Phase-field modelling of multi-phase solidification and polycrystalline grain structure evolution

Britta Nestler

Gießerei-Institut, RWTH Aachen, Intzestr. 5, D–52072 Aachen, Germany;
Fax: +49 241 8888 276, Email: b.nestler@gi.rwth-aachen.de

Adam A. Wheeler

Faculty of Mathematical Studies, Highfield, Southampton SO17 1BJ, U.K.;
Email: aaw@maths.soton.ac.uk

Abstract

A new phase-field model for a general class of metallic alloys is used to describe both, multi-phase solidification phenomena as well as polycrystalline grain structures. The model serves as a computational method to simulate the motion and kinetics of multiple phase boundaries and enables the visualization of the diffusion processes and of the phase transformations. In the asymptotic limit of vanishing interfacial thickness, the diffuse interface (phase-field) model can be related to classical sharp interface models. This analysis ensures that the phase-field model recovers physical laws at phase boundaries and multiple junctions. Numerical simulations are presented which illustrate the capability of the phase-field model to recover a variety of complex experimental growth structures. In particular, the phase-field model is used to simulate phase transformations and microstructure evolutions in eutectic, peritectic and monotectic alloys. A first application of the model to multi-component (ternary) multi-phase systems will be shown. In addition, polycrystalline grain structures with effects such as wetting, grain growth, coarsening, symmetry properties of adjacent triple junctions in thin film samples and stability criteria at multiple junctions are described by phase-field simulations.