

MM 56: Phase Transformations II

Time: Thursday 11:45–13:00

Location: H26

MM 56.1 Thu 11:45 H26

Dendrite growth kinetics of undercooled Iron-based alloy melts — ●CHRISTIAN KARRASCH^{1,2}, THOMAS VOLKMANN¹, and DIETER M. HERLACH^{1,2} — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany — ²Institut für Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum, Germany

Dendritic growth is the major crystal growth mode controlling the evolution of the microstructure during solidification of metallic alloys. In order to verify models for dendritic growth in undercooled melts growth velocities were measured on pure Fe and Fe-based alloy melts. We analyse the effect of solute redistribution on the growth of Fe-B revealing a small partitioning coefficient. Electromagnetic levitation technique is applied to undercool droplets of metallic melt accessible for in-situ diagnostics of the solidification processes. Deep undercoolings of more than 200 K prior to solidification are achieved, which leads to rapid growth of dendrites with velocities of several m/s. The temperature-time profile is measured by a pyrometer while rapid solidification is monitored by a high-speed video camera. The contrast between the liquid and solid phase is visible due to the release of latent heat during recalescence. Experimental results will be presented and discussed in the frame of current model for dendritic growth in undercooled melts.

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MM 56.2 Thu 12:00 H26

Simulation of rapid crystallization in phase change materials by means of phase field modeling — ●FATEMEH TABATABAEI¹, MARKUS APEL², and EFIM BRENER¹ — ¹Peter Grünberg Institut (PGI-2), Forschungszentrum Jülich, 52428 Jülich — ²Access e.V., RWTH Aachen, 52072 Aachen

Phase change materials (PCM) are employed in data-storage applications extensively. A stable crystalline and a metastable amorphous state can be utilized for the data recording. To obtain a quantitative understanding of the kinetics of writing and erasing data, it is essential to gain insights into the energy transport and phase boundary movement during the phase transformation. We applied phase field modeling as a continuum simulation technique in order to study rapid crystallization processes in AgInSbTe. The simulation model is adapted to the experimental conditions, in particular the geometrical arrangement used for measurements of crystallization rates by a laser pulse technique. Simulations are performed for substrate temperatures close to the melting temperature of AgInSbTe down to low temperatures when an amorphous state is involved. Different growth regimes are identified by calculating crystallization velocity as a function of undercooling. We discussed the role of interface mobility on solidification kinetics by determining the mobility as a function of temperature. Furthermore, the role of nucleation of the crystalline phase as well as temperature dependent thermophysical properties are investigated.

MM 56.3 Thu 12:15 H26

Spinodal decomposition versus nucleation and growth mechanism of phase separation in nonstoichiometric silicon oxide films during high temperature annealing — ●ANDREY SARIKOV — V. Lashkarev Institute of Semiconductor Physics NAS Ukraine, 45 Nauki avenue, 03028 Kiev, Ukraine

This work is devoted to the study of the thermodynamic mechanisms of phase separation in the nonstoichiometric silicon oxide films during high temperature anneals. Based on the obtained earlier expression for the Gibbs free energy of nonstoichiometric silicon oxide phase,

the binodal and the spinodal characteristics of silicon oxide as well as the regions of stoichiometry indexes corresponding to the stability, metastability, and instability of silicon oxide phase with respect to the phase separation as the functions of temperature are determined. The regions of the phase separation process taking place according to the spinodal decomposition and according to the nucleation and growth mechanism are presented. Obtained results are useful for the development of the kinetic theory of phase separation in nonstoichiometric silicon oxide films and the formation of the structures consisting of Si nanoinclusions in the silicon oxide matrix.

MM 56.4 Thu 12:30 H26

Experimental examination of the MacPherson-Srolovitz prediction for grain growth kinetics — ●JULES DAKE¹, JETTE ODDERSHEDE², SØREN SCHMIDT², and CARL KRILL¹ — ¹Institute of Micro and Nanomaterials, Ulm University, Germany — ²Department of Physics, Technical University of Denmark, Denmark

The long-sought extension of the von Neumann relation to 3D — recently achieved by MacPherson and Srolovitz — constitutes a major advance in the field of materials modeling. If, however, this new relation is to serve as the basis for predicting microstructural evolution, then it must be tested against real three-dimensional coarsening data, which has proven stubbornly difficult to come by. Fortunately, the recently developed technique of three-dimensional x-ray diffraction microscopy (3DXRD) has made it possible to map the 3D microstructure of a polycrystalline sample nondestructively, delivering exactly the kind of experimental data required to test the MacPherson-Srolovitz relation. In a previous attempt, the authors successfully mapped and characterized a polycrystalline Al-1wt.% Mg specimen before and after heat treatment at 350°C. Regrettably, the annealing step (90 min) was too long, rendering an analysis of the local growth kinetics impossible. This time, we repeated the experimental procedure using intervals just 10 min in duration, and we extracted the local growth kinetics from a total of 9 time steps. The measured growth rates of individual grains are finally compared to predictions of the MacPherson-Srolovitz relation.

MM 56.5 Thu 12:45 H26

Impact of the inclination dependence of grain boundary energy on faceting and kinetics of grain boundaries in Aluminum — ●JANN-ERIK BRANDENBURG, DMITRI A. MOLODOV, and LUIS A. BARRALES-MORA — Institute of Physical Metallurgy and Metal Physics, RWTH-Aachen University

The motion and faceting behaviour of <100> tilt and mixed tilt-twist grain boundaries with misorientations in the range between 4° and 23° were investigated in situ in a scanning electron microscope at elevated temperatures. The results revealed that tilt boundaries with misorientations lower than 15° did not assume a curved shape and did not move under a capillary driving force at any temperature. In contrast, all investigated low angle boundaries with mixed tilt-twist geometry (20° twist component) were observed to attain a smoothly curved shape and moved under a curvature force. Molecular static simulations provided evidence that the experimentally observed behaviour is due to the inclination dependence of grain boundary energy, which is very pronounced for pure tilt (low angle) boundaries but becomes nearly isotropic for mixed boundaries with the same rotation angle. The influence of the energy anisotropy on grain boundary migration during grain growth was investigated by molecular dynamic simulations of shrinking initially circular grains encircled by tilt and mixed boundaries. The results showed an influence of the inclination dependent energy on the shape of the grains during shrinking as well as on the shrinking rate itself.