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Velocity selection in 3D dendrites: Phase field computations and microgravity experiments

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Abstract

The growth of a single needle of succinonitrile (SCN) is studied in three-dimensional (3D) space by using a phase field model. For realistic physical parameters, namely, the large differences in the length scales, i.e., the capillarity length (10^{-8}–10^{-6} cm), the radius of the curvature at the tip of the interface (10^{-3}–10^{-2} cm) and the diffusion length (10^{-3}–10^{-1} cm), resolution of the large differences in length scale necessitates a 500^3 grid on the supercomputer. The parameters, initial and boundary conditions used are identical to those of the microgravity experiments of Glicksman et al. for SCN. The numerical results for the tip velocity are (i) largely consistent with the Space Shuttle experiments, (ii) compatible with the experimental conclusion that tip velocity does not increase with increased anisotropy, (iii) different for 2D versus 3D by a factor of approximately 1.9, (iv) essentially identical for fully versus rotationally symmetric 3D.

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1. Introduction

The temporal evolution of an interface during solidification has been under intensive study by physicists and material scientists for several decades. The interface velocity and shape have important consequences for practical metallurgy, as well as the theory, e.g., velocity selection mechanism and nonlinear theory of interfaces.

The simplest observed microstructure is the single needle crystal or dendrite, which is observed to be a shape resembling a paraboloid (but not fully rotationally invariant away from the tip) growing at a constant velocity, v_0, with tip radius, R_0.

An early model of this phenomenon by Ivantsov [19] stipulated the heat diffusion equation in one of the phases and imposed latent heat considerations at the interface. With the interface assumed to be at the melting temperature, the absence of an additional length scale implies the existence of an infinite spectrum of pairs of velocities and tip radii, (v_0, R_0). Since the experimental results have shown that there is a unique pair (v_0, R_0) that is independent of initial conditions, there has been considerable activity toward uncovering the theoretical mechanism for this velocity selection (see, for example [5,6,21,27]). The emergence of the capillarity length associated with the surface tension as an additional length scale has provided an explanation for the selection mechanism. Advances in computational power and a better understanding of interface models and their computation have opened up the possibility of comparing experimental values for the tip velocity with the numerical computations. This is nevertheless a difficult computational issue in part due to the large differences in length scales that range from 1 cm for the size of the experimental region, to 14 μm for the radius of curvature near the tip, 10^{-6} cm for the capillarity length, to 10^{-8} cm interface thickness length.

One perspective into the theoretical and numerical study of such interfaces has been provided by the phase field model introduced in [7,8] in which a phase, or order parameter, φ, and temperature, T, are coupled through a pair of partial differential equations described below (see also more recent papers [2,18,23]). In physical terms, the width of the transition region exhibited by φ is Angstroms. In the 1980s three key results facilitated the use of these equations for computation of physical phenomena. If the equations are properly scaled one can (i) identify each of the physical parameters, such as the surface tension, (ii) and attain the sharp interface problem as a limit [9], and (iii) use the interface thickness, ε, as a free parameter, since the motion of the interface is independent of this parameter [12]. This last result thereby opened the door to computations with realistic material parameters, by removing the issue of small interface thickness. However, the difference in scale between the radius of the curvature and overall dimensions still pose a computational challenge. More recently, several computations, have been done using the phase field model [1,20,28,29,31,32], with some three-dimensional (3D) computations in [20] utilizing the model and asymptotics of [11], that will be compared with our results below. Also, George and Warren studied [14] the simulation of dendritic growth in 3D space using a phase field model.

Our work differs from the works referenced above in many aspects. However, the main difference arises from the adaptation of the experimental conditions in the simulation of dendritic growth. Most importantly, we use true values of physical parameters which are obtained from the microgravity experiment for SCN [24]. In order to deal with different