MM 21: Microstructure and Phase Transformations II

Time: Tuesday 10:15–11:45 Location: H 0106

MM 21.1 Tue 10:15 H 0106

A phase-field simulation of directional solidification in ternary Al-Cu-Ni alloys — •Julia Kundin[1], Henning Hörstermann[1], Rainer Schmid-Fetzer[2], and Heike Emmerich[1] — [1]Material- und Prozesssimulation, Universität Bayreuth, 95448 Bayreuth, Germany — [2]TU Clausthal, Institute for Metallurgy, 38678 Clausthal-Zellerfeld, Germany

A precise calculation of the directional solidification based on a reliable thermodynamic description is carried out in a ternary Al-Ci-Ni alloy. A comprehensive understanding of the interplay between the phases in the three-phase peritectic reaction and in the four-phase transition reaction, and their influence on the nucleation kinetics and the resulting microstructure evolution is of great interest. A three-phase peritectic reaction in a ternary system is no longer invariant but a univariant reaction, which means, the equilibrium compositions of all phases vary with the temperature. For a four-phase reaction $L + \alpha \rightarrow \beta + \gamma$, there are two product phases, which have an effect on the nucleation. If the product phase β first precipitates via heterogeneous nucleation on the primary phase α, these precipitates of β may be also a potent nucleant for the other product phase γ. The microstructure formation of a ternary Al-Cu-Ni alloy during the directional solidification with a three-phase peritectic reaction and a four-phase transition reaction is simulated by a quantitative multi-phase multi-component phase-field model. The refined thermodynamic description of the system as well as other input data for the phase-field model are discussed.

MM 21.2 Tue 10:30 H 0106

Comparative investigation of phase-field models based on free energy and grand potential formulations — •Oleg Tschukin[1], Abhik Choudhury[2], and Britta Nestler[1,2] — [1]IMP - Hochschule Karlsruhe Technik und Wirtschaft — [2]IAM - Zuverlässigkeit von Bauteilen und Systemen, Karlsruher Institut für Technologie

We present a comparison between a phase-field model for multi-component solidification based on a grand potential functional constructed out of the thermodynamic chemical potential μ: $f\left(c\left(\mu,T\right),T\right)-\mu c\left(\mu,T\right)$[1] and the free energy functional of the average concentration [2]. Contrary to formally used free energy functionals, when the evolution equations are derived from the grand potential formulation, there exist certain advantages: length scales of simulations can be upscaled and surface as well as kinetic properties can be easily calibrated. We perform a quantitative evaluation of both methodologies by applying them to common problems of multi-phase solidification (eutectic and peritectic solidification). While both methods can be used to derive the same physics, we point out the efficiencies and advantages of the grand potential formalism.

[1] A. Choudhury *et al.*: Grand potential formalism for multi-component phase transformations along with thin-interface asymptotics of the double obstacle potential, submitted to Physical Review E (2011)

[2] H.Garcke *et al.*: A diffuse interface model for alloys with multiple components and phases, SIAM J Appl. Math. 64 775-799 (2004)

MM 21.3 Tue 10:45 H 0106

A phase-field study of morphology effects in heterogeneous nucleation — •Henning Hörstermann, Julia Kundin, and Heike Emmerich — Material- und Prozesssimulation, Universität Bayreuth, 95448 Bayreuth, Germany

The effect of the morphology of the primary phase on heterogeneous nucleation in peritectic materials is studied using a quantitative phase-field method on an example of an Al-Ni peritectic alloy based on the refined thermodynamic data related to the Gibbs energies of the phases. The nucleation energy barrier of the peritectic Al_3Ni_2 phase is estimated by determining the critical nucleus radius in three dimensions for different shapes and curvatures of the primary Al_3Ni seed. The undercooling of the peritectic reaction used in the simulations was taken from DSC experiments. The nucleation energy and the contact functions calculated from the phase-field simulations are compared to predictions from classical nucleation theory.

