MM 50: Methods in Computational Materials Modelling II: Microstructure evolution

Time: Thursday 10:15–11:45 Location: H53

MM 50.1 Thu 10:15 H53

Atomistic insight into the structure and shape of growing nuclei during solidification in Ni — •Grisell Diaz Leines, Ralf Drautz, and Jutta Rogal — Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany

A crucial stage during solid-liquid phase transformations is the initial nucleation of a stable phase within a metastable medium. Molecular dynamics simulations provide an atomistic picture of solidification, but the modelling of the initial nucleation is hampered by the extended timescale of the process. In this work we employ an advanced computational method, transition path sampling (TPS), to enable the investigation of nucleation in elemental nickel on the atomistic level. We initially focus on homogeneous nucleation. Here, a comparison of the temperature dependence of the free energy barriers to the predictions of classical nucleation theory is discussed. As a second step, we extend our study by including small Ni-clusters as seeds during heterogeneous nucleation. The analysis of the transition path ensemble (TPE) obtained from our simulations indicates the presence of fcc and hcp crystalline structures and nonspherical shapes of the clusters. Furthermore, critical nuclei sizes, free energy barriers and rates, as well as optimal candidates for reaction coordinates based on local structural parameters are identified in the TPE. These results provide fundamental understanding of the nucleation mechanisms and can help to validate and improve existing thermodynamic models describing nucleation in metals.

MM 50.2 Thu 10:30 H53

Derivation of TTT diagrams with kinetic Monte-Carlo simulations — •Ankit Gupta, Biswanath Dutta, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany

Al-based light-weight alloys are promising for structural applications. A critical strengthening mechanism in these alloys is precipitate formation and thus the inherent evolution of the precipitates over time plays a key role in governing the mechanical behaviour of these alloys. Therefore, in order to fine tune the mechanical properties, an in-depth understanding of the precipitation kinetics is crucial. In this work, we study the precipitation kinetics in a model Al-Sc system employing kinetic Monte-Carlo (kMC) simulations. A linear bond-cutting model has been used to describe the underlying energetics. The kinetics has been analysed in terms of size distribution of the precipitates and their temporal evolution. The final results have been plotted as time-temperature-transformation (TTT) diagrams. The critical factors controlling the key features of the fully atomistically derived TTT diagrams such as asymptotic and nose temperature are discussed. Since the key observations are independent of the specific material system, they can be applied to tailor the precipitation kinetics in many applications.

MM 50.3 Thu 10:45 H53

On the Propagation of two en passent cracks upon mutual interaction: A phase field study — •Michael Fleck, Markus Thäter, Martin Lautenschläger, and Heike Emmerich — Materials and Process Simulation, University of Bayreuth, Germany

A phase field model for the simulation of crack propagation in brittle materials is applied to the problem of two mutually interacting "en passent" cracks. Thereby, crack growth is described as a first order phase transformation process, where the solid parent phase transforms into an infinitely weak "broken" phase, driven by elastic energy dissipation. We discuss the problem of "en passent" cracks in a two dimensional plain strain geometry, subjected to a constant uniaxial pulling velocity of mode I type. Our model reproduces a number of basic features that are also observed in corresponding experimental setupsInitially, when the two cracks propagate independently, they approach each other along straight paths. Then, during the early stage of the mutual interaction and for certain geometrical circumstances the principle of local symmetry may even force the cracks to turn slightly away from each other. When the line connecting the two crack tips alines with the pulling direction, the two cracks curve towards each other upon mutual tip-tip interaction until each crack tip reaches the other's crack tail, finally releasing a lenticular fragment. Here, we investigate the crack propagation dynamics as well as the chosen crack paths as a function of all relevant physical dependences, with the aim to elucidate the governing mechanisms that allow to classify the observed kinetics.

MM 50.4 Thu 11:00 H53

Laser Ablation of Alloys and Layered Materials — •Johannes Roth[1], Dennis Rapp[2], Alexander Kiselev[1], and Hans-Rainer Trebin[1] — [1]FMQ, Universität Stuttgart — [2]IWMF, Universität Stuttgart

We have studied laser ablation of Al-Ni alloys and layers using MD simulations combined with a two-temperature model (TTM) to describe the influence of the electrons. First the simulation program had to be adapted to alloys and the parameters for the electronic contribution had to be determined. After tests with pure Al and Ni melting depths and ablation thresholds for AlNi, $AlNi_3$ and Al_3Ni have been determined. For $AlNi_3$ we observe a change in ablation mechanism at high fluences and for the orthorhombic Al_3Ni a phase transition to a cubic $L1_2$ phase. Unfortunately there are nearly no experimental data avaialable to compare with.

Al layers on Ni substrates have also been studied. A thin layer of Al melts first, the Ni substrate follows, then the Al is ablated completely. A thicker Al layer absorbs a lot of laser energy and delays the melting of the Ni substrate to considerably higher fluences. At fluences low above the ablation threshold the thick Al layer is ablated as a whole as before, but at higher fluence the ablation depth is reduced due to vaporization of Al which cools the sample. The diffusion assisted formation of AlNi alloys has been observed in the thin layer case for fluences close to the ablation threshold. The structure of the compounds is fcc as in AlNi, but the composition varies from pure molten Al to solid Ni.

MM 50.5 Thu 11:15 H53

Impurity diffusion in bcc-iron from first-principles — •Casper Versteylen[1] and Marcel Sluiter[2] — [1]Mekelweg 2, 2628 CD Delft, the Netherlands — [2]Mekelweg 15, 2629 JB Delft, the Netherlands

Since detailed knowledge of impurity diffusivities is vital in the design of new steel compositions and microstructures, substitutional diffusion in bcc-iron has been studied comprehensively. Calculating diffusivities at temperatures relevant for realistic applications is difficult for several reasons; accurate excess entropies must be determined for vacancy formation and element specific vacancy binding while accounting for magnetic disordering. Sophisticated techniques have been developed to evaluate the influence of magnetism on total energies, but to do so for a large number of impurity elements in iron is expensive. Therefore a method was developed that links first principles results to the semi-empirical Girifalco model. A general method to evaluate the influence of magnetic disordering on impurity diffusivities has been applied to 28 impurity elements in bcc-iron and to iron self-diffusion.

15 min. coffee break