ELSEVIER

Journal of Crystal Growth 222 (2001) 677–684

JOURNAL OF CRYSTAL GROWTH

www.elsevier.nl/locate/jcrysgro

Numerical simulation of magnetic field design for damping thermocapillary convection in a floating half-zone

K. Li, W.R. Hu*

National Microgravity Laboratory, CAS; Institute of Mechanics, CAS, Beijing 100080, People's Republic of China

Received 10 April 2000; accepted 14 November 2000
Communicated by T. Hibiya

Abstract

The magnetic fields produced by electrical coils are designed for damping the thermocapillary convection in a floating half-zone in microgravity. The fields are designed specially to reduce the flow near the free surface and then in the melt zone by adjusting the longitudinal coil positions close to the melt zone. The effects of the designed magnetic fields on reducing the flow velocity and temperature distribution non-uniformity in the melt zone are stronger than those of the case of an uniform longitudinal magnetic field obtained by numerical simulation, particularly at the melt-rod interface. It brings fundamental insights into the heat and mass transfer control at the solidification interface by the magnetic field design for crystal growth by the floating full-zone method. © 2001 Published by Elsevier Science B.V.

Keywords: Floating half-zone; Magnetic field; Numerical simulation

1. Introduction

The floating full-zone method is a crucible-free process for the growth of high-quality single crystal because the melt zone is confined by the melt surface tension. However, the diameter of the grown crystal is limited under the terrestrial condition. The microgravity environment provides the possibility of growing large size crystals by the floating full-zone method. In this method, the thermocapillary convection driven by the surface tension gradient is dominant in the melt zone, and the buoyancy-driven convection is greatly reduced. The thermocapillary convection may be unsteady, and induces the impurity striations. In order to suppress the unsteady thermocapillary convection in the melt, a steady magnetic field, in many cases an uniform longitudinal magnetic field, is often used [1–3]. The unsteady flow in the core region of the melt zone is damped out and the impurity striations in the according part of the grown crystal is eliminated when the longitudinal magnetic field is strong enough. The longitudinal magnetic field reduces effectively the flow across the force-lines, but has less influence on the flow along the force-lines such as on the free surface, where the thermocapillary convection is driven, even when the magnetic field is stronger. The relatively strong convective recirculations still persist near the free surface while the weak flow occupies the core region of the melt zone. Such a flow structure will induce non-uniformity in large concentration distribution in the melt zone,

*Corresponding author. Fax: +86-10-626-15530.
E-mail address: wrhu@imech.ac.cn (W.R. Hu).

PII: S0022-0248(00)00985-4

particularly at the solidification interface which results in the large radial macro-segregation in the grown crystal [3]. It is important to improve the concentration distribution non-uniformity at the solidification interface by a suitable flow structure in the melt zone. This cannot be achieved by merely increasing the strength of the longitudinal magnetic field [3,4].

As the first step of the study, the paper presents a discription of how axis-symmetric non-uniform magnetic fields produced by electrical coils are designed for damping the convection in the floating half zone in microgravity which is often used to investigate the thermocapillary convection in the floating zone [5–11]. The magnetic fields are designed specially to reduce the flow near the free surface and then in the melt zone by adjusting the longitudinal coil positions close to the melt zone. The effects of the designed magnetic fields on reducing the flow velocity and temperature distribution non-uniformity are obtained by numerical simulation. It brings fundamental insights into the heat and mass transfer control at the solidification interface by magnetic field design for crystal growth by the floating zone method.

2. Model

The model of the floating half-zone is described in a cylindrical coordinate system (r, θ, z) and is assumed to be axis-symmetric, $\partial/\partial\theta = 0$, as shown in Fig. 1. A cylinder liquid bridge is floating between rod-melt interfaces at $z = 0$ and $z = L$, respectively, with the same radius R_0 under microgravity condition. The melt–rod interfaces are assumed to be flat with constant temperatures T_0 at the lower rod and $T_0 + \Delta T$ at the upper rod, respectively. Adiabatic ambient temperature distribution near the free surface is adopted for the first step.

The designed magnetic fields in the present paper are produced by several electrical coils, which are located axis-symmetrically at adjusted positions and close to the free surface. The diameter of the coils is small and assumed to be zero for simplification. The coils are located axis-symmetrically. The magnetic fields produced by the electrical currents of the coils are computed based on the Biot–Savart's law. Because the magnetic Reynolds number is very small, the induced magnetic field can be neglected. Furthermore, the induced electrical current is adopted as zero because of the arrangement of the magnetic field. The purpose of the present paper is to study the design of the magnetic field for a more suitable flow structure while damping the thermocapillary convection.

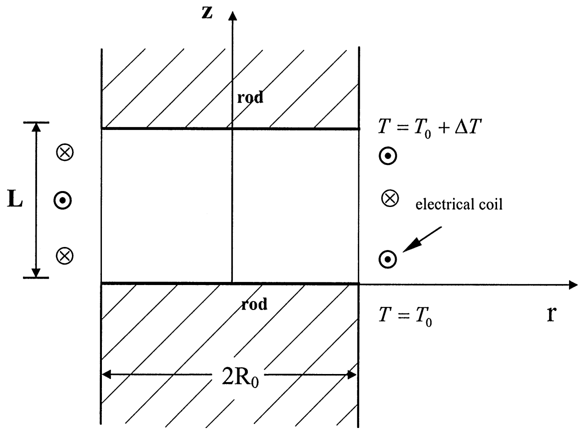

Fig. 1. The schematic diagram of a floating half-zone with three electrical coils.

