

MM 21: Topical Session: Thermodynamics at the nano scale I - Kinetics, nucleation, grain growth, segregation

Time: Tuesday 10:15–11:30

Location: BAR 205

Topical Talk MM 21.1 Tue 10:15 BAR 205
Nucleation and growth in small systems — ●CHRISTOPH DELLAGO — University of Vienna, Vienna, Austria

Under suitable conditions, first order phase transitions such as the freezing of a liquid or the structural transformation of a solid occur via a nucleation and growth mechanism, in which a nucleus of the stable phase is formed in the metastable phase. For systems with sizes in the nanometer regime, the nucleation mechanism and its kinetics are strongly affected by finite size effects. I will address this issue using melting/freezing of gold nanoparticles and the Wurtzite-to-rocksalt transition in CdSe nanocrystals as illustrative examples. Based on the results of transition path sampling simulations, I provide a picture of the transition mechanism paying particular attention to the structure of the critical nuclei. The role of the reaction coordinate in the investigation of the transition mechanism is discussed.

MM 21.2 Tue 10:45 BAR 205

Observing steady-state coarsening: From nanocrystalline to normal grain growth — ●DANA ZÖLLNER and PETER STREITENBERGER — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

It is well-known that normal grain growth is characterized by a parabolic growth law and self-similar scaling resulting in a universal, time-independent grain size distribution as well as in a self-similar topology of the polycrystalline grain microstructure. In the present work we show by theoretical considerations and modified Potts model simulations that self-similarity is also a feature of junction controlled grain growth as it can be found in nanocrystalline materials.

To this aim, the influence of the grain junctions - boundary faces, triple lines and quadruple points - on the growth kinetics is analyzed by attributing each type of boundary junction an own specific energy and mobility. This strategy results in nine size-dependent types of growth kinetics, each characterized by a self-similar scaling form of the growth law and corresponding self-similar grain size distributions. For the three limiting cases of grain growth controlled by the specific grain boundary energy in conjunction with the mobility of grain boundaries, triple lines or quadruple points the analytical results are in good agreement with those obtained by Potts model simulations. In particular, we show that triple and quadruple junction controlled coarsening is characterized by a series of quasi-steady-states reaching for long-time annealing the characteristics of normal grain growth.

MM 21.3 Tue 11:00 BAR 205

Segregation at and structure of iron grain boundaries using parameterized electronic description. — ●GEORG K. H.

MADSEN¹, JINGLIANG WANG¹, NICHOLAS HATCHER^{1,2}, and RALF DRAUTZ¹ — ¹ICAMS, Ruhr-Universität Bochum, 44780 Bochum, Germany — ²QuesTek Innovations LLC, Evanston, IL 60201, USA

We employ a recently developed iron carbon orthogonal tight-binding model of grain boundaries (GBs) in the iron-carbon system. Bulk electron states are captured in this model as it is applied to systems containing over 5,000 ferromagnetic atoms. A strategy for a systematic screening of grain boundary energies has been applied to BCC-Fe. We show how the Fe-Fe tight binding model is able to pre-screen the rigorous coincidence site lattice GBs and apply it to calculate the stable $\Sigma < 15$ GBs in α -Fe.

The properties of carbon near and on the $\Sigma 5$ (310)[001] symmetric tilt GB are calculated and it is found that a carbon atom lowers the GB energy by 0.29 eV/atom in accordance with the DFT value of 0.23 eV. Carbon segregation to the GB is analyzed, and we find an energy barrier of 0.92 eV for carbon to segregate to the carbon-free interface while segregation to a fully-filled interface is disfavored. We isolate two different mechanisms governing carbon's behavior in iron: a volumetric strain which increases the energy of carbon in interstitial α -iron and a non-strained local bonding which stabilizes carbon at the GB.

MM 21.4 Tue 11:15 BAR 205

Solid state amorphization of thin metal films embedded in bulk metallic glass — ●TOBIAS BRINK¹, DANIEL ŞOPU^{1,2}, and KARSTEN ALBE¹ — ¹Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany — ²now at ICAMS, Ruhr-Universität Bochum, Germany

Metals commonly appear in crystalline phases. Even thin films of metal stay crystalline on a variety of substrates. In contrast, it was recently observed experimentally, that thin metal layers embedded in a bulk metallic glass matrix become amorphous if they are thin enough (Ghafari *et al.*, Appl. Phys. Lett. **100** (2012), 203108). The resulting multilayer systems have possible applications in the realm of materials for magnetic tunnel junctions, among others. We reproduced this effect in a series of molecular dynamics simulations and investigated the driving force behind it. We show that thin amorphous metal nanolayers in our model system are thermodynamically stable. We present a model based on a competition between the excess energy of the amorphous phase and the interface energy. We show that the glass-glass interface has lower potential energy than the corresponding crystal-glass interface. Our model correctly predicts the critical thickness under which amorphization occurs. These results suggest that other technologically relevant systems with amorphization of metallic nanolayers may exist. The results are also of interest for the study of crystalline phases in bulk metallic glasses.