A Phase-Field/Fluid Motion Model of Solidification: Investigation of Flow Effects During Directional Solidification and Dendritic Growth

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The phase-field model of solidification is extended to include the effects of fluid flow in the melt. The phase-field model is based on coupling the equations for heat flow in the liquid and solid phases with an auxiliary equation that describes the evolution of the phase-field variable, which is a non-conserved order parameter indicating the local phase, solid or liquid, at each point of the material. The solid-liquid interface is then represented by a diffuse transition layer in which the phase-field variable changes rapidly between its values in the bulk phases.

The model is extended to include fluid flow by a further coupling to the Navier-Stokes equations. Preliminary studies have been performed for a model in which the solid phase is treated as a liquid of high viscosity compared to the actual liquid phase. The main coupling in the Navier-Stokes equations is then through an additional term in the stress tensor that depends on the gradients of the phase-field variable, representing the effects of capillary forces within the diffuse interface.

Fluid motion in the context of diffuse interface models has been treated previously[1,2] for two-fluid systems in which the flow equations are coupled to a conserved order parameter that satisfies a convective form of the Cahn-Hilliard equation, as in the Model H of Hohenberg and Halperin.[3] In this case, the capillary forces within the diffuse interface are known as the Korteweg stress.[4] Similar terms also arise in models in which the mass density is used as the conserved order parameter;[5,6] in that case the coupling is through the continuity equation rather than a Cahn-Hilliard equation. In our work, we consider coupling through the non-conserved phase-field variable in order to make contact with previous diffuse interface treatments of the solidification of a pure material, in which neither the density nor a concentration variable are appropriate order parameters. This allows us to model systems with either constant or variable density in a single component system. In addition, the phase-field model can be used to incorporate the effects of anisotropic surface tension by using the appropriate generalization[7] of the Cahn-Hoffman ξ-vector,[8] even if the solid is approximated by a highly viscous liquid. Related models have been derived using the formalism of two-phase flows,[9] in which the phase-field variable plays a role analogous to the solid fraction.

An important area of application is the study of flow effects on microstructure during solidification. For example, many experimental investigations, both in terrestrial and microgravity environments, have studied the selection of tip radius and velocity during dendritic growth. Previous theoretical studies of dendritic growth that include fluid motion in the liquid have been able to make predictions about how the growth rate of the tip is affected by the flow but have not, for example, been able to address the effects of fluid motion on the development of side branches. Phase-field models of solidification have been a useful tool in assessing the complicated morphologies associated with dendritic growth when diffusion (heat or solute) is the dominant growth mechanism but have not included the effects of fluid motion. This research therefore aims to provide a theoretical model which will allow the modelling and computation of complex interfacial structures in realistic growth configurations. This will allow the assessment of flow effects on interfacial morphology in both terrestrial and microgravity environments.

Our preliminary work has resulted in a derivation of the governing equations for coupled fluid flow and the phase-field evolution that is based on principles of irreversible thermodynamics. We have investigated simple solutions to these equations in order to assess the capabilities of the model. The model provides a reasonable description of the flow normal to a solid-liquid interface that is generated by a density change upon solidification, and also provides a good description of shear flow tangential to the interface. In both cases, the sensitivity of the results to the magnitude of the artificial viscosity in the solid phase has been examined.

The principal objective of this research is to develop an anisotropic phase-field model for the solidification of a single-component material which incorporates flow in the melt. We will apply this model to solidification and crystal growth situations in order to investigate the effect of fluid motion in the melt on the growth characteristics as well as the microstructure formed in the solid. In particular, we will study hydrodynamic effects during directional solidification, coarsening, and dendritic growth, where complicated interface morphologies and flows may be present. Finally, we will extend the model to solidification of a binary alloy with fluid flow in the melt.

References

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