Commun. Comput. Phys.
doi: 10.4208/cicp.300612.210313a

Vol. **15**, No. 1, pp. 76-92
January 2014

A Phase-Field Model Coupled with Lattice Kinetics Solver for Modeling Crystal Growth in Furnaces

Guang Lin[1,*], Jie Bao[2], Zhijie Xu[1], Alexandre M. Tartakovsky[1] and Charles H. Henager Jr.[3]

[1] *Computational Mathematics Group, Pacific Northwest National Laboratory, Richland, WA 99352 USA.*
[2] *Fluid and Computational Engineering Group, Northwest National Laboratory, Richland, WA 99352 USA.*
[3] *Engineering Mechanics and Structure Materials Group, Northwest National Laboratory, Richland, WA 99352 USA.*

Received 30 June 2012; Accepted (in revised version) 21 March 2013

Communicated by Peter Jimack

Available online 26 July 2013

Abstract. In this study, we present a new numerical model for crystal growth in a vertical solidification system. This model takes into account the buoyancy induced convective flow and its effect on the crystal growth process. The evolution of the crystal growth interface is simulated using the phase-field method. A semi-implicit lattice kinetics solver based on the Boltzmann equation is employed to model the unsteady incompressible flow. This model is used to investigate the effect of furnace operational conditions on crystal growth interface profiles and growth velocities. For a simple case of macroscopic radial growth, the phase-field model is validated against an analytical solution. The numerical simulations reveal that for a certain set of temperature boundary conditions, the heat transport in the melt near the phase interface is diffusion dominant and advection is suppressed.

AMS subject classifications: 35Q20, 74N20, 74N05, 65Y05

Key words: Phase-field, crystal growth, diffusion, convection, lattice kinetics, modeling.

1 Introduction

Numerical simulations of crystal growth from the melt in vertical gradient furnaces [1, 2] has attracted significant attention due to the importance of crystals in a number of medical imaging applications and for radiation detection [3–5].

*Corresponding author. *Email addresses:* guang.lin@pnnl.gov (G. Lin), jie.bao@pnnl.gov (J. Bao), zhijie.xu@pnnl.gov (Z. Xu), alexandre.tartakovsky@pnnl.gov (A. M. Tartakovsky), chuck.henager@pnnl.gov (C. H. Henager Jr.)

Vertical growth methods include both high-pressure and ambient pressure methods with recent advances in ambient pressure methods coming to the fore [5]. Ambient pressure methods offer reduce experimental complexity and have been shown to produce large single crystal volumes with properties as good or better than high-pressure methods, thus, there has been a shift towards low-pressure methods using vertical gradient furnaces and sealed ampoule growth [5]. However, material uniformity, property homogeneity, and crystal defects remain difficult problems to solve for certain systems grown in this manner, such as Cd-Zn-Te (CZT). Modeling and simulation techniques have been advanced as a route to understanding the solidification process in complex systems and are thought to provide a more systematic method for determining optimal growth conditions and improved materials.

Recent advances in computer models for growth processes in the vertical gradient furnace have been useful in understanding the general effects of furnace operating conditions on the growth of crystals [6]. As such, computer models became a valuable tool in the furnace design and optimization of operating conditions [7–11]. At the same time, most existing models use a simplistic description of crystal/melt interface and its dynamic. Furthermore, in these models it was assumed that the latent heat dissipates without disturbing the continuity of the heat fluxes at the interface. This approach fails to account for the effects of crystal anisotropy and solidification kinetics, which may be important in the simulations of crystal dendritic growth or lateral overgrowth [12,13]. Here, we have developed a phase-field based model to simulate crystal growth in the vertical gradient furnace. The model takes into account the effects of anisotropy in kinetic and interfacial free energy coefficients as well as the effect of front curvature on crystal growth. The model was used to study the effects of operating and boundary conditions on crystal growth in a prototypical vertical gradient furnace.

The phase-field method has become a standard tool to tackle free-boundary problems and simulate interfacial pattern formation phenomena in solidification and other systems [14–16]. The phase-field method avoids explicit front tracking by replacing sharp interfaces with spatial-smoothly diffused boundaries between bulk phases. Thus, the phase-field method is suitable for simulating time-dependent free-boundary problems, especially when complex geometries are present. In a phase-field model, an order parameter, phase-field variable ψ is introduced to smoothly vary from one value in the liquid region to another one in the solid region. This method is not only used to simulate solidification but is also able to track solid-solid phase transformations and is suitable for general microstructural evolution problems. Thus, solidification and subsequent microstructural coarsening during high-temperature furnace processing can all be addressed within the same simulation framework.

The main difficulty for simulating the fluid field in the liquid region is the time-dependent growth interface between the liquid and solid phase. Hence a semi-implicit lattice kinetics model [17] based on the Boltzmann equation method [18–21]is used for solving the fluid flow instead of using the traditional computational fluid dynamics (CFD) method based on solving Navier-Stokes equations. One of the advantages of the