

Phase-field simulations of 3D crystal growth in a channel

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Abstract

Quite generally, solidification patterns of an undercooled melt result from a competition between confinement effects and directional properties of the material or imposed experimental conditions. In particular, constant-velocity patterns grow in an originally homogeneously undercooled environment with a velocity that is governed by the anisotropy of the interfacial material properties or by the confining geometry, and possibly by a compromise between them.

There are good analytical theories describing free growth of dendritic structures in two and three dimensions; for other structures such as double fingers or for crystal growth in channel geometries, only the two-dimensional theory has been developed substantially. The talk will report on phase-field simulations of solidification in three-dimensional channels of differently shaped cross section. Results from these simulations may serve as input for the development of an analytic description aimed at a detailed understanding of confinement effects, which become the more important, the smaller the channel diameter (“nanotubes”).

As it turns out, the three-dimensional situation differs from the two-dimensional one not only in allowing a richer variety of patterns. Our simulations suggest that the value $\Delta = 1/2$ of the nondimensional undercooling loses the significance for the case of isotropic surface tension that it has in 2D. The influence of the energy conservation law on the ratio of the cross section of stationary patterns to that of the channel is subtly different in the 3D situation from the 2D case. We find bifurcations from symmetric to asymmetric fingers to be always continuous, whereas analogous bifurcations in 2D have been claimed to be discontinuous, and the bifurcation leading from the dendrite to the doublon most certainly is discontinuous. On the other hand, we observe coexistence of chaotic patterns with steady-state fingers in a certain parameter range.