MM 27: Phase Transformations II

Time: Wednesday 14:30–15:45 Location: IFW D

MM 27.1 Wed 14:30 IFW D

In-situ characterization of embedded metallic nano-clusters with a positron beam. — •Philip Pikart[1,2] and Christoph Hugenschmidt[1,2] — [1]ZWE FRM-II, Garching, Germany — [2]Technische Universität München, Physikdepartment E21, Garching, Germany

Positron measurements on model systems of aluminum with thin embedded layers (0.5nm to 100nm) of different materials (Au, Cr and Cu) are reported. It is shown how the positron affinity of different metals affects the measurements sensitivity. It is demonstrated that temperature dependent Doppler broadening on gold clusters embedded in aluminum reveals clustering and re-organization processes.

When a positron is implanted into a sample, it thermalizes rapidly (within ps) and starts to diffuse over up to several hundred lattice constants. During the diffusion it can be trapped at irregularities in the crystal matrix. Hence it acts as a "nanoprobe" with a highly increased sensitivity e.g. for vacancy-like defects and metallic agglomerations. The non-destructiveness of this method enables in-situ observation of agglomeration growth at different temperatures. The usage of a mononergetic positron beam assures the positron implantation into the bulk where surface effects do not influence the measurement.

MM 27.2 Wed 14:45 IFW D

Morphological study of a peritectic Al-Ni alloy by a quantitative phase-field simulation — •Julia Kundin and Heike Emmerich — 1Material and Process Simulation (MPS), University Bayreuth, Germany, Nürnberger str.38(4) 95448 Bayreuth

A phase field model of simulating peritectic and eutectic growth is described, which is applied to the investigation of the peritectic microstructure in an Al-Ni alloy during directional solidification. The presented model is an extension of the multiphase-field approach [I. Steinbach, Physica D 94 (1996), R. Folch and M. Plapp, Phys. Rev. E 72, 011602 (2005)] to study the solidification of multiphase systems based on the real free energy functions. It is shown, that the model is a reliable and powerful numerical approach to simulate the solidification of alloys involving more than one solid phase at nonisothermal conditions. The model is verified on an example of the Al-Ni system for which the morphology of the peritectic structure during the process of the directional solidification is investigated. The proposed model is also extended to multi-component systems.

MM 27.3 Wed 15:00 IFW D

Phase-field simulation of dendritic growth in the system Al-Si — •Sebastian Schulz, Abhik Choudhury, and Britta Nestler — Institute of Materials and Processes, Karlsruhe, Germany

The strength of the phase-field method to simulate material alloy systems has been demonstrated over the years. The method however, requires the knowledge of the Gibbs-free energy of the phases involved in the transition which can be derived via the Calphad method. In the present study, we build the methodology for the direct use of thermodynamic databases in the simulation of material alloys, using the phase-field method. Using this set-up, we investigate the effect of small additions of a third component on dendritic growth in the cast Al-Si system. In particular, we study the effect of these additions on the dendritic arm spacing, in a directional solidification setup and attempt to derive relationships between the amount of additions of the third component and the physical parameters like interfacial surface tensions, through systematic parameter studies and comparison with experiments.

MM 27.4 Wed 15:15 IFW D

Recrystallization of a deformed 3D microstructure studied by macro-micro simulations — •Alexander Vondrous[1], Michael Selzer[1], Britta Nestler[1], Pierre Bienger[2], and Simone Schendel[3] — [1]Institute of Materials and Processes, University of Applied Sciences, Karlsruhe, Germany — [2]Fraunhofer Institut for Machanics, Freiburg, Germany — [3]Institute for Reliability of Components and Systems KIT, Karlsruhe, Germany

Cold rolling of sheet metal introduces a high amount of dislocations, which lead to significant changes of the material properties. During annealing, to obtain the initial properties, dislocations are reduced by nucleation and growth of the nuclei driven by the stored energy (recrystallization). A dislocation density triggered nucleation of recrystallizing grains is introduced to simulate stored energy driven nuclei growth of cold rolled sheet metal for static recrystallization. The phase-field model incorporating additional equations for the stored energy driving force is introduced. Growth kinematics depend on the crystallographic orientations and the stored energy distribution. The starting point of the microstructure simulation is a macroscopic finite element simulation containing the corresponding deformation texture and accumulated plastic slip. A comparison with experimental measurements is achieved by evaluating the pole figures of the polycrystalline material at different stages of the process. The comparison serves as a validation of the micro-macro approach.

MM 27.5 Wed 15:30 IFW D

On the Growth Behaviour of Individual Grains in Polycrystals — •Dana Zöllner[1], Peter Streitenberger[1], and Iain Fielden[2] — [1]Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield, UK

A 3D grain growth model is developed allowing the prediction of the growth history of individual grains. The model - based on a generalised mean-field approach - represents data of 3D grain growth - simulated by a Monte Carlo Potts model algorithm - very well. The parameters from the obtained grain size distribution are then used to calculate an analytic function describing the individual growth history of all grains. A comparison with simulation results of normal grain growth shows good agreements for the temporal development of grain sizes of single grains as well as for the prediction of their life span.

On the other hand, the monitoring of the motion of individual quadruple points and triple junctions in 2D sections of the simulated 3D microstructures shows a highly discontinuous movement. Based on a stochastic grain growth model the diffusivity of the Brownian-like motion can be related to the average growth rate providing a possibility to determine the average growth law of the grain ensemble solely from the stochastic growth behaviour of single grain features.

In addition, the simulation results - compared with real-time in-situ SEM observations of grain growth - show a good qualitative agreement of the temporal movement of grain boundary junctions.