MM 60: Phase Transitions II

Time: Thursday 15:30–17:00 Location: H5

MM 60.1 Thu 15:30 H5

Colloidal model systems for undercooled metallic melts — •Ina Klassen[1], Patrick Wette[1], Dirk Holland-Moritz[1], Thomas Palberg[2], and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55128 Mainz, Germany

Due to their mesoscopic length scales, colloidal suspensions are ideal model systems to address fundamental issues in condensed matter physics such as liquid ordering, nucleation and crystallization. Colloidal particles are several orders of magnitude larger than atoms in metals and their relaxation behavior is very sluggish compared to atomic systems. Due to the possibility of tunable interaction, systematic investigations of the short-range order in a charged colloidal silica system far from equilibrium state are presented. Therefore, time-dependent structure factors in the undercooled state were measured applying Ultra Small Angle X-ray Scattering. The results of these investigations are compared to measurements on metallic systems represented by an undercooled Ni melt applying neutron scattering. The measured structure factors of both physically different systems are analyzed using the same evaluation method which reveals icosahedral short-range order in the melt phase of both systems, colloids and pure metals as well. In addition, due to the variation of the interaction potential from soft repulsive to hard-sphere like bahavior, icosahedral short-range order is replaced by a fcc structure near the solid-fluid phase boundary.

MM 60.2 Thu 15:45 H5

Crystallization in a model system of charged colloidal particles: How do larger particles influence the crystallization process and therefore the resulting microstructure? — •Andreas Engelbrecht and Hans Joachim Schöpe — Johannes Gutenberg-University, 55099 Mainz, Germany

Characteristics of a material often depend on the microstructure of the material (i.e. the grain size in metals,) therefore the control of the crystallization process allows access to new materials of desired properties. Colloidal suspensions of spherical particles are widely used as model system for molecular and atomic systems - especially for metals. Progress understanding the solidification process has been made in recent years studying colloidal suspensions.

The formation of crystals from the melt can be controlled either by the required activation energy or by the rate of particles attaching to the crystal liquid interface. Adding just small amounts (less than 1%) of a larger and higher charged spherical particles to colloidal suspension of charged spheres we observe a drastic variation of the crystallization process and for this reason the resulting microstructure of the solidified material is changing its appearance. Expressed in terms of the classical nucleation theory the observed enormous effect on crystal nucleation is not exclusively induced by a significant change of the nucleation barrier height, but by a modification of the kinetic prefactor. A variation in the transport mechanism of particles form the melt towards the crystals modifies the kinetic prefactor of the classical nucleation theory as well as the crystal growth.

MM 60.3 Thu 16:00 H5

Competition between heterogeneous and homogeneous nucleation near a flat wall — Andreas Engelbrecht, Roushdey Salh, and •Hans Joachim Schöpe — Johannes Gutenberg-University, 55099 Mainz, Germany

The physical and chemical properties of solidified crystalline materials depend in a crucial way from the conditions of crystal nucleation. In order to improve the conditions of production processes and even to develop novel materials with extraordinary properties a detailed knowledge of the nucleation process is most desired.

We studied the competition between heterogeneous and homogeneous nucleation in colloidal model systems of charged spheres close to the container walls as function of metastability.

Our results show some unexpected behaviour: Although the appearing polycrystal displays a high amount of wall crystal we find that the heterogeneous nucleation at the container walls is delayed in comparison to the homogeneous bulk nucleation and its rate density appears surprisingly slightly smaller demonstrating the complexity of the observed crystallization process.

MM 60.4 Thu 16:15 H5

Bulk liquid undercooling and nucleation in Nickel — •Joachim Bokeloh, Anna Moros, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

While classical nucleation theory is widely accepted textbook knowledge, it is somewhat lacking with regard to the atomistic details of the nucleation and growth mechanisms. Right now, there are many efforts in exploring these details with computational methods. However, only few experimental methods that can corroborate these results are available. The best known of these experimental methods are containerless processing in levitation melting and the investigation of fine droplet dispersions.

We present here data on the liquid undercooling behaviour of Ni obtained by repeated melting and crystallization in a DTA. This method allows to acquire a statistically meaningful data set under clean and reproducible conditions, while still allowing reasonable sample sizes, thus combining several advantages of the two methods mentioned above. Ni was chosen as a model system because it shows good levels of undercooling and because it is well suited for computer simulations due to its relatively low number of electrons.

MM 60.5 Thu 16:30 H5

Investigation of nucleation in undercooled metal melts — •Stefan Klein[1,2] and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — [2]Institut für Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Containerless processing is an effective tool for undercooling metallic melts far below their equilibrium melting temperatures. By using such levitation techniques the dominating heterogeneous nucleation on container walls is completely eliminated. Furthermore, if the experiments are performed under clean environmental conditions, heterogeneous nucleation on free surfaces is also greatly reduced. In this work both electromagnetic and electrostatic levitation techniques are used for a comparative investigation of nucleation in undercooled metallic metals. In case of electromagnetic levitation samples in a diameter of 7 mm are processed within high purity inert gas atmosphere while in case of electrostatic levitation samples in a diameter of 2 mm are processed in ultra high vacuum. With a modified model by Skripov a statistical analysis of the distribution function of the undercoolings measured in one experiment run consisting of at least 100 undercooling cycles is conducted which provides information about the physical nature of different nucleation mechanism depending on experiment conditions.

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MM 60.6 Thu 16:45 H5

Neural Network Potential-Energy Surfaces for Materials Simulations — Nongnuch Artrith, Tobias Morawietz, and •Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Artificial neural networks represent a very flexible class of mathematical functions, which is well suited for the construction of potential-energy surfaces by interpolating a set of reference energies obtained from accurate electronic structure calculations. Recently, the applicability of neural network potentials has been extended to high-dimensional energy surfaces of condensed systems. By incorporating long-range electrostatic interactions also multicomponent systems can be addressed. Using semiconductors, oxides and metals as benchmark systems we show that neural networks provide reliable potentials for a wide range of materials. Since analytic gradients are readily available to calculate the forces, neural network potentials can be used to carry out efficient molecular dynamics simulations.