MM 45: Phase Transitions III

Time: Thursday 15:15–16:30 Location: IFW B

MM 45.1 Thu 15:15 IFW B

Colloidal model systems for undercooled metallic melts — •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, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Physik, Johannes-Gutenberg-Universität Mainz, — [3]HASYLAB, DESY, 22603 Hamburg, Germany

The knowledge of short-range order and nucleation behavior in a liquid is of fundamental importance for understanding the crystallization process of metals. To get a valuable insight in this process on the atomic length scale, we chose the way of analyzing a colloidal model system of charged silica spheres in aqueous solution. Its interaction can be controlled in a precise way by varying sodium hydroxide concentration. This colloidal system is characterized by convenient time scales between seconds and minutes and particle distances up to 500nm and is thus accessible by simple, yet powerful optical techniques. In addition to this, USAXS technique was used to determine the short-range order and nucleation behavior far from equilibrium state. These results are compared particularly with regard to those of a metallic system and show similarities which verify the chosen colloidal system as a good model system for metals.

MM 45.2 Thu 15:30 IFW B

Crystal growth in metallic melts: A computer simulation study — •Roberto Rozas Cardenas and Jürgen Horbach — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

The crystal growth of Ni is studied using molecular dynamics computer simulation. The interactions between the particles are modeled by a potential of the embedded atom type. To this end, we consider the direct simulation of crystal growth through the movement of a planar solid-liquid interface at different temperatures. The kinetic growth coefficients and the melting temperature are estimated from an analysis of the interface growth velocity. The resulting melting temperature is at 1748 K, close to the experimental one at 1728 K. The crystal growth coefficient is about two orders of magnitude larger than in the intermetallic alloy $Al_{50}Ni_{50}$. We show that in the latter system crystal growth is driven by diffusion in the solid-liquid interface region, whereas for pure Ni phononic degrees of freedom lead to the much faster crystal growth kinetics.

MM 45.3 Thu 15:45 IFW B

Investigation of nucleation in undercooled melts of pure metals — •Stefan Klein[1,2] and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 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 7mm are processed within high purity inert gas atmosphere while in case of electrostatic levitation samples in a diameter of 2mm 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 45.4 Thu 16:00 IFW B

Undercooling and solidification of Ni_2B under different conditions of convection — •Sven Binder[1,2], Jianrong Gao[3], and Dieter M. Herlach[1] — [1]Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany — [2]Institut für Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Key Laboratory of Electromagnetic Processing of Materials, Northeastern University, Shenyang 110004, China

We investigate the kinetics of crystal growth by measurements of the dendrite growth velocity as a function of undercooling during non-equilibrium solidification. Measurements are conducted under different conditions of convection. The liquid samples are levitated and undercooled in strong alternating electromagnetic fields leading to forced convection. Inductive stirring is avoided by processing the samples in a liquid or glassy slag where only natural convection is present. Forced convection and natural convection can be reduced by performing undercooling experiments in reduced gravity. The experimental results obtained under different conditions are compared to each other in order to investigate the influence of convection on the growth dynamics of dendrites in undercooled melts. The congruently melting compound Ni_2B is chosen as sample system. It forms an intermetallic phase with growth velocities that are comparable to the fluid flow velocities in electromagnetically levitated melts. The results are analyzed within dendrite growth models and reveal that the growth velocity is essentially influenced by forced convection in strong electromagnetic fields. The present work is supported by DFG under contract HE1601/22.

MM 45.5 Thu 16:15 IFW B

Crystal growth in undercooled NiZr melt: Linking phase-field modeling to molecular dynamics simulations — •Mohammed Guerdane[1], Denis Danilov[1], Frank Wendler[1], Helmar Teichler[2], and Britta Nestler[1] — [1]Institute of Computational Engineering, Karlsruhe University of Applied Sciences, Germany — [2]Institute of Materials Physics, University of Göttingen, Germany

Propagation of a planar solidification and dissolution front in a two-phase crystal-melt structure under non-equilibrium conditions (supersaturated solution) is considered by molecular dynamics (MD) simulations and phase-field modeling (PFM). The MD simulations are carried out with interatomic potentials for the NiZr alloy and provide the thermophysical data required for setting up the PFM simulations. Results are presented showing a comparison of concentration profiles across the crystal-melt interface and of the growth velocity obtained from MD and PFM methods. By considering different approximations of the free energy density in the PFM, we analyze the contribution of the activity coefficient in the chemical potential and of the solute-solvent interdiffusion in the growth dynamics.