Available online at www.sciencedirect.com
ScienceDirect
Trans. Nonferrous Met. Soc. China 25(2015) 936−943
Transactions of Nonferrous Metals Society of China
www.tnmsc.cn

Effects of static magnetic fields on melt flow in detached solidification

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Received 8 April 2014; accepted 8 August 2014

Abstract: A series of three-dimensional numerical computations were conducted to understand the effects of different static magnetic fields on thermal fluctuation and melt flow during the detached solidification of CdZnTe. Numerical calculations were carried out by three different configurations of magnetic field: without magnetic field, with an axial magnetic field (AMF) and with a cusp-shaped magnetic field (CMF). The results reveal that the magnetic fields can effectively suppress the melt flow and thermal fluctuation and the suppression effect of the AMF is stronger than that of the CMF. Besides, the physical mechanism of thermocapillary−buoyancy convection instability was discussed and the effects of magnetic field on the critical Marangoni number were also obtained.

Key words: detached solidification; static magnetic field; thermocapillary−buoyancy convection; numerical simulation; CdZnTe

1 Introduction

The technological potential of CdZnTe is great due to its excellent physical properties in the area of medical imaging and photorefractive sensors. Furthermore, CdZnTe is a tricky material in terms of crystal growth, the traditional available growth techniques are unsatisfactory because of its thermal sensitivity. Since the first observation of detachment on skylab in 1974 by accident, it attracted much attention for its remarkable performance in crystallography [1]. As described in Ref. [2], since the absence of the stress produced by differential thermal contraction of the crystal and ampoule, the dislocation density is tremendously reduced. Based on the model proposed by DUFFAR et al [3−5], detached solidification can be achieved by applying a gas pressure between the ampoule and the crystal.

However, melt flow still has a fundamental influence on the crystal quality in detached solidification. To obtain the high-quality crystal, the accurate control of melt flow and thermal fluctuation is essential [6,7].

A substantial amount of progress has been made in the past decades in understanding the influence of magnetic fields on the melt flow and thermal distribution in the crystal growth [8−10]. LIU et al [11,12] studied the effects of magnetic field on the turbulent convection and thermal fluctuation. They found that the cusp-shaped magnetic field (CMF) provides stronger suppression effect on thermal instability than the transverse magnetic field (TMF). JABER et al [3] indicated that the melt flow can be effectively suppressed by the axial and rotating magnetic field during GeSi crystal growth. SADRHOSSEINI and SEZAI [14] found that the suppression effect of magnetic field on the melt flow is enhanced with the increase of *Ha*. CEN et al [15] compared the effect of the static magnetic field on the melt flow and found that the axial magnetic field is more effective in suppressing the convection than the cusp magnetic field.

As the CdZnTe melt is electrically conductive, the application of magnetic field is identified as an effective way to weaken the melt flow. PENG et al [16] conducted a two-dimensional global simulation of detached solidification under a cusp magnetic field and the results exhibited that the cusp magnetic field has a suppression effect on the melt flow. LI et al [17] studied the effects of geometric parameters and axial magnetic field on thermocapillary−buoyancy convection during detached solidification. The results indicated that the inhibition effect of axial magnetic field is enhanced as the *Ha* increases.

Foundation item: Project (51276203) supported by the National Natural Science Foundation of China
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DOI: 10.1016/S1003-6326(15)63682-2

In this work, to make a comprehensive analysis of the influence of static magnetic field on the flow behavior and the temperature fluctuation of molten CdZnTe in detached solidification, the three-dimensional numerical simulations were performed for three configurations: without magnetic field, with axial magnetic field (AMF) and with cusp-shaped magnetic field (CMF). Meanwhile, the evolution of flow pattern and the physical mechanism of unstable Marangoni convection were explored. And magnetohydrodynamic (MHD) effects on the critical Marangoni number (*Ma*) were also discussed.

2 Physical and mathematical models

The schematic diagrams for three configurations: without magnetic field, with AMF and with CMF are plotted in Fig. 1. In addition, the cusp-shaped magnetic field adopted in the simulation was produced by two identical solenoids carrying equal but counter-rotating currents [18]. The aspect ratio *A* (height/radius) of the crucible equals 1, and the non-dimensional width of the gas gap (*S*) equals 0.1. The physical properties of CdZnTe are listed in Table 1.

