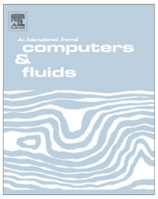
Computers & Fluids 103 (2014) 204–214

Contents lists available at ScienceDirect

Computers & Fluids

journal homepage: www.elsevier.com/locate/compfluid



A three-dimensional phase field model coupled with a lattice kinetics solver for modeling crystal growth in furnaces with accelerated crucible rotation and traveling magnetic field

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ARTICLE INFO

Article history:
Received 7 November 2013
Received in revised form 17 July 2014
Accepted 25 July 2014
Available online 7 August 2014

Keywords:
Phase field
Crystal growth
Accelerated crucible rotation technique (ACRT)
Traveling magnetic field (TMF)
Lattice Kinetics
Modeling

ABSTRACT

In this study, we present a new three-dimensional numerical model for crystal growth in a vertical solidification system. This model accounts for buoyancy, accelerated crucible rotation technique (ACRT), and traveling magnetic field (TMF) induced convective flow and their effect on crystal growth and the chemical component's transport 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. A one-way coupled concentration transport model is used to simulate the component fraction variation in both the liquid and solid phases, which can be used to check the quality of the crystal growth. Numerical results indicate that ACRT can slightly increase the quality of grown crystal, but the effect of TMF on quality of grown crystal depends on the temperature profile of the ampoule wall. Finally, excellent scalability of our developed parallel methods is demonstrated on the three-dimensional cases.

1. Introduction

Due to the importance of crystals in a number of medical imaging applications and radiation detection [1–3], numerical simulations of crystal growth from the melt in vertical gradient furnaces [4,5] have attracted significant attention.

Vertical growth techniques include both high- and ambient-pressure methods with recent advances in ambient-pressure methods at the forefront [3]. Ambient-pressure methods offer reduced 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 toward low-pressure methods using vertical gradient furnaces and sealed ampoule growth [3]. However, material uniformity, property homogeneity, and crystal defects remain difficult problems to solve for certain systems grown in this manner, such as cadmium zinc telluride (CZT). Modeling and simulation techniques are promoted as vehicles toward 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 have become a valuable tool in furnace design and the optimization of operating conditions [7–11]. At the same time, most existing models use a simplistic description of the crystal/melt interface and its dynamic. Furthermore, in these models, it is assumed that 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]. Applying a traveling magnetic field (TMF) to the vertical-gradient furnace is a direct way to introduce a body force in the direction of gravity [14–16]. TMF can adjust the magnitude of the force by adjusting the strength of the electric current. As such, we believe TMF can be used to affect crystal quality in the vertical solidification system. The accelerated crucible rotation technique (ACRT) is applied to the vertical solidification system to improve mixing in the melt [17–21], which can increase the quality of crystal growth. Already, we have developed a phase-field-based model to simulate crystal growth in the vertical gradient furnace [22]. The model accounts for 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 ACRT and TMF on crystal growth in a prototypical vertical gradient furnace.

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http://dx.doi.org/10.1016/j.compfluid.2014.07.027
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Nomenclature

