MM 23: Topical Session Heterogeneous Nucleation and Initial Evolution of Microstructure - Poster

Time: Tuesday 14:45–16:30 Location: P4

MM 23.1 Tue 14:45 P4

Scale-bridging phase-field simulations of microstructure responses on nucleation in metals and colloids — •Denis Danilov and Britta Nestler — Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Germany

Phase-field simulations from atomic to mesoscopic length scales are used to analyse the microstructure responses on heterogeneous nucleation, both in metallic as well as in colloidal systems. The scale-bridging from 1 nm to 10 μm in metals is achieved either by combining Molecular Dynamics (MD) and Phase-field (PF) simulations or by hybrid PF modelling. Essential for three dimensional numerical computations is the employment of performance optimized simulation techniques and adaptive multigrid methods. The microstructure responses on the parameter sets, on the shape of the nuclei and on the characteristic properties of the substrate are systematically investigated in PF simulations. Large-scale simulations of microstructure formations are compared with experimental observations.

MM 23.2 Tue 14:45 P4

Colloidal model system for undercooled metals — •Ina Klassen[1], Patrick Wette[1], Dirk Holland-Moritz[1], Thomas Palberg[2], Stephan V. Roth[3], and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, — [2]Institut für Physik, Johannes-Gutenberg-Universität Mainz, — [3]HASYLAB, DESY, 22603 Hamburg, Germany

Model systems are often used to describe equilibrium properties of simple fluids and solid materials. Charged colloidal spheres in aqueous dispersion show a rich phase behavior and many phenomena known from metals are also observed here, like selection of the metastable phase at large undercoolings. By contrast to metals heterogeneous nucleation can either be efficiently suppressed or, if present, clearly discriminated and separated from data evaluation. Our colloidal particles are characterized by convenient time scales (seconds) and particle distances (300-500nm) and thus accessible by optical techniques. Microscopy and light scattering yield complementary information on equilibrium properties and crystallization kinetics from real and reciprocal space (phase behavior, solidification mechanisms, growth velocities, nucleation rate densities). Structural changes of the melt with increased undercooling and the corresponding changes of the solidification can be monitored by Ultra Small Angle X-Ray Scattering (USAXS) performed at HASYLAB (Hamburg).

MM 23.3 Tue 14:45 P4

Heterogeneous nucleation in charged colloidal model systems using spherical seeds: Controlling the crystallization kinetics — •Andreas Engelbrecht, Roushdey Salh, Thomas Palberg, and Hans Joachim Schöpe — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudinger Weg 7, 55099 Mainz, Deutschland

In the classical crystallization scenario three processes can be discriminated: crystal nucleation, growth and ripening. The crystallization kinetics and the resulting morphology of the polycrystalline material are given by a complex interplay of these mechanisms. Controlling nucleation and growth is one key to create new materials. A great deal of progress has been made in recent years using colloidal suspensions as model systems studying crystallization. Close analogies to atomic systems are observed which can be exploited to address questions not accessible in atomic solidification. We here present systematic measurements controlling the crystallization kinetics of a charged colloidal model system by adding small amounts of a second higher charged component. Using small amounts of the second component the nucleation rate is strongly accelerated whereas crystal growth is only slightly influenced. At large amounts the crystallization process is overshadowed by fractionation of the supersaturated fluid: nucleation is delayed and crystal growth slowed down. The average crystal size of the resulting polycrystalline material can be changed by a at least one order of magnitude. The crystal size distribution is strongly influenced in its shape as well.

MM 23.4 Tue 14:45 P4

Surface Tension of Liquid Al-Cu Alloys — •Julianna Schmitz, Jürgen Brillo, and Ivan Egry — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany

Precise surface tension data of liquid Al-Cu alloys are fundamental for our purpose of studying the interaction of the liquid with differently oriented single crystalline sapphire surfaces. These data were measured for the entire Al-Cu liquid alloy system as a function of temperature and composition. Contamination of the sample from contact with container walls had to be avoided. Thus, measurements were performed in an inert gas atmosphere using an electromagnetic levitation furnace. From surface oscillations of the levitated droplet the surface tension was determined by means of the oscillating drop method. Hence, we obtained precise data of the entire Al-Cu system within a wide temperature range with only a small scatter of 3%. A linear temperature dependence with a negative slope was found for all stoichiometric compositions whereas the surface tension monotonically decreases with increasing aluminium concentration. The observed behaviour with respect to both, temperature and concentration, is in agreement with thermodynamic model calculations using the regular solution approximation. Additionally, we give an outlook on the measurement of contact angles and the work of adhesion as a function of the crystalline substrate orientation performed with a sessile drop apparatus whose construction is about to be finished. Combining this with the surface tension data we are able to estimate solid-liquid interfacial energies.

