MM 16: Methods in Computational Materials Modelling (methodological aspects, numerics)

Sessions: Nucleation; Interfaces

Time: Tuesday 10:15–13:15   Location: H45

MM 16.1 Tue 10:15 H45

Atomistic mechanism of nucleation in Ni: the role of pre-structuring and seeding in polymorph selection — •Grisell Díaz Leines and Jutta Rogal — Ruhr-Universität Bochum, Universitätsstrasse 150, 44780 Bochum, Germany

Understanding the fundamental principles of polymorph selection during crystal nucleation is essential in the control and prediction of materials properties. However, to obtain a precise knowledge of the crystallization mechanism is often challenging as most physical systems exhibit polymorphic transitions and are often heterogeneously seeded by the presence of impurities. Here we employ transition path sampling together with maximum likelihood estimation to analyze the atomistic mechanism of crystal nucleation in Ni. We further investigate the effect of small pre-structured seeds on the crystallization process. The analysis of the transition path ensemble reveals that the pre-structured liquid region that surrounds the nucleus plays a crucial role in the description of the nucleation process together with the amount of fcc particles in the core of the crystal cluster. Consistent with our interpretation of the nucleation mechanism, we demonstrate that seeds with structures compatible with those observed in the growing nucleus (fcc and pre-structured liquid) facilitate the nucleation and determine the polymorph selected, while seeds with hcp and icosahedral structures have neither an effect on the nucleation rate nor on the mechanism. Our results shed light on the atomistic processes of polymorph selection during crystallization in Ni.

MM 16.2 Tue 10:30 H45

Transition path sampling of homogeneous nucleation during solidification in molybdenum — •Sarath Menon, Grisell Diaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum

The investigation of nucleation during solidification on an atomic scale is challenging for both experimental and theoretical methods due to the involved time and length scales. Since nucleation time scales are many orders of magnitude larger than the ones achieved by classical molecular dynamics, we employ transition path sampling, an atomistic simulation method that generates an ensemble of dynamical trajectories between the liquid and the solid state. From the path ensemble, thermodynamic and kinetic properties such as the free energy barrier and the nucleation rate are calculated. We study homogeneous nucleation in Mo at various undercoolings and compare the effect of the interatomic potential on the calculated properties. Furthermore, we employ transition path sampling for analysis of the nucleation mechanisms by studying the polymorphs that are generated during the initial stages of nucleation and growth. The crystal core originates in a region of pre-ordered liquid, with BCC being the most abundant phase throughout nucleation. We further compare the nucleation mechanisms in molybdenum and nickel to reveal that the final bulk structure emerges at an early stage of nucleation.

MM 16.3 Tue 10:45 H45

Hysteretic phase transitions of IrTe2: a unified picture from ab initio approaches — •Gabriele Saleh and Sergey Artyukhin — Istituto Italiano di Tecnologia, Via Morego 30, Genova 16163 Italy

A number of metal dichalcogenides are promising candidates for cutting-edge applications [1]. IrTe2 displays peculiar temperature-induced phase transitions to phases with Ir-Ir dimers [2] that can be tuned by doping and triggered by photoexcitation [3]. These transitions display hysteresis and they are accompanied by a change in the physical properties of the material, thus opening possibilities for technological applications. The various phases differ by the length of certain Ir-Ir and Te-Te bonds, that change up to 25% [3]. While a wealth of experimental results exist, the atomic-level understanding of transitions in IrTe2 is still poor. Here we present an in-depth computational investigation of the electronic structure and lattice dynamics of IrTe2. We demonstrate, through the combined use of several chemical bonding analysis approaches, that the electronic stability of low-T phases is determined by the formation of Ir2Te2 4-centre bonds. The high-T phase, instead, is stabilized by the higher entropic contribution of its phonons. We rationalize the observed hysteresis by analyzing

the energetics of phase transitions through the Nudged Elastic Bands method. Finally, we present our preliminary results on the effect of doping on both the band structures and the phonon spectra of the IrTe2 phases. REFERENCES: [1] C. Tan et al. , Adv. Mater., 29(37), 1701392 (2017). [2] Q. Li et al. , Nat. Comm., 5, 5358 (2014). [3] S. I. Ideta et al. , Sci. Adv., 4(7), eaar3867 (2018).

