MM 30: Phase transitions III

Time: Thursday 10:15–11:15 Location: H4

MM 30.1 Thu 10:15 H4

nucleation kinetics analysis of pure liquid Gold * a model case? — •Gerhard Wilde[1] and John Perepezko[2] — [1]Institut für Materialphysik, Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany — [2]Department of Materials Science and Engineering, University of Wis-consin-Madison, 1509 University Avenue, Madison 53706, USA

Flux treatments with a molten glass slag are commonly used to promote deep liquid undercooling or even bulk glass formation. Although the technique has demonstrated frequently the capability to yield large under-cooling, the underlying mechanisms remain uncertain. There are sugges-tions of flux induced *nucleant removal* or *surface site deactivation* interactions, but the effectiveness and operation of these processes have not been identified clearly. As a model system, the undercooling response of pure Au encased in Pyrex glass was studied systematically to develop a consistent record of the undercooling behavior. Nucleation kinetics analy-ses of statistically significant sets of measurements performed under strictly controlled conditions reveal the presence of a new mechanism based on gas-solid interactions that trigger nucleation through a nucleant precipitation reaction as the first step of the interaction. A new model, based on thermodynamic considerations and on the nucleation kinetics data is proposed that accounts for the undercooling increase including initial conditioning, atmosphere effects and undercooling saturation in a self-consistent manner.

MM 30.2 Thu 10:30 H4

The effect of melt convection on the secondary dendritic arm spacing of Nd-Fe-B alloys — •Kaushik Biswas[1], Regina Hermann[1], Horst Wendrock[1], Gunter Gerbeth[2], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Forschungszentrum Rossendorf (FZR), Institute of Safety Research, P.O. Box 510119, 01314 Dresden, Germany

Dendritic microstructure is one of the major microstructural constituents of peritectic alloys. In the present work, the effect of melt convection on the secondary dendritic arm spacing (SDAS) and phase fraction of properitectic α-Fe was investigated during solidification of stoichiometric Nd-Fe-B alloys under forced crucible rotation technique. The resulting microstructure of the alloy in consideration of melt convection has been investigated using scanning electron microscopy and optical microscopy. The average SDAS was determined for each sample from the whole cross-section of the cylindrical test samples using image analysing software LEICA QWIN. A detailed statistical analysis of the spacing distribution was performed on the basis of the variation of SDAS values averaged from about 80 to 120 dendrites in different zones. The α-Fe volume fraction measured by vibrating sample magnetometer (VSM) reduces with increasing crucible rotation frequency. Similarly, the SDAS values decrease with increasing rotation frequency. These results are explained from the viewpoint of a reduced melt convection state under steady forced crucible rotation leading to a reduced effective mass transfer coefficient.

MM 30.3 Thu 10:45 H4

Molecular dynamics simulations for calibrating a phase-field model of solidification in Ni-Zr alloys — •Britta Nestler[1], Denis Danilov[1], Hamid Guerdane[2], and Helmar Teichler[2] — [1]Institute for Computational Engineering, Karlsruhe University of Applied Sciences, Karlsruhe, Germany — [2]Institut für Materialphysik, Universität Göttingen

Atomic-scale simulations of crystal-melt interfaces in Ni-Zr alloys are performed to determine the energy densities and material parameters for phase-field modelling of solidification microstructures. To set up the phase-field (PF) model, quantities such as the free energy density functions related to the liquidus and solidus lines of the phase diagram, the diffusion coefficients and the interface thickness are calculated from molecular dynamics (MD) simulation data. The kinetic coefficient is approximated by comparing interfacial positions of MD and PF simulations. Direct comparison of PF and MD simulations show a disagreement in the dynamics of the interface motion. To match PF and MD results the diffusion coefficients of the solid and liquid phases in the PF model have been calibrated using a two-sided analytical sharp interface solution. Results of simulated solid-liquid interfaces are presented showing a comparison of concentration profiles across the crystal-melt interface and of the growth dynamics obtained from MD and PF simulations.

MM 30.4 Thu 11:00 H4

Influence of Strain on Phase Transitions in Solids — •Robert Spatschek[1], Efim Brener[1], and Vladimir Marchenko[2] — [1]Institut für Festkörperforschung, Forschungszentrum 52425 Jülich — [2]P.L. Kapitza Institute for Physical Problems, RAS 119334, Kosygina 2, Moscow, Russia

Many magnetic, superconducting and structural phase transitions in solids are accompanied by small lattice distortions which lead to the presence of elastic deformations. In some cases, these effects are of minor influence and can be ignored, but nevertheless for many applications the elastic strain causes qualitatively new and observable effects.

We consider a sharp interface kinetic model of phase transitions accompanied by elastic strain, together with its phase-field realization. Quantitative results for the steady-state growth of a new phase in a strip geometry are obtained and different pattern formation processes in this system are investigated. We consider the case of a dilatational mismatch and a transition in hexagonal crystals involving shear strain as particular applications of this minimum model.