Phase-field simulation of morphology evolution during eutectic solidification

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Abstract

The results of this work are thematically split between two technologically important eutectic systems, Mg-Al and Pt-C:

In the first part of the work, the simulation of freezing and melting of the eutectic phase transitions in the Pt-C system using the multi-phase field model is presented.

In contrast to most simulations of eutectic solidification presented in the literature treating equal fraction of 50%/50% in a two dimensional lamellar growth mode, in this work, kinetics of solidification and melting have been obtained in 3D, incorporating the realistic extreme differences in the volume fractions (98%/2%) of the FCC-α-Pt phase on the one hand and graphite (C) on the other. The simulations reproduce reasonable offsets in temperature for freezing and melting with respect to the equilibrium eutectic temperature.

The simulations reproduce experimentally observed needle/rod-like morphology for different heat-extraction rates. The transition from needle to rod-like was shown to be sensitive on the degree of local carbon saturation of the melt.

A seemingly anomalous peak, observed in the experimental freezing curves, is recovered in the simulations. It is ascribed to the speed up of the solidification process due to the curvature effect. This effect is more pronounced with increasing cooling rates, in agreement with the experimental results.

Melting was simulated starting from a frozen structure produced by a freezing simulation as well as an alternative set up. The resulting simulations reproduce the experimental melting curves and, together with the simulated freezing curves, help to understand the phase transition of the Pt-C eutectic.

Finally the effect of metallic impurities was investigated briefly. As demonstrated for Au, impurities affect the morphology of the eutectic structure. Their impact increases with the impurity content, thus they can act as modifiers of the structure, as earlier reported for irregular eutectics.
In the second part of the work, simulations of the solidification process of Mg-Al alloys are presented. This is followed by an outlook towards a novel approach to virtually tensile test the resulting microstructure using the same software.

The nucleation and equiaxed dendritic growth of the primary HCP $\alpha$-Mg followed by eutectic solidification is simulated on a large scale in 3D using state of the art parallel computing methods. Realistic cast microstructures with grain sizes depending on the applied cooling-rate and corresponding temperature curves were simulated. The results are in remarkable qualitative and quantitative agreement with accompanying experiments. Also, segregation and effects of back-diffusion are investigated and discussed.

The interdendritic eutectic is fully resolved using a multiscale approach. To this end, we consider a zoomed in region of a melt channel under eutectic conditions. The eutectic growth of $\alpha$- and $\beta$-Mg phases between primary $\alpha$-phase dendrites is studied in detail. Based on these results and the accompanying experiments, we propose a nucleation sequence and nucleation position of the divorced eutectic.

As an outlook, we use a virtual mechanical testing process to assess the quality of the resulting microstructure of the alloy. The utilized approach intentionally follows the spirit of usual experimental sequence of work and defines a possible computational workflow, which corresponds to modeling of a material processing chain. The two parts, solidification as well as tensile testing, are executed within the phase-field framework implemented inside OpenPhase with all the advantages such as its morphology describing potential and mathematical simplicity. Because of the realistic model parametrization, the obtained simulated and experimental results are in good agreement to each other.

The obtained results give insight into the solidification processes governing the microstructure formation, allowing targeted design for different applications.