MM 16.4 Tue 11:00 H45

Atomistic Modelling of Early Stage Clusters In Al-Mg-Si alloys — •David Kleiven[1] and Jaakko Akola[1,2] — [1]Norwegian University of Science and Technology, Trondheim, Norway — [2]School of Chemical Technology, Aalto University, Aalto, Finland

Aluminium alloys are essential in a variety of industrial applications, including cars and aeroplanes. The mechanical properties, such as hardness and strength, depend heavily on the formation of beneficial precipitates from solute species. Interestingly, the precipitation process (and prior nucleation) can be manipulated via thermomechanical treatment. We apply the Cluster Expansion formalism as implemented in CLEASE (CLuster Expansioin in ASE) to construct a DFT-parametrised energy model for Al-Mg-Si alloys, which we further apply in finite temperature statistical simulations. Even though Al-Mg-Si is a common industrial alloy, the mechanisms behind the precipitation process are still not fully understood. In this contribution, the stable phases on the FCC lattice, which are important intermediates for needle-like precipitates, are identified with high accuracy (~5 meV/atom). We assess the role of various effects such as solute ordering and direction-dependent surface tension of solute clusters. Via this approach we obtain quantitative results for the thermodynamics of early stage clusters in Al-Mg-Si alloys which paves way for understanding the precipitation process at atomic level.

MM 16.5 Tue 11:15 H45

Atomistic Study of Nucleation and Growth in Ni$_3$Al — •Yanyan Liang, Grisell Díaz Leines, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum

The initial stages of nucleation and growth are a crucial step during solidification. Atomistic insight into nucleation, in particular for binary alloys, still remains elusive due to the extended timescales and the complexity of the process. In this study, we focus on the binary alloy Ni$_3$Al which is a key component in high-temperature superalloys. We employ transition path sampling to generate an ensemble of molecular dynamics trajectories, from which we extract thermodynamic and kinetic properties of the nucleation process. For Ni$_3$Al, we obtain two different nucleation pathways that resemble the competition between two distinct bulk crystal structures, face-centred cubic and body-centred cubic. The size of the critical nucleus commonly used as reaction coordinate strongly depends on the structural composition and is therefore not sufficient to describe the nucleation in this binary system. Both the size and crystal structure of the growing nucleus need to be explicitly taken into consideration as reaction coordinates. Furthermore, we observe that the competition between diffusion and interface growth velocities has a decisive impact on the chemical order. In Ni$_3$Al, the growth velocity surpasses the diffusion even for small undercooling of 1% which leads to disorder trapping with partial chemical order.

15 min. break

MM 16.6 Tue 11:45 H45

Machine learning and the thermodynamics of grain boundary segregation — •Liam Huber, Raheleh Hadian, Blazej Grabowski, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Solute-grain boundary (GB) interaction critically impacts the evolution and stabilization of grain structure and thus has a strong impact on the final material properties. At the atomic scale, structural disorder at the GB can create a wide variety of local environments for segregating atoms, and thus a wide distribution of segregation energies. Using classical molecular statics, we perform high-throughput

calculations of six solutes to 38 different boundaries in Al obtaining 1.4 million segregation energies. With this rich dataset, we demonstrate that the traditional Langmuir-McLean model, which approximates solute-GB interaction with a single effective energy, is insufficient. By applying machine learning techniques, we provide a new and computationally highly efficient path to obtain the full energy distribution of the solvents. Extending this approach we have also calculated a corresponding set of surface segregation energies. Using a similar distribution-based approach provides us with a direct route to assess the role of solutes on GB embrittlement.

MM 16.7 Tue 12:00 H45
Development of a layer-specific surface segregation model based on atomistic simulations beyond McLean — Tamara Krauss and •Sebastian Eich — Institut für Materialwissenschaft, Lehrstuhl für Materialphysik, Universität Stuttgart, Deutschland

In this atomistic study, layer-specific segregation to the surface is investigated for an exemplary (100) surface in iron–chromium alloys. Segregation is simulated in the semi-grand canonical ensemble using a thermodynamically accurate iron–chromium embedded-atom potential[1]. Through a continuous variation of the chemical potentials, the full composition range is explored in the temperature range from 400 K to 1400 K, enabling the analysis of surface segregation below and above the critical temperature of the miscibility gap. Taking the surface tensions into account, the change in surface formation energy according to the interfacial adsorption equation[2] is confirmed excellently.

With the obtained dependence of layer-specific segregation on bulk composition, it is shown that segregation cannot be described sufficiently by the single-parameter McLean model. Thus, an analytic layer-specific model of surface segregation is proposed which is capable of reproducing the simulated segregation data over the whole composition range with high accuracy. Using the modeled segregation curves, the change in formation energy can be described in an accurate manner as well.