MM 23.5 Tue 14:45 P4

Heterogeneous nucleation undercooling and kinetics analysis — •Charuayporn Santhaweesuk[1], John H. Perepezko[1], Joachim Bokeloh[2], and Gerhard Wilde[2] — [1]University of Wisconsin-Madison, Department of Materials Science and Engineering, Madison, USA — [2]University of Münster, Institute of Materials Physics, 48149 Münster, Germany

For large liquid volumes it is essential to remove or to deactivate heterogeneous nucleation sites in order to achieve large undercooling values. An effective method of melt conditioning for nucleant removal is based upon flux treatments, but the mechanism that is responsible for the large undercooling is not properly understood. Recent experiments and analyses of the undercooling behavior in flux treated pure Cu have provided new results as well as confirmation for a model of nucleant refining that accounts for the undercooling behavior including initial conditioning, atmosphere effects and saturation in a self-consistent manner. Moreover, the statistical analysis of the undercooling data that has been developed during the initial work on pure Au can yield nucleation rates that are independent of the choice of a specific nucleation kinetics model. These results are also discussed in comparison with a description based on classical nucleation theory.

MM 23.6 Tue 14:45 P4

Binary Mixtures of Charged Colloidal Suspensions and their Role as Model Systems — •Nina J. Lorenz[1], Patrick Wette[2], Thomas Palberg[1], Hans Joachim Schoepe[1], and Tsuneo Okubo[3] — [1]Institute of Physics, University Mainz, Germany — [2]Institute for Raumsimulation DLR Cologne, Germany — [3]Cooperative Research Centre, Yamagata University, Yonezawa, Japan,

We investigate colloidal charged sphere mixtures in aqueous dispersion, exploring their possible use as conveniently accessible models for metallic binary mixtures. Using static and dynamic light scattering, torsional resonance spectroscopy and optical microscopy we investigate the structure, elasticity and solidification kinetics of mixtures with different size- and charge ratio. We find a rich variety of binary phase diagrams similar to those in metal systems including spindle, azeotropic and eutectic types [1, 2]. Eutectic-like behaviour is found for large asymmetries in the mixtures and demixing confirmed by diffusion experiments. The independent solidification of the segregating components is monitored with time resolved elasticity measurements. In addition we find interesting morphologies not unlike those in metal eutectics, but still considerably altered due to the different system dynamics. [1] T. Palberg, N. Lorenz, H.J. Schoepe, P. Wette, I. Klassen, D. Holland-Moritz, D.M. Herlach, in D. Herlach et. al.: Solidification in multicomponent melts, VCH-Wiley Weinheim, 2008, pp. 185-212, Solidification experiments in single component and binary colloidal melts [2] N. Lorenz, J.Liu, T. Palberg: Phase behaviour of binary

mixtures of colloidal charged spheres, Colloids Surf. A 319, 109 (2008)

MM 23.7 Tue 14:45 P4

Numerical Simulation of Heterogeneous Nucleation and Microstructure Formation in Al-Ni Alloy System — •Ricardo Siquieri[1], Evelyn Doernberg[2], Heike Emmerich[1], and Rainer Schmid-Fetzer[2] — [1]Computational Materials Engineering, Center of Computational Engineering Science and Institute of Minerals Engineering, RWTH Aachen, Mauerstrasse 5, D-52064 Aachen, Germany — [2]Institut für Metallurgie, Robert-Koch-Straße 42, 38678 Clausthal-Zellerfeld, Germany

Many important technological materials including magnetic and superconducting alloys are produced through solidification in peritectic systems. Although this class of materials is very important for the industry, many aspects of its solidification process are still unclear. To help with gaining a comprehensive and reliable understanding of this process, we will present numerical investigation of peritectic solidification for the system Al-Ni alloy in this contribution. For this purpose, recent developments of phase-field field techniques will be combined with thermodynamic precision data aiming a systematic investigation of all stages of peritectic solidification: Heterogeneous nucleation, peritectic reaction, peritectic transformation, and direct growth of the peritectic phase. This model approach allows us to make conclusions based on its comparison with experimental measurements as well as employ it to obtain new relations between processing parameters and the resulting kinetics and dynamics of the phase-transformation process during all of the four stages above.

