Journal of Crystal Growth 385 (2014) 82–87

Contents lists available at ScienceDirect

Journal of Crystal Growth

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

Numerical investigation of heat and mass transfer during vertical Bridgman crystal growth under rotational vibrations

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ARTICLE INFO

Available online 20 June 2013

Keywords:
A1. Convection
A1. Directional solidification
B1. Alloys

ABSTRACT

The paper deals with the numerical investigation of convective flows and heat and mass transfer in the directional solidification of binary melts in the presence of rotational vibrations of finite amplitude and frequency. The study is performed in the framework of the Boussinesq approximation and unsteady axisymmetric approach, taking into account the existence of the two-phase zone. The simulation is conducted for binary melt with low phase change temperature (succinonitrile with ethanol), using ANSYS Fluent package which realizes the finite volume method. The data on the temporal evolution of velocity, temperature and solute concentration fields in the melt and on the solute distribution in the grown crystal with and without vibrations are obtained. It is demonstrated that the vibrations make strong stabilizing effect; they reduce the radial segregation and prevent the pit formation and solidification front breakdown, which leads to a substantial increase of grown crystal homogeneity.

1. Introduction

In the process of solidification of binary alloys by the vertical Bridgman method [1] the crystallization temperature does not remain constant, it depends on the concentration of solute at the crystal/melt interface. The radial inhomogeneity of the melt temperature, resulting from the difference in thermal conductivities of the melt and crystal and heat release of the phase transition, leads, on the one hand, to the curvature of the crystallization front, and on the other hand, to the onset of convective flows [1]. The influence of these flows on the binary melt crystallization may result in the local solute accumulation and pit formation at the crystallization front which accelerates the morphological instability due to the constitutional supercooling [2–5]. The key factor in the formation of pit is the radial flow generated in the vicinity of the front and directed toward the axis [5]. If the radial flow is suppressed or pushed away from the front to a distance greater than the thickness of the diffusion layer, the pit formation could be prevented or at least its depth could be reduced.

Thus, convective flows occurring in the melt can provoke the morphological instability and solute segregation and it is important to find the ways for controlling these flows. As one of the methods to control the melt flows, the application of magnetic fields was suggested (see, for example [6–9]). Another, more recently proposed method is the vibrations exposure technique. In [10], in the framework of simplified model, it was shown that the high-frequency small-amplitude horizontal vibrations of crucible in the vertical Bridgman method may lead to a substantial reduction of intensity of the melt flow near the front. Lyubimov et al. [11] investigated the effect of high-frequency small-amplitude translational vibrations of linear polarization on morphological stability of the infinite plane crystallization front moving with constant velocity. They found that the tangential vibrations (parallel to the crystal-melt interface) exert a stabilizing effect, which well corresponds to the results [10], and the normal vibrations play a destabilizing role. Destabilizing effect of high-frequency small-amplitude translational vibrations normal to the interface was also confirmed for vertical Bridgman growth [12].

Another type of the vibration action on the melt flows was considered in [13]. In that case, vibrational flow was induced by the submerged vibrator. It was shown that the vibrations generate the mean flows near the crystallization front which may reduce the thickness of the boundary layers near the front.

The melt flows induced by finite-frequency translational vibrations of linear and circular polarizations and finite-frequency rotational vibrations were studied in [14] from the viewpoint of using applied vibrations as a means of flow control. It was found that circular-polarized translational vibrations and rotational vibrations result in more intensive melt flows than linear-polarized translational vibrations.

Scheel [15] proposed a modification of the vertical Bridgman method where the ampoule rotation is set by the various periodic

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http://dx.doi.org/10.1016/j.jcrysgro.2013.04.063

functions. This method called Accelerated Crucible Rotation Technique (ACRT) is based on the Ekman time scale for rotational spin up. Accelerated rotation leads to effective stirring of the melt. It results in a rapid equalization of the concentration (and temperature) and prevents a constitutional supercooling.

In [16] an average approach was developed and implemented for the investigation of flow patterns and heat/mass transfer during crystal growth by the vertical Bridgman method in the presence of low-amplitude, high-frequency rotational vibrations about the ampoule axis. Differing from ACRT where the ampoule completes several revolutions before its direction is reversed, in the rotational vibration technique (RVT) the direction of rotation is reversed after only partial rotation of the ampoule. As it was shown in [16], rotational vibrations lead to the generation of mean flow localized near the crystallization front, the direction of this flow is opposite to that of buoyancy-induced convective flow. As the result, the buoyancy-induced flow is pushed away from the crystallization front. Based on these results it was concluded that the rotational vibrations may lead to a stabilization of morphological instability of front during directional solidification of binary alloys. This conclusion was confirmed in [17–20], where the effect of rotational vibrations on the melt flow in the directional solidification of binary alloys was studied experimentally and numerically in the framework of time-average approach and on the basis of the full equations and boundary conditions.

Comparative analysis of the accelerated crucible rotation technique (ACRT) and the rotational vibration technique (RVT) performed in [21] has demonstrated that RVT is more efficient for radial segregation control.

In the present work, we study heat and mass transfers during directional solidification of binary melts with low phase change temperature (succinonitrile (SCN) containing ethanol) subjected to rotational vibrations, taking into account the existence of the two-phase transition zone.