[1] S. M. Eich, D. Beinke, and G. Schmitz, Comput. Mater. Sci. 104, 185 (2015).
[2] T. Frolov and Y. Mishin, Phys. Rev. B 85, 224106 (2012).

MM 16.8 Tue 12:15 H45
Atomistic simulation of bulk and grain boundaries diffusion in iron — •Sergei Starikov, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-University, Bochum, Germany

In this work, we have studied the grain boundary (GB) diffusion of the point defect and self-diffusion in pure iron. We performed the simulations with different interatomic potentials. The results of classical molecular dynamics were compared with the data calculated with DFT and BOP models. As results we have obtained that GB self-diffusion is controlled by self-interstitial atoms, while the vacancies play major role at bulk diffusion. In addition, exchange mechanism of atomic diffusion takes place for the GB with high energies. Such defectless mechanism of diffusion leads to large self-diffusion coefficient that is in 5-7 orders higher that the bulk one. The comparison with available experimental data was performed.

MM 16.9 Tue 12:30 H45
Modelling of Magnetic Driving Force in Grain Boundary Migration: Using Multi-Phase Field Method — •Liu Huo, Raphael Schiedung, and Ingo Steinbach — Interdisciplinary Centre for Advanced Materials Simulation

We provide a method which combines the dynamical solution of the magnetic moments and multi-phase field method. In our work we solve the motion of magnetic moments using either Time-Dependent Ginzburg Landau equation or Landau-Lifshitz-Gilbert equation. Meanwhile, by taking advantage of the multi-phase field method, we can solve the magnetic driving force by simply calculate the functional derivative with respect to the phase field for each terms of magnetic free energy so that we are able to solve the magnetic driven grain boundary migration simultaneously. With this method it is possible to simulate some magnetic dependent problems such as the orientation selection in external magnetic field during annealing and the magnetostriction. Our code is implemented in Openphase (www.openphase.de).

MM 16.10 Tue 12:45 H45
Determining mobilities and anisotropic grain boundary energies from MD simulations of shrinking grains — •Adrian A. Schratt and Volker Mohles — ICAMS, Ruhr-Universität Bochum

A new technique to determine average grain boundary (GB) mobilities and energies for arbitrary grain misorientations from molecular dynamics (MD) simulations has been developed. The shrinkage velocity of a cylindrical or spherical grain (2D/3D) allows to calculate the reduced mobility of the GB. From an isotropic model for the capillary driving force we can also derive the average energy of the GB during the shrinkage. The connection between the shrinkage velocity, the GB stiffness and the mobility is exploited to compute the latter. The technique is free of possible artefacts from synthetic driving forces as the GB is only driven by its curvature. In addition, information on the anisotropy of the GB energy can be derived: during shrinkage, the initially cylindrical or spherical shape becomes slightly facetted. This can be expressed as an occurrence frequency of GB plane orientations, which in turn can be used to formulate the GB energy as a function of the plane normal direction. This can be used for instance in mesoscopic models of GB motion.

MM 16.11 Tue 13:00 H45
Simulations of anisotropy effects of interface energies — •Volker Mohles and Adrian A. Schratt — ICAMS, Ruhr-Universität Bochum

Grains and particles of secondary phases control numerous properties of metallic materials. For instance, the interaction between particles and grain boundaries affects recrystallization during heat treatments of manufacturing in a very sensitive manner, which in turn control the material strength and formability. In general, the interface energy of particles and grain boundaries depends on their local orientation in relation to crystallographic planes. This anisotropy strongly affects the equilibrium shapes of particles and grains, hence it can influence the overall properties. In the present contribution, new mesoscopic 2-D and 3-D front tracking simulations of grain boundaries and particle interfaces are presented in which the anisotropy of the interface energy is fully taken into account. It is demonstrated that anisotropic interface energies derived from Molecular Dynamics simulations can be used directly to simulate the resulting particle or grain shapes. The facetting observed in the mesoscopic simulations agrees very well with the corresponding MD simulations. Hence together these simulations provide a multi-scale path toward an improved quantitative understanding of recrystallization kinetics or grain growth, which, for instance, helps improving manufacturing processes of e.g. aluminium sheet. Also, the mesoscopic simulations allow to interpret anisotropic grain boundary energies directly from experimentally observed particle or grain shapes.