Phase-Field Study of the Cellular Bifurcation in Directional Solidification

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The cellular structures that arise during the directional solidification of alloys above a critical growth velocity have been extensively studied since their first description by Rutter and Chalmers[1]. The basic physical mechanisms that lead to their formation are well understood, and there exist numerous theoretical and numerical models that are able to predict some features of cellular growth. However, many questions remain open, both concerning the properties of individual cells, such as their precise shape and tip radius, and concerning phenomena that result from the interaction between numerous cells, such as the selection of a characteristic spacing, the structure and dynamics of the cellular array, and the morphological transitions and instabilities.

The phase-field method has emerged in recent years as a new and powerful tool to investigate such questions[2]. It avoids the numerical difficulties linked to the tracking of a sharp solidification front by introducing a phase field, which takes constant values in the bulk phases and varies smoothly through diffuse interfaces of a typical width W. The complete dynamics of the solidification front can be easily simulated in three dimensions on the scale of a few cells. However, a direct quantitative comparison with experiments is generally difficult. The reason is that for typical parameters of slow directional solidification, the size of the cells is of the order of 100 μm, whereas the solid-liquid interfaces have a typical thickness of the order of 1 nm. Because it is unfeasible to resolve numerically both of these scales at the same time, even with the help of modern multiscale algorithms, the interface width W of the phase-field model has to be chosen orders of magnitude larger than the thickness of the physical solid-liquid interfaces. This generally makes the results of simulations depend on the interface thickness. However, for a few special cases, such as the symmetric and the one-sided model of solidification, improved phase-field models have been developed that eliminate all undesired effects that scale linearly with W, which has opened the way to quantitative phase-field modeling of microstructure formation in pure substances and dilute binary alloys[3].

Here, we present the results of phase-field simulations in both two and three dimensions which are used to investigate the microstructures that form closely above the threshold of the Mullin-Sekerka instability in the directional solidification of dilute binary alloys. It is found that in this regime of shallow cells the simulation results strongly depend on the thickness of the diffuse interfaces even for model parameters that yield quantitative results for deep cells. For the material parameters of a dilute Sn-Bi alloy, the bifurcation is found to be supercritical, whereas weakly nonlinear amplitude expansions[4] predict a subcritical bifurcation. Furthermore, an oscillatory instability of the cell grooves is found, which leads to the pinch-off of liquid inclusions even for relatively shallow cells. Finally, in three dimensions, three different morphologies are found, in agreement with experiments and previous numerical studies: regular hexagons, elongated cells ('stripes'), and inverted hexagons ('node' or 'pox' structure, a hexagonal array of local depressions of the solidification front). Nodes and stripes are stable steady-state solutions only very close to the bifurcation[5].

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