MM 51: Computational Materials Modelling - Mechanical Properties

Time: Thursday 10:15–11:30 Location: IFW B

MM 51.1 Thu 10:15 IFW B

Atomic scale investigation of internal friction in austenitic steels — •Osamu Waseda, Tilmann Hickel, and Jörg Neugebauer — MPIE Düsseldorf

Internal friction measurements are a powerful method for the identification of the nature of point defects and complex short range order of solute atoms in austenitic steels. Whereas it is possible to identify point defect interactions that contribute to internal friction, it is difficult to decompose experimental results into each cause, as the complex interactions and the stochastic nature of solute diffusion smear out different contributions. Therefore, the interpretation of experimental results requires assumptions that are currently a matter of discussion. Correspondingly, a theoretical model that yields quantitative agreement with experiments is still missing for austenite. In this study, we developed a novel thermodynamic method conjugated with ab initio calculations to understand the short range ordering generated by vacancies and carbon atoms. This model not only accounts for the variation of solute interactions due to material deformation, but also the variation of migration energies due to solute interactions. In this way, it removes the commonly known discrepancy between empirical models and experimental results. This model, therefore, enables us to decompose experimental internal friction results into each contribution of point defect interactions. This clarifies the nature of short range order of carbon and vacancies in austenite, which is decisive for their mechanical performance.

MM 51.2 Thu 10:30 IFW B

Closing the gap between atomic-scale lattice deformations and continuum elasticity within the phase-field crystal framework — •Marco Salvalaglio[1], Ken Elder[2], and Axel Voigt[1] — [1]Institute of Scientific Computing, TU Dresden — [2]Department of Physics, Oakland University, Rochester, Michigan, USA

The Phase-Field Crystal (PFC) model allows for describing atoms in a lattice through a continuous probability density and focusing on diffusive time scales. In the amplitude expansion of the PFC model (APFC), a coarse-grained description of the atomic probability density is obtained by focusing on its complex amplitudes and, in turn, on their dynamics. These amplitudes vary on length scales larger than the atomic spacing but still retain details of the crystal lattice. Numerical simulations based on the APFC model and exploiting the Finite Element Method are shown to reproduce defects structures in two and three dimensions for different crystal symmetries as well as their dynamics. The derivation of continuous deformation fields from the complex amplitudes, their connections with the elasticity theory, and the characterization of dislocations by the Burgers vector density are also discussed. These findings assess the APFC model as a reliable coarse-graining of the PFC model. More importantly, the description of crystal structures through amplitudes is shown to provide a natural framework connecting atomic-scale lattice deformations and continuum elasticity.

MM 51.3 Thu 10:45 IFW B

Two mechanisms of anomalous slip in bcc metals — •Roman Gröger[1] and Vaclav Vitek[2] — [1]Czech Academy of Sciences, Institute of Physics of Materials and CEITEC IPM, Brno, Czech Republic — [2]University of Pennsylvania, Department of Materials Science and Engineering, Philadelphia, PA, USA

Many body-centered cubic metals and alloys exhibit anomalous slip of $1/2\langle 111\rangle$ screw dislocations on {110} planes with very low Schmid factors. The origin of this phenomenon is still unknown but there is a growing pool of evidence linking it to core structures of these dislocations and their transformations under applied load. Here, we identify two possible mechanisms leading to the anomalous slip for uniaxial loading in the center of the stereographic triangle. The first originates from the glide of $1/2[111]$ and $1/2[\bar{1}11]$ screw dislocations on their most highly stressed planes, as proposed by the Schmid law. This inevitably leads to their intersection and formation of [100] screw junctions, as proposed previously in the co-planar double slip model. If this junction is strong, the three dislocations have to move on their common $(0\bar{1}1)$ plane, which results in anomalous slip. The second mechanism is based on a hypothesis that the two $1/2\langle 111\rangle$ screw dislocations may move directly on the $(0\bar{1}1)$ plane in contradiction to the Schmid law. Using atomistic simulations, we investigate which of these two mechanisms is operative at 0 K in the five non-magnetic bcc metals (V, Nb, Ta, Mo, W), magnetically isotropic state of Cr, and in ferromagnetic α-Fe. The predictions of both models are compared with available low-temperature experiments on high-purity single crystals.

MM 51.4 Thu 11:00 IFW B

Synergetic effects of solute and strain in biocompatible Zn-based and Mg-based alloys — •Shihao Zhang[1,2], Yuanqi Guo[1], Irene J. Beyerlein[3], Dominik Legut[2], Shunli Shang[4], Zi-Kui Liu[4], and Ruifeng Zhang[1] — [1]School of Mat. Sci. and Eng., Beihang University, China — [2]IT4Innovations, VSB-TU Ostrava, Czech Republic — [3]University of California at Santa Barbara, USA — [4]Pennsylvania State University, USA

Zn and Mg alloys are considered highly promising biodegradable materials for cardiovascular stent applications; however, their poor strength has prevented this application. Via first-principles calculations and Peierls-Nabarro model, we investigate the coupled effect of the solute element and mechanical straining on the stacking fault energy (SFE), dislocation core structure, and Peierls stress in Zn and Mg alloys. Several biocompatible solute, i.e., Li, Al, Mn, Fe, Cu, Mg and Zn, were considered. It is suggested that some elements, like Fe, can potentially enhance strength in both Zn and Mg alloys, while other elements, like Li, can lead to opposed effects. The effect of solute strengthening and longitudinal straining on SFEs is much stronger for the Zn alloys than for the Mg alloys. Investigations on electronic structure and bond lengths reveal a coupled chemical-mechanical effect of solute and strain on electronic polarization, charge transfer, and bonding strength, which can explain the weak mechanical effect on Zn alloys and the variable strengthening effect among these solutes. These findings provide critical information needed in solute selection in Zn and Mg alloy design for biomedical applications.

MM 51.5 Thu 11:15 IFW B

The emergence of small-scale self-affine surface roughness from deformation — •Wolfram Nöhring[1], Adam Hinkle[1,2], Richard Leute[1], Till Junge[6], and Lars Pastewka[1,3,4,5] — [1]Department of Microsystems Engineering, University of Freiburg, Germany — [2]Materials, Physical and Chemical Sciences Center, Sandia National Laboratories, USA — [3]Institute for Applied Materials, Karlsruhe Institute of Technology, Germany — [4]Freiburg Materials Research Center, University of Freiburg, Germany — [5]Cluster of Excellence livMatS, University of Freiburg, Germany — [6]Department of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland

Surfaces in nature and engineering are often rough across many length scales, with self-affine scaling of heights. There is presently no unifying theory for the origin of roughness and self-affinity. One likely contributor is plastic deformation. In this work, the link between plastic deformation and self-affine roughness is investigated using molecular dynamics simulations. Three different materials are considered, single-crystal Au, the High Entropy Alloy $Ni_{36.67}Co_{30}Fe_{16.67}Ti_{16.67}$, and amorphous $Cu_{50}Zr_{50}$. Bi-axial compression of initially atomically flat surfaces of these materials is simulated. A self-affine topography emerges in all cases during plastic deformation, despite differences in composition, structure, and deformation mechanisms. Moreover, it is shown that non-affine displacements in the bulk scale self-affinely as well. The results indicate that self-affinity of plastic deformation is sufficient to explain the emergence of self-affine surface roughness.