MM 35 Growth

Time: Thursday 14:45–16:30 Room: IFW B

MM 35.1 Thu 14:45 IFW B

Investigation of the initial transient in directional solidification of a binary AlCu alloy — •Anne Drevermann, Nils Warnken, Laszlo Sturz, and Gerhard Zimmermann — ACCESS e.V., Intzestr. 5, 52072 Aachen

For the formation of microstructures the initial transient, i.e. the very beginning of solidification, is of major relevance. At this stage a complex interaction between the velocity of the solidification front, the concentration pile-up and the temperature gradient takes place. In this work these three main variables and their coupling are investigated in experiments and numerical simulations.

Directional solidification experiments are carried out thermosolutally stable in a Bridgman-Stockbarger furnace with cylindrical Al-1.3wt.%Cu samples. During solidification the solidification velocity and the temperature profile are measured insitu while the concentration profile is determined afterwards in the processed sample by SEM/EDX analysis.

Numerical simulations were performed according to the Coriell model and with the phase field method. The Coriell simulations consider thermal diffusion in the liquid and the solid and solutal diffusion in the liquid while the phase field simulations consider only solute diffusion. The calculated transient solidification velocities and concentration profiles are in good agreement with the experimental results.

MM 35.2 Thu 15:00 IFW B

Crystal growth in undercooled Ti-Al-Nb melts — •Dirk Holland-Moritz and Thomas Volkmann — DLR, Institut für Raumsimulation, D-51147 Köln, Germany

Investigations on the solidification behaviour of undercooled Ti-Al-Nb melts are presented. The liquids are undercooled by application of the electromagnetic levitation technique. Maximum levels of undercooling of up to 320 K are achieved. Crystal growth during solidification of the undercooled melts is observed using a high-speed video camera at frame rates of 30000 frames per second. At small undercoolings an irregular shape of the solidification front is found. At larger levels of undercooling the growth front is smooth, but exhibits a pronounced anisotropy. From the recorded video sequences the growth velocities are determined as a function of the undercooling.

This work was financially supported by the IMPRESS Integrated Project (Contract NMP3-CT-2004-500656) that is co-funded by the European Commission in the 6th Framework Programme, the European Space Agency and the Swiss Government.

MM 35.3 Thu 15:15 IFW B

Molecular dynamics simulation of the nucleation and growth of platinum clusters — •Norbert Lümmen and Thomas Kraska — Physical Chemistry, University Cologne, Luxemburger Str. 116, D-50939 Köln, Germany

The formation of platinum clusters in an inert gas aggregation source is investigated by molecular dynamics simulation. At the beginning of the simulation the platinum atoms are in a highly supersaturated vapour state embedded in the carrier gas argon acting as a heat bath. The interactions of the metal atoms are modelled by the commonly used embedded atom method. Once the simulations are started the metastable phase remains for some time until clusters are formed by homogenous nucleation.

The nucleation rates are calculated from the cluster size statistics. Using a correlation of the nucleation rates as function of the supersaturation and the nucleation theorems the critical cluster size as well as the excess energy of the critical clusters are estimated. Also the continuation of the growth process by coalescence is traced in the simulations. In this context it is shown that coalescence can be the cause for a structural transition of a cluster. Even, or rather especially small clusters, which are often at high temperature, can be responsible for such transition.

Further results on the extension of the methodology on the investigation of nano alloy formation of will be reported. This will include the simulation of the formation process itself and the structural analysis of the resulting clusters.

MM 35.4 Thu 15:30 IFW B

Grain growth of two-dimensional grain structures with surfaces: a vertex dynamics approach — •Daniel Weygand — IZBS, Kaiserstr. 12, University of Karlsruhe, 76133 Karlsruhe

The time evolution of a two dimensional grain structure in presence of surfaces, e.g. a fibre geometry, is investigated. The influence of surface grooving and inhomogeneous heat treatments on the final microstructure is modelled using an enhanced vertex dynamics simulation. It is shown that, starting from a populations obtained by normal grain growth, the microstructure evolves toward a bamboo structure with interesting properties, e.g. depending on grooving parameter, grains with an non-uniaxial shape factor in the range of 1 to 7 occur. The grain size distribution is broader and larger grains are able to keep their size advantage due to the presence of the surfaces.

MM 35.5 Thu 15:45 IFW B

Dendritic Solidification of undercooled Ni-based alloy melts — •Sven Reutzel[1,2], Peter K. Galenko[2], and Dieter M. Herlach[2] — [1]Ruhr-University, Institute of Experimental Physics IV, 44780 Bochum — [2]German Aerospace Center (DLR), Institute of Space Simulation, 51170 Cologne

Morphology and size of dendritic microstructures sensitively depend on the solidification conditions, in particular on the crystallisation dynamics of the melt. Depending on the velocity with which a dendrite propagates into the undercooled melt a great spectrum of non-equilibrium phenomena can occur. For instance, if the velocity comes of comparable order with the atomic diffusive speed (1 - 10 m/s) solute trapping leads to the formation of supersaturated solutions and disorder trapping in intermetallic alloys produces disordered superlattice structures with completely different mechanical properties as the ordered counterparts. Also, as investigated in the present work grain refined alloys are solidified from the undercooled melt.

For a quantitative description of non-equilibrium solidification processes the growth velocity of the propagating dendrites in undercooled Ni and selected Ni-based alloy melts is experimentally determined as a function of undercooling on electromagnetically levitated drops. High accuracy measurements are realised even at small growth/undercooling values by applying a high speed camera technique, which allows for direct observation of morphology and dynamics of the solidification front. The analysis will be important to investigate and understand the development of various microstructures in as solidified materials.

MM 35.6 Thu 16:00 IFW B

Suppression of eutectic precipitation in rapid solidification of a binary system — •Peter Galenko and Dieter Herlach — Intitut für Raumsimulation, DLR, 51170 Köln, Germany

Experimental results on rapid solidification for binary systems in a range of eutectic concentration are analysed. Conditions at which eutectic precipitation is suppressed are found. A model for rapid crystal growth in a binary system of eutectic composition is developed. Analytical solutions of the model allow to predict beginning solidification of supersaturated solid solution without eutectic precipitation. It occurs at a solidification velocity equal to solute diffusion speed in bulk liquid. Within this point, a solute diffusion-limited growth is finishing with an onset of diffusionless solidification of the supersaturated solid solution. In such a case, complete solute trapping proceeds and eutectic solidification does not occur. The work was supported by DFG under contract No. He 1601/13.

MM 35.7 Thu 16:15 IFW B

Three dimensional normal grain growth: mean-field theory and Monte Carlo Potts model simulation — •Dana Zöllner and Peter Streitenberger — Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Abteilung Materialphysik, PF 4120, D-39016 Magdeburg

Normal grain growth in three dimensions has been studied on the basis of large-scale 3D Monte Carlo Potts model simulations, which enabled an extensive statistical analysis of the growth kinetics and topological properties of the microstructure within the quasi-stationary self-similar coarsening regime. It is shown that three dimensional normal grain growth can adequately be described by an average scaled growth law, which is

a quadratic function of the relative grain size. A generalized analytic mean-field theory based on this growth law yields a scaled grain size distribution function that is in excellent agreement with the simulation results. The problem of the existence of a sharp cut-off in the simulated microstructure is discussed.