MM 36: Topical Session: Interface-dominated phenomena - Theoretical Approaches

Time: Wednesday 11:45–13:00 Location: IFW A

Topical Talk MM 36.1 Wed 11:45 IFW A

Computational methods for grain boundary engineering — Daniel Scheiber, Vsevolod Razumovskiy und •Lorenz Romaner — Materials Center Leoben Forschung GmbH, Leoben, Austria.

Segregation of solute elements to grain boundaries plays an important role for the physical properties of many technologically relevant materials. For example, it can induce intergranular embrittlement in steels, copper, nickel-based alloys or refractory metals. Furthermore, also nanocrystalline stability, grain growth, phase transformations and electrical properties can be steered via segregations. Controlling such phenomena provides a lever for developing materials with superior or targeted properties.

In this talk we will present our recent activities regarding grain boundary engineering. This involves the development of computational methodologies providing direct coupling of atomistic grain boundary simulations with thermo-kinetic modeling. With such approaches, we describe the evolution of grain boundary chemistry during heat treatment, analyze depletion zones next to grain boundaries and explore the relationship with precipitation kinetics. The methods are applied to steels and refractory metals to show how chemical composition, grain size and heat treatment can be designed to reduce the propensity for intergranular cracking. As a last point we present the development of our software tool SEGROcalc and conclude with an outlook on challenges for future segregation modeling.

MM 36.2 Wed 12:15 IFW A

Towards large-scale atomistic calculations with quantum-mechanical accuracy: the QM/MM route — •Gehringer Dominik[1], Liam Huber[2], Jörg Neugebauer[2], and David Holec[1] — [1]Department Materials Science, Montanuniversität Leoben, Franz-Josef-Straße 18, 8700 Leoben — [2]Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf

Although ab-initio methods such as Density Functional Theory (DFT) provide a powerful tool to investigate materials science problems, they are also a limiting factor in terms of tractable system sizes, especially when one moves on to extended defects (interfaces, grain boundaries, dislocations). In constrast to DFT molecular dynamics (MD) is also well suited to properly describe temperature and mechanical properties, since simulations can handle thousands of atoms needed for describing extended defects. On the other hand, since in MD simulations do not consider the electronic structure but rather rely on interatomic potentials, the accessible chemistry is restricted by the availability of those. This is a limiting factor for e.g. segregation studies.

In the present contribution we will describe our developments for linking quantum mechanical calculations with molecular mechanics. While MM is applied to matrix regions, QM is used to treat chemical impurities and extended defects such as interfaces for which interatomic potentials are not available. After introducing the methodology and its implementation within the pyiron framework, we will show an example of linking LAMMPS and VASP calculations on an example of segregation to phase boundaries in γ/α_2 structured TiAl alloys.

MM 36.3 Wed 12:30 IFW A

Characterization of the stability of metal/metal interfaces by atomistic simulations — •Daniel F. Urban[1], Oskar Till[2], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]University of Freiburg, FMF, Germany

The reliable prediction of the adhesion and mechanical stability of interfaces between two metal phases from density functional theory (DFT) calculations remains a challenge. One possible approach to systematically address this issue is an idealized cleavage simulation analysed in terms of the Rose-Ferrante-Smith universal binding energy relationship (UBER) which results in a measure for the ideal work of separation and the maximum tolerable normal strain. Another approach is the study of the gamma surface, i.e. the generalized stacking fault energy, as function of lateral displacement, which yields information on the critical resolved shear stress of dislocation motion.

Here we study a variety of coherent interfaces between fcc and hcp metals in terms of the above mentioned methods. We analyze the interface energy in terms of coupled tensile and shear displacements which include the effect of the tension softening of the interface. Furthermore, the influence of an additional lateral mechanical strain on the two phases, as often present in experimentally grown thin layers, is examined.

MM 36.4 Wed 12:45 IFW A

Comparative atomistic-continuum modeling and experimental characterization of dislocation-solute interaction in binary alloys — •Jaber R. Mianroodi[1,2], Pratheek Shanthraj[2,3], Xuyang Zhou[2], Gregory B. Thompson[4], and Bob Svendsen[1,2] — [1]RWTH Aachen University, Aachen, Germany — [2]Max-Planck-Institut fur Eisenforschung, Dusseldorf, Germany — [3]The University of Manchester, Manchester, UK — [4]The University of Alabama, Tuscaloosa, USA

The purpose of the current work is a comparative modeling and experimental investigation of the interaction between defects and chemistry in metallic alloy systems at the nanoscopic scale. On the modeling side, three approaches are employed and compared. These include (i) hybrid Monte-Carlo molecular dynamics (e.g., [1]), (ii) diffusive molecular dynamics (e.g., [2]), and (iii) atomistic phase-field chemomechanics (e.g., [3]). All these are energy-based approaches. In the first two, the energy is determined by an interatomic potential. For (quantitative) comparability, the same potential is used to calibrate the phase-field energy model. In the current work, these three methods are applied to the modeling of solute segregation to dislocations in the binary system Pt-Au. Corresponding simulation results are compared with analogous experimental results from atom probe tomography and precession electron diffraction. Among others, these include in particular results on solute segregation to the dislocation core as well as on maximum segregation to dislocations at different bulk compositions.