MM 15: Interfaces I

Time: Monday 14:45–16:00 Location: H5

MM 15.1 Mon 14:45 H5

Ab initio characterisation of the mechanical behavior of grain boundaries — Naveed Ahmed, •Rebecca Janisch, and Alexander Hartmaier — ICAMS, Ruhr-Universität Bochum, 44780 Bochum

Multiscale modeling of polycrystals requires knowledge of the elastic and plastic properties of the interfaces in their microstructure. To capture the physics of grain boundary sliding, migration, and decohesion, these processes should be investigated by atomistic calculations. Especially if the influence of segregated impurities, which can alter the bond character, shall also be described, a quantum mechanical treatment is necessary. However, the construction of continuum constitutive laws for grain boundaries from the results of ab initio calculations still requires sampling a five parameter space: the orientation of the grain boundary plane, the misorientation axis and the misorientation angle. This remains a formidable task, even with today's computers. In this paper we will introduce our investigation of the mechanical properties of grain boundaries in aluminum, which aims at replacing such a comprehensive sampling by as few representative calculations as possible. On the one hand we are investigating discriminating features in the elastic and plastic response of tilt and twist grain boundaries. On the other hand we are looking for common behavior that enables a unified treatment and a separation of variables.

MM 15.2 Mon 15:00 H5

Non-equilibrium grain boundary segregation of phosphorus in nickel-base superalloy — Lei Zheng[1] and •Tingdong Xu[2] — [1]Institute for materialphysics, university of Muenster, wilhelm-klemm-str. 10, 48149, Muenster, Germany — [2]Superalloy department, Central iron and steel research institute, xueyuan nanlu 76, 100081, Beijing, China

Applying Auger electron spectroscopy, the levels of grain-boundary segregation of phosphorus in a Ni-based superalloy are measured after solution treatment at 1200 °C for 9.8 h or at 1020 °C for 68.5 h and subsequent aging at 720 °C for 2 h. It is found that the levels of segregation increase with the solution treatment temperature. The measurement results are interpreted by the laws of equilibrium and non-equilibrium segregation. Based on this analysis, the concept of non-equilibrium grain-boundary segregation of phosphorus in a superalloy is confirmed for the first time.

MM 15.3 Mon 15:15 H5

Line stress of step edges — •weina li[1,2], huiling duan[2], and jörg weissmüller[1,3] — [1]Karlsruher Institut für Technologie, Institut für Nanotechnologie, Karlsruhe, Germany — [2]Peking University, Beijing, P.R.China — [3]Universität des Saarlandes, Saarbrücken, Germany

It is well known that the surface of a solid interact with the underlying volume phase by a mechanical force, which is quantified by the surface stress. By analogy, the line elements at solid surfaces, such as triple lines, edges, or steps may also interact mechanically with the bulk. The forces originating from lines may be derived by taking the derivative of the line tension - an excess in energy per line length - with respect to the strain. The resulting 'line stress', $\mathbf{t}$, has not been systematically investigated so far. Consider of dimensionality, line stress should be represented by a scalar describing the magnitude of a stress directed along the line. However, it's well known that parallel step edges at planar surfaces interact via stress fields in the substrate that are dominated by normal stress components. The standard (dipole-) models [1] of step stress predict that line stress is zero. We present molecular statics computations of vicinal surfaces that show a nonzero value, with parallel and normal components. We also present a continuum model which explains the observations in terms of the extra surface stress at the inclined (up- or down-) face of the step edge. The assistance by Karsten Albe in setting up the numerical simulation is greatly acknowledged.

[1] P. Müller, A. Saul, Sur. Sci. Rep 54 (2004), 157.

MM 15.4 Mon 15:30 H5

Interfacial properties of metallic systems from molecular dynamics simulation — •Jürgen Horbach and Roberto E. Rozas — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

Using molecular dynamics (MD) computer simulation, interfacial properties of crystal-liquid interfaces are investigated for the one-component metallic systems Ni and Ti. The interactions between the atoms in these systems are modeled by potentials of the embedded atom type (EAM). Inhomogeneous systems are simulated where the crystal phase in the middle of an elongated simulation box is surrounded by the liquid phase and separated by two interfaces (due to periodic boundary conditions in all Cartesian directions). The melting temperature and crystal growth coefficients are determined. At coexistence, we demonstrate how one can accurately obtain interfacial free energies from a detailed analysis in the framework of capillary wave theory.

MM 15.5 Mon 15:45 H5

Ordering dynamics of snow under isothermal conditions — •Henning Löwe, Johanna Spiegel, and Martin Schneebeli — WSL Institute for Snow and Avalanche Research SLF, Davos, Switzerland

We have investigated the morphological evolution of laboratory snow at different temperatures by means of X-ray tomography. The collective dynamics of the bicontinuous ice-vapor system is monitored by the evolution of the two-point correlation function $C(\mathbf{r},t)$ and an ice thickness distribution. We observe the absence of dynamic scaling and reveal fundamentally different classes of length scales: The first class comprises the mean ice thickness and the ice volume per surface area. Both follow a power law $l \sim t^{1/z}$ in time, where $z \approx 3$ is in accordance with coarsening of a locally conserved order parameter. A second class of length scales is defined by the inverse partial derivatives of $C(\mathbf{r},t)$ at the origin. The second class shows a slower growth with anomalous power law scaling $z \approx 5$. The two different power laws are consistent with fractal coarsening and reveals the persistence of long-range correlations from initial, dendritic conditions. A third class of length scales is defined by the first zero crossing of $C(\mathbf{r},t)$ on the coordinates axes which display a non-monotonic evolution with a strong anisotropy between vertical and horizontal directions. We attribute this behavior to larger scale structural relaxations of the ice network which apparently leave the small scale, interfacial relaxations unaffected. However, vice versa it poses the question how structural mobility is induced by coarsening.