α	thermal diffusion coefficient [$m^2\ s^{-1}$]
α_l	thermal diffusion coefficient of liquid phase [$m^2\ s^{-1}$]
α_s	thermal diffusion coefficient of solid phase [$m^2\ s^{-1}$]
β	kinetic coefficient [$s\ m^{-1}$]
β_T	coefficient of thermal expansion [K^{-1}]
Δt	time step interval [s]
Δx	mesh size [m]
ϵ	phase field model parameter
η	derivative of pressure with respect to density [$m^2\ s^{-2}$]
Γ	interface between liquid and solid phases
λ	parameter that controls the strength of the coupling between the phase and diffusion fields
μ	liquid dynamic viscosity [$kg\ m^{-1}\ s^{-1}$]
μ_m	magnetic permeability [$H\ m^{-1}$]
∇	differential operator in Cartesian coordinate system
∇^2	second-order differential operator in Cartesian coordinate system
$\nabla^2_{r,z}$	second-order differential operator in axisymmetric coordinate system
Ω	entire domain containing both liquid and solid phase
ω	electric current angular frequency [Hz]
Ω_g	domain occupied by new grown solid phase
Ω_l	domain occupied by the liquid phase
Ω_s	domain occupied by the solid phase
ϕ_n	electric current phase shift between coils
ψ	phase field
ρ	density [$kg\ m^{-3}$]
ρ_l	density of liquid [$kg\ m^{-3}$]
ρ_s	density of solid [$kg\ m^{-3}$]
σ	electrical conductivity [$s\ m^{-1}$]
τ	characteristic time of attachment of atoms at the interface [s]
$\tau_{sl,1}, \tau_{sl,2}$	tangential coordinates of curvilinear coordinate system moving with the interface [m]
Υ	linear relaxation parameter
ς	values at the beginning of the time step
$\varsigma + 1$	values at the end of the time step
ϑ	surface tension [$kg\ s^{-2}$]
$\vec{e}_z$	unit vector of z direction [m]
$\vec{e}_{il}$	particle velocity [$m\ s^{-1}$]
$\vec{F}$	total external forces [$kg\ m^{-2}\ s^{-2}$]
$\vec{F}_L$	time-averaged Lorentz force per volume [$kg\ m^{-2}\ s^{-2}$]
$\vec{g}$	gravity acceleration [$m\ s^{-2}$]
$\vec{n}_{sl,x}$	x component of normal direction of the solid–liquid interface [m]
$\vec{n}_{sl,y}$	y component of normal direction of the solid–liquid interface [m]
$\vec{n}_{sl,z}$	z component of normal direction of the solid–liquid interface [m]
$\vec{n}_{sl}$	normal direction of the solid–liquid interface [m]
$\vec{S}_0$	total momentum source term [$kg\ m^{-2}\ s^{-1}$]
$\vec{S}_{0b}$	momentum source caused by buoyancy force [$kg\ m^{-2}\ s^{-1}$]
$\vec{S}_{0L}$	momentum source caused by Lorentz force [$kg\ m^{-2}\ s^{-1}$]
$\vec{u}$	velocity vector [$m\ s^{-1}$]
$\vec{u}_p$	velocity of particles in Boltzmann equation [$m\ s^{-1}$]
$\vec{u}_{wall}$	velocity of the ampoule wall [$m\ s^{-1}$]
$\vec{x}$	position vector in Cartesian coordinate system [m]
$\widetilde{F}_{il}$	external forces in lattice scheme [$kg\ m^{-3}\ s^{-1}$]
A_1	in-phase components of magnetic potential [$V\ s\ m^{-1}$]
a_1	phase field model parameter
A_2	out-of-phase components of magnetic potential [$V\ s\ m^{-1}$]
a_2	phase field model parameter
a_s	anisotropy strength
c	non-dimensional chemical components' concentration
$c\vert_l$	non-dimensional chemical components' concentration at solid–liquid interface in liquid side
$c\vert_s$	non-dimensional chemical components' concentration at solid–liquid interface in solid side
C_p^l	specific heat capacity of liquid [$J\ kg^{-1}\ K^{-1}$]
C_p^s	specific heat capacity of solid [$J\ kg^{-1}\ K^{-1}$]
c_r	reference chemical components' concentration
c_{lks}	lattice sound speed [$m\ s^{-1}$]
c_{lk}	reference lattice speed [$m\ s^{-1}$]
d_0	capillary length [m]
D_l	chemical component diffusion coefficient in liquid phase [$m^2\ s^{-1}$]
D_s	chemical component diffusion coefficient in solid phase [$m^2\ s^{-1}$]
f	particle distribution function [$kg\ m^{-3}$]
f_{il}^{eq}	discretized equilibrium Maxwell distribution [$kg\ m^{-3}$]
$f_{il,\rho}$	discretized particle distribution function for density [$kg\ m^{-3}$]
$f_{il,\vec{u}}$	discretized particle distribution function for velocity [$kg\ m^{-3}$]
f_{il}	discretized particle distribution function [$kg\ m^{-3}$]
H	height of ampoule [m]
h	heat transfer coefficient [$W\ m^{-2}\ K$]
J_0	electric current density [$A\ m^{-2}$]
k	segregation coefficient
K_l	thermal conductivity of liquid [$W\ m^{-1}\ K^{-1}$]
K_s	thermal conductivity of solid [$W\ m^{-1}\ K^{-1}$]
L	latent heat [$J\ kg^{-1}$]
N	total number of lattice directions excluding the stationary 0 direction
n	norm coordinate of ampoule wall [m]
n_{sl}	norm coordinate of curvilinear coordinate system moving with the interface [m]
R	radius of ampoule [m]
r	r direction in axisymmetric coordinate system, distance from the centerline of ampoule [m]
S_ψ	thermal source term caused by phase filed transition [$K\ s^{-1}$]
T	temperature [K]
t	time [s]
T_0	reference temperature [K]
T_c	cold end temperature [K]
T_h	hot end temperature [K]
T_i	interface temperature [K]
T_m	melting temperature [K]
T_w	ampoule wall temperature [K]
U	magnitude of velocity [$m\ s^{-1}$]
u	velocity component in x direction [$m\ s^{-1}$]
U_{pull}	ampoule pulling speed [$m\ s^{-1}$]
v	velocity component in y direction [$m\ s^{-1}$]
V_i	normal interfacial velocity [$m\ s^{-1}$]
W	interface thickness [m]
w	velocity component in z direction [$m\ s^{-1}$]
W_0	phase field model parameter for interface thickness [m]
$x,\ y,\ z$	coordinates in Cartesian coordinate system [m]
z_i	position of solid–liquid interface [m]
z_{i0}	initial position of solid–liquid interface [m]