MM 23.8 Tue 14:45 P4

Elastic effects on heterogeneous nucleation and microstructure formation — •Robert Spatschek[1], Efim Brener[2], Michael Fleck[2], Clemens Gugenberger[2], Claas Hüter[2], Heiner Müller-Krumbhaar[2], Denis Pilipenko[2], and Alain Karma[3] — [1]ICAMS, Ruhr-Universität Bochum — [2]IFF-3, Forschungszentrum Jülich — [3]Northeastern University Boston

Elastic effects due to lattice strain modify the local equilibrium conditions at solid-solid interfaces compared to classical dendritic growth. We present results on the influence of dilatational and shear strain on the kinetics of these phase transitions and discuss its relevance for the selection properties.

The description of surface-diffusion controlled dynamics via the phase-field method is less trivial than it appears at first sight. Numerical simulations of a standard and a more sophisticated model from the literature as well as of two new models are performed to assess the relative merits of each approach.

On small scales, the overlap of interface profiles can lead to attractive and repulsive forces, which are important for the understanding of heterogeneous nucleation processes. They are related to lattice incompatibilities due to a misorientation or grain shifts, and provoke elastic deformations and the formation of dislocations. Using concepts from the classical density functional theory and amplitude equations we shed light on the forces between solid-melt interfaces on an analytical and numerical level.

MM 23.9 Tue 14:45 P4

Derivation of the phase field crystal model for colloidal solidification — •Sven van Teeffelen[1], Rainer Backofen[2], Axel Voigt[2], and Hartmut Löwen[1] — [1]Institute for Theoretical Physics II: Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf — [2]Institute of Scientific Computing, Technical University Dresden, D-01062 Dresden, Germany

The phase-field crystal model is by now widely used in order to predict crystal nucleation and growth. For colloidal solidification with completely overdamped individual particle motion, we show that the phase-field crystal dynamics can be derived from the microscopic Smoluchowski equation via dynamical density functional theory. The different underlying approximations are discussed. In particular, a variant of the phase-field crystal model is proposed which involves less approximations than the standard phase field crystal model. We finally test the validity of these phase-field crystal models against dynamical density functional theory. In particular, the velocities of a linear crystal front from the undercooled melt are compared as a function of the undercooling for a two-dimensional colloidal suspension of parallel dipoles. Good agreement is only obtained by a drastic scaling of the free energies in the phase field crystal model in order to match the bulk freezing transition point.

MM 23.10 Tue 14:45 P4

Computer simulation studies of heterogeneous nucleation in the hard spheres and colloid-polymer mixtures. — •Tatyana Zykova-Timan[1], Juergen Horbach[2], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz — [2]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

Using Monte Carlo simulations in $NP(z)T$ ensemble a growth of the crystalline germ on the planar walls is modeled. Both hard spheres and colloid-polymer mixtures were considered. The latter was represented by one-component colloid system described by an effective Asakura-Oosawa potential. The repulsive interactions between the wall and colloids were tuned such that no wetting layer was allowed. We show how to stabilize the solid nucleus on the wall and analyze its morphology.

MM 23.11 Tue 14:45 P4

Phase field modeling vs. molecular dynamics simulations: Crystal growth kinetics of Ni — •Roberto Rozas Cardenas[1], Denis Danilov[2], Britta Nestler[2], and Jürgen Horbach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln — [2]Institute of Computational Engineering (ICE), Karlsruhe University of Applied Sciences, Moltkestrasse 30, 76133 Karlsruhe

Growth of crystal seeds in the undercooled melt of pure Nickel is simulated by means of molecular dynamics simulations and phase-field modeling. In order to establish a direct comparison between the two methods the lower length-scale limit of the phase field modeling is extended up to the scale of typical molecular simulations, i.e. about 100 Å. The input variables of the phase field modeling such as interface tension and transport properties, and initial configurations, are obtained from molecular dynamics simulations. We present results for the growth velocities of crystal seeds of Ni at different undercoolings. The validity of the assumptions of the phase modeling at nanoscopic scale is discussed.