2. Problem formulation. Governing equations and boundary conditions

Let us consider the process of directional solidification of a binary alloy by the vertical Bridgman technique [1]. The equations, describing convective flows during solidification in the axisymmetric case, are written as

– for the radial velocity component u

$$\frac{\partial u}{\partial t}+v\frac{\partial u}{\partial z}+u\frac{\partial u}{\partial r}-\frac{w^2}{r}=-\frac{1}{\rho}\frac{\partial p}{\partial r}+\frac{\nu}{r^2}\frac{\partial}{\partial z}\left[\left(\frac{\partial u}{\partial z}+\frac{\partial v}{\partial r}\right)\right]+\frac{2\nu}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right)-2\nu\frac{u}{r^2} \quad (1)$$

– for the azimuthal velocity w

$$\frac{\partial w}{\partial t}+\frac{\partial}{\partial z}(uw)+\frac{1}{r}\frac{\partial}{\partial r}(rvw)=\nu\frac{\partial^2 w}{\partial z^2}+\frac{\nu}{r^2}\frac{\partial}{\partial r}\left[r^3\frac{\partial}{\partial r}\left(\frac{w}{r}\right)\right]-\frac{vw}{r} \quad (2)$$

– for the axial velocity component v

$$\frac{\partial v}{\partial t}+v\frac{\partial v}{\partial z}+u\frac{\partial v}{\partial r}=-\frac{1}{\rho}\frac{\partial p}{\partial z}+\nu\left(\frac{\partial^2 v}{\partial z^2}+\frac{\partial^2 v}{\partial r^2}\right)+\frac{\nu}{r}\frac{\partial v}{\partial r}-g(\beta_T T_l-\beta_C C) \quad (3)$$

here r, z are radial and vertical coordinates, ρ is the density, ν is the kinematic viscosity of the melt, g is the gravitational acceleration, β_T is the volumetric thermal expansion coefficient, β_C is the concentration coefficient of volumetric expansion, T_l is temperature of melt.

The continuity equation

$$\nabla\cdot\vec{v}=\frac{\partial u}{\partial r}+\frac{\partial v}{\partial z}+\frac{u}{r}=0 \quad (4)$$

The energy equation is written in terms of the enthalpy H

$$\frac{\partial}{\partial t}(\rho H)+\nabla\cdot(\rho\vec{v}H)=\nabla\cdot(k\nabla T) \quad (5)$$

The medium enthalpy is calculated as a sum of apparent enthalpy h and latent heat ΔH.

$$H=h+\Delta H \quad (6)$$

where $h=h_{ref}+\int_{T_{ref}}^{T}C_p dT$, h_{ref} is the initial value of the enthalpy, T_{ref} is the reference temperature, C_p is the specific heat capacity at constant pressure.

In the two-phase zone which is formed between the melt and crystal the latent heat of the medium is written in terms of the latent heat of the examined material Lt:

$$\Delta H=\beta Lt \quad (7)$$

where β is the parameter determining the fraction of a substance in a liquid state:

$$\beta=\begin{cases}0, & T<T_{solidus}\\ 1, & T>T_{liquidus}\\ \frac{T-T_{solidus}}{T_{liquidus}-T_{solidus}}, & T_{solidus}<T<T_{liquidus}\end{cases} \quad (8)$$

Here, $T_{solidus}$ is the solidus temperature, $T_{liquidus}$ is the liquidus temperature. The quantity ΔH takes zero value in a crystal and the value Lt in a melt and monotonically changes from 0 to Lt in a transition zone.

For two-component system the solidus temperature $T_{solidus}$ and liquidus temperature $T_{liquidus}$ are defined by

$$T_{solidus}=T_{melt}+mY/K$$
$$T_{liquidus}=T_{melt}+mY \quad (9)$$

where T_{melt} is the melting temperature of the pure material, K is the coefficient of segregation, which is equal to the ratio of concentrations of liquid- and solid phases at the interface; Y is the mass fraction of the solute and m is the liquidus slope.

The equation of solute transport is written as

$$\frac{\partial Y}{\partial t}+\nabla\cdot(\beta\vec{v}_{liq}Y_{liq}+(1-\beta)\vec{v}_p Y_{sol})=-\frac{1}{\rho}\nabla\cdot\vec{J} \quad (10)$$

where

$$\vec{J}=-\rho[\beta D_{m,liq}\nabla Y_{liq}+(1-\beta)D_{m,sol}\nabla Y_{sol}] \quad (11)$$

here $D_{m,liq}$ and $D_{m,sol}$ are the dopant diffusivities in the melt and crystal respectively, $Y=\beta Y_{liq}+(1-\beta)Y_{sol}$, Y_{liq} and Y_{sol} are interrelated by the proportionality formula

$$Y_{sol}=KY_{liq} \quad (12)$$

$\vec{v}_{liq}$ is the melt flow velocity, $\vec{v}_p$ is the pulling rate. The melt flow velocity is defined as

$$\vec{v}_{liq}=\frac{\vec{v}-\vec{v}_p(1-\beta)}{\beta} \quad (13)$$

for hydrodynamic boundary conditions we use the no-slip conditions at all ampoule walls.

The thermal boundary conditions are as follows:

– continuity condition for the temperature and heat flux at the melt-ampoule interface;
– zero heat flux condition at the upper ampoule wall;