The main assumptions adopted in the simulation are summarized as follows: 1) The CdZnTe melt is incompressible Newtonian fluid; 2) The free surfaces of the gas gap and the top of melt are adiabatic; 3) All boundaries are electric insulators; 4) The induced field caused by electromagnetic field is ignored; 5) On the free surface, the thermocapillary force is taken into account, and at other solid−liquid boundaries, the no-slip condition is applied; 6) The surface tension is linear function of the temperature.

Table 1 Physical properties of CdZnTe melt [19,20]

Parameter	Symbol	Value
Temperature coefficient/(N·m^{-1}·K^{-1})	γ_T	0.14×10^{-3}
Thermal expansion coefficient/K^{-1}	β	5.0×10^{-4}
Density of melt/(kg·m^{-3})	ρ	5.68×10^{3}
Thermal conductivity/(W·m^{-1}·K^{-1})	k	1.09
Melting temperature/K	T_m	1364
Specific heat/(kJ·kg^{-1}·K^{-1})	c_p	0.187
Kinematic viscosity/(m^2·s^{-1})	ν	4.16×10^{-7}
Prandtl number	Pr	0.4

Based on the above assumptions, the melt flow is described by the dimensionless three dimensional continuity, Navier−Stokes and energy equations are in the domain $0 \le Z \le H, 0 \le R \le 1, 0 \le \theta < 2\pi$.

$$\nabla \cdot \boldsymbol{V} = 0 \tag{1}$$

$$\frac{\partial \boldsymbol{V}}{\partial \tau} + \boldsymbol{V} \cdot \nabla \boldsymbol{V} = -\nabla P + \nabla^2 \boldsymbol{V} + \boldsymbol{F} + Gr\Theta \tag{2}$$

$$\frac{\partial \Theta}{\partial \tau} + \boldsymbol{V} \cdot \nabla \Theta = \frac{1}{Pr} \nabla^2 \Theta \tag{3}$$

where $\boldsymbol{V}$, P and Θ are non-dimensional velocity, pressure and temperature, respectively. The dimensional scales of the time, the velocity, the pressure and the temperature are as follows:

$$\tau = \frac{t}{r_o^2/\nu}, \quad (U,V,W) = \frac{(u,v,w)}{(\nu/r_o)}, \quad P = \frac{p}{\rho\nu^2/r_o^2},$$

$$\Theta = \frac{T - T_m}{T_h - T_m}$$

where r_o is the radius of ampoule; T_h is the temperature of ampoule wall; U, V, W are three velocity components.

Other parameters are Grashof number $Gr = g\beta(T_h - T_m)r_o^3/\nu^2$, Prandtl number $Pr=\nu/a$. Special note is that under the condition of microgravity, the gravity acceleration (g) can be considered zero, thus, the term of buoyancy is negligible.

According to the Ohm's law, the electric current ($\boldsymbol{J}$) induced by the interaction of the magnetic field and the melt flow can be expressed as $\boldsymbol{J} = \sigma(\boldsymbol{V} \times \boldsymbol{B} - \nabla\psi)$, where σ is electric conductivity of the melt, ψ is stream function and $\boldsymbol{B}$ is magnetic field intensity. The

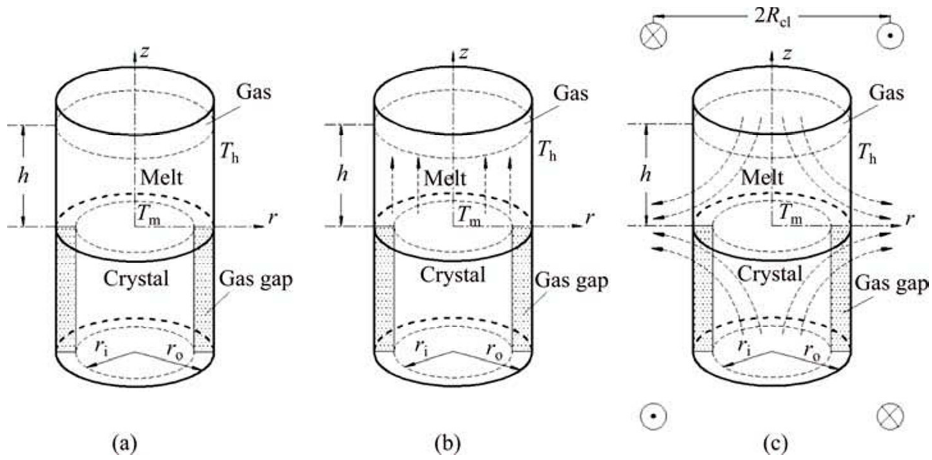

Fig. 1 Physical model of simulation system: (a) Without magnetic field; (b) With AMF; (c) With CMF