials — •Tatiana Kostiuchenko[1], Alexander Shapeev[1], Fritz Körmann[2,3], and Jörg Neugebauer[2] — [1]Skolkovo Institute of Science and Technology, Moscow, Russia — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [3]Delft University of Technology,The Netherlands

High-entropy alloys (HEA) is a class of materials which consist of at least four different chemical elements and have a specific structure. These alloys have high ductility and yield strengthening, they are widely used as construction and heat-resistant materials. Experimental methods of HEAs investigation are time-consuming, and by this reason, computational methods of HEAs investigation are of the high interest. In this work, a new data-driven approach for investigation of solid solution stability in HEA is proposed. It is based on Canonical Monte Carlo algorithm with the use of machine-learning potential, namely low-rank potential (LRP) [Shapeev A., 2017]. The approach was examined by comparing it with the existing works. The key difference of the LRP from the other "on-lattice" models is its ability to take into account local lattice distortions, which is critical for the materials behavior. The parameters of the LRP were fitted on quantum-mechanical data, the LRPs prediction accuracy was 1 meV/atom. Thus, the temperature of the order/disorder phase transition was accurately calculated for the equiatomic NbMoTaW system. The low-energy structures and the mechanisms of chemical ordering were also investigated.