

**REPRESENTING REALISTIC COMPLEXITY IN MODELS
OF MELT CRYSTAL GROWTH: THREE-DIMENSIONAL AND
TIME-DEPENDENT FLOWS, PHASE BOUNDARIES, AND FURNACES**

A. Yeckel, A. Pandey, and J.J. Derby

Department of Chemical Engineering and Materials Science
The University of Minnesota
Minneapolis, MN 55455-0132
derby@umn.edu

With the continuing advance of hardware and algorithms, large-scale numerical simulation is proving to be an increasingly useful approach to understand the growth of crystalline materials. The use of realistic theoretical models is extending the traditional paradigm of experimental investigation and process development, thereby accelerating the development and optimization of crystal growth processes. Representing realistic complexity in numerical models of crystal growth systems depends on a self-consistent coupling of many nonlinear interactions. Of special importance is the ability to represent three-dimensional and transient continuum transport (incompressible flows, heat and mass transfer), phase-change phenomena (thermodynamics and kinetics), and system design (such as furnace heat transfer during melt growth).

We present an overview of a new finite element model for the parallel computation of three-dimensional flows, segregation, and solidification during Bridgman crystal growth. The model features a self-consistent coupling between the field phenomena and interfacial effects via ALE, front-tracking techniques. We also discuss coupling the code to a sophisticated furnace model, the CrysVUN++ code of Müller et al., to provide realistic heat transfer boundary conditions. Results from simulating various systems will be discussed, including a model microgravity growth system and an industrial-scale system for the growth of cadmium zinc telluride.