Solidification, Crystal Growth and Casting

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Overview of Current Investigations

Directional solidification techniques are the most widely used methods for preparing high quality single crystals of metallic, electronic, and opto-electronic materials. In order to obtain optimum microstructure and properties in the solidified material, it is important to maintain a uniform distribution of solute/dopants and a flat solidification interface during a growth process. Such ideal conditions are difficult to achieve in practice because of an unavoidable heat exchange between the crucible and the sample. This heat exchange leads to radial temperature gradients and subsequent fluid flow. The results are non-planar solidification fronts and potentially severe axial and radial solute segregation.

Since there is a close relationship between growth conditions and the microstructure and properties of solidified materials, there has been an extensive amount of investigation of both sharp-interface and phase-field, directional solidification configurations. Exact solutions to these classes of problems are generally restricted to unbounded domains and are subject to limitations on the boundary conditions. For this reason, a variety of approximate analytical and numerical approaches have been developed to examine domains and boundary conditions that more closely simulate actual growth conditions.

Our work falls into the category of developing analytical approaches for a variety of crystal growing configurations. We have examined time-dependent and steady-state convective-diffusive transport of heat and solute in directional solidification systems. The solution procedure involves a coupled asymptotic/numerical approach. The asymptotic expansions are based upon the assumptions that the ampoule aspect ratio, the heat exchange between the ampoule and sample, and the slope of the liquidus line are small. These scalings lead to boundary layer solutions around the solidifying front. The solidifying interfacial shape, thermal, flow, and solutal profiles are analytically evaluated as functions of the heater temperature profile, heater translation rate, and material properties of the system. The axial and radial segregation, and morphological stability of these systems are predicted.

Publications

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2. "Directional Solidification with Buoyancy in Systems with Small Segregation Coefficient," G. W. Young and S. H. Davis, *Physical Review B.*, Vol. 34, September 1986, pp. 3388-3396.

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