MM 21.4 Tue 11:00 H 0106

Abnormal grain growth of Goss grains in grain-oriented electrical steel — •Wei Guo[1] and Wei-min Mao[2] — [1]Department of Microstructure Physics and Alloy Design,Max-Planck Institute for Iron Research GmbH, Duesseldorf, Germany — [2]2, School of Materials, University of Science and Technology, Beijing, Beijing, China

Strong Goss texture {110}<001> in grain-oriented electrical steels forms by abnormal grain growth during high temperature recrystallization annealing. However, the cause of this abnormal growth has been disputed for more than 70 years. The various explanations include high fraction of high angle boundaries, high mobility of coincidence site lattice boundaries, size effects and so on. However, none of these explanations address the internal environment of Goss oriented grains. Here we use electron back scattering diffraction techniques and field emission microscopy to show that some Goss oriented grains in matrix have higher secondary particle densities than their neighbors during final annealing at 875 degree C before secondary recrystallization. Since regions with higher second phase particle density offer a high resistance to grain boundary migration, Goss oriented grains ought to grow more readily towards regions with lower secondary particle density. Therefore, we conclude that second phase particle densities must play a vital role in the growth of Goss oriented grains. This findings may shed light on optimizing Goss texture and improve magnetic properties of grain oriented electrical steels.

MM 21.5 Tue 11:15 H 0106

Investigation of Grain Growth in $SrTiO_3$ by diffraction contrast tomography and modelling — •Daniel Weygand[1], Melanie Syha[1], Wolfgang Rheinheimer[1], Wolfgang Ludwig[2], Erich Lauridsen[3], and Peter Gumbsch[1,4] — [1]KIT, IAM, Karlsruhe, Germany — [2]ESRF, Grenoble, France — [3]Risoe National Lab., Roskilde, Denmark — [4]IWM, Freiburg, Germany

The grain growth dynamics of bulk $SrTiO_3$ samples have revealed a puzzling growth behaviour, the sudden decrease of the growth rate with increasing temperature [1]. Metallographic analysis of two-dimensional sections through the bulk samples has not revealed any specific quantities, related to this growth acceleration.

Therefore diffraction contrast tomography measurements and subsequent reconstructions of the three dimensional grain structures in $SrTiO_3$ and three dimensional grain growth modelling have been employed to characterize the grain structure. Samples have been analysed at different states of the heat-treatment. This allows determining the growth dynamics of specific grains, knowing the geometry and crystallographic orientations of the surrounding grains.

[1] Bäurer, M., Weygand, D., Gumbsch, P. and Hoffmann, M.J.: Grain growth anomaly in strontium titanate, Scripta Mat. 61 (2009),584.

[2] M. Syha, W. Rheinheimer, M. Bäurer, E.M. Lauridsen, W. Ludwig, D. Weygand, P. Gumbsch, Three-dimensional grain structure of sintered strontium titanate from X-ray diffraction contrast tomography, Script Mat. 66 (2012) 1.

MM 21.6 Tue 11:30 H 0106

Measuring dihedral angles in polycrystalline grain microstructures — Stefan Schäfer and •Dana Zöllner — Abteilung Materialphysik, Institut für Experimentelle Physik, Otto-von-Guericke-Universität, 39106 Magdeburg

Dihedral angles in polycrystalline grain microstructures are known to control the morphology of the structure and therewith also the microstructural evolution during grain growth. Hence they play an important role in grain growth theories, but are rarely measured. For exact measurements two problems have to be considered. First, assumptions have to be made regarding the shape of the grain boundaries and their triple junctions. Secondly, in digital discretised grain microstructures grain boundaries usually do not have a physical representation in the images but are defined to be between two grains of unlike orientation and are - due to the use of pixels in 2D and voxels in 3D - not smooth but rather staircase-shaped.

In this work we discuss a method to measure dihedral angles in two and three dimensional discretised (digital) grain microstructures based on trisections of circles resp. spheres. Measuring errors are examined and the method is applied to grain structures obtained by Monte Carlo Potts model simulations.