The non-dimensional quantities and parameters are defined as follows:

$$r^* = \frac{r}{R_0}, \quad z^* = \frac{z}{R_0}, \quad u^* = \frac{u}{U_0}, \quad v^* = \frac{v}{U_0},$$

$$p^* = \frac{p}{\rho U_0^2}, \quad T^* = \frac{T - T_0}{\Delta T}, \quad \boldsymbol{B}^* = \frac{\boldsymbol{B}}{B_0},$$

$$\Gamma = \frac{L}{2R_0}, \quad \mathrm{Re} = \frac{\rho U_0 R_0}{\eta},$$

$$\mathrm{Ma} = \frac{U_0 R_0}{\kappa}, \quad \mathrm{Ha} = B_0 R_0 \sqrt{\sigma_e/\eta}, \tag{2.1}$$

where $(u, 0, v)$ are the velocities in (r, θ, z) direction; L is the height of the floating half-zone; Γ is the geometrical aspect ratio; p, T and ρ are the pressure, temperature and density of the melt respectively; ΔT the applied temperature difference between the rods; η, κ and σ_e the melt viscosity, the thermal diffusion coefficient and the electric conductivity respectively. The characteristic velocity is defined as $U_0 = |\gamma_T|\Delta T/\eta$, where γ_T is the gradient of surface tension. The characteristic magnetic field $B_0 = \mu_r\mu_0 I_0/\pi R_0$, where μ_r is the relative magnetic permeability of the melt and $\mu_r = 1$; μ_0 is adopted as $4\pi \times 10^{-7}$ H/m; I_0 is the electric current intensity in a single coil. The superscript "*" denotes non-dimensional quantities and will be omitted hereafter for simplification. The thermocapillary convection in the melt zone is assumed to be a steady and axial symmetric process. The non-dimensional governing equations are written as follows, and the gravity term is omitted under the microgravity condition:

$$\frac{1}{r}\frac{\partial}{\partial r}(ru) + \frac{\partial}{\partial z}(v) = 0. \tag{2.2}$$

$$\frac{1}{r}\frac{\partial}{\partial r}(ru^2) + \frac{\partial}{\partial z}(vu) = -\frac{\partial p}{\partial r} + \frac{1}{\mathrm{Re}}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) + \frac{\partial^2 u}{\partial z^2} - \frac{u}{r^2}\right] + \frac{\mathrm{Ha}^2}{\mathrm{Re}}\left(vB_rB_z - uB_z^2\right), \tag{2.3}$$

$$\frac{1}{r}\frac{\partial}{\partial r}(ruv) + \frac{\partial}{\partial z}(v^2) = -\frac{\partial p}{\partial z} + \frac{1}{\mathrm{Re}}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v}{\partial r}\right) + \frac{\partial^2 v}{\partial z^2}\right] + \frac{\mathrm{Ha}^2}{\mathrm{Re}}\left(uB_rB_z - vB_z^2\right), \tag{2.4}$$

$$\frac{1}{r}\frac{\partial}{\partial r}(ruT) + \frac{\partial}{\partial z}(vT) = \frac{1}{\mathrm{Ma}}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right]. \tag{2.5}$$

The non-dimensional boundary conditions are written as:

$$r = 0,\ z \in (0, \Gamma) : u = 0,\ \frac{\partial v}{\partial r} = 0,\ \frac{\partial T}{\partial r} = 0, \tag{2.6}$$

$$r = 1,\ z \in (0, \Gamma) : u = 0,\ \frac{\partial v}{\partial r} = -\frac{\partial T}{\partial z},\ \frac{\partial T}{\partial r} = 0, \tag{2.7}$$

$$z = 0,\ r \in (0, 1) : u = 0,\ v = 0,\ T = 0, \tag{2.8}$$

$$z = \Gamma,\ r \in (0, 1) : u = 0,\ v = 0,\ T = 1. \tag{2.9}$$

3. Numerical simulation results

A strong uniform longitudinal magnetic field can be produced approximately by four electrical coils with $I_0 = 4.0 \times 10^4$ A in the same direction in each coil, the magnetic field strength in the melt zone is 0.988 T [12]. To design the non-uniform magnetic field, the coils are located near the free surface with each carrying an equal electric current $I_0 = 2.0 \times 10^3$ A in the opposite direction compared with its neighbour coil, and a horizontal plane of purely radial magnetic field appears between the coils as shown in Fig. 2. It may be practically difficult to carry the large electric currents in such small electrical coils, but in the present study, such coil design is simply used to generate the non-uniform magnetic field with the required configuration and the characteristic that only the designed field at the purely horizontal plane of the radial magnetic field near the free surface has the similar field strength in comparison with the longitudinal magnetic field, while the field strength is much weaker in other regions.

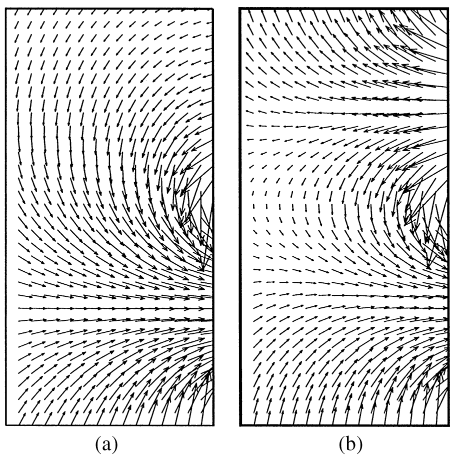

Fig. 2. The schematic diagrams of the designed magnetic field produced by (a) two coils and (b) three coils, respectively.

The steady governing equations are treated as "pseudo-unsteady" equations and discretized on the staggered grids by the finite control volume difference method [13]. Fully implicit time marching is used with first order in time term. Hybrid scheme is adopted in writing the coefficients of convection and diffusion term. The "block modification" method [14] is used to solve the problem of difference equations. The boundary conditions are discretized with second order accuracy. The total grid meshes are 32×64. The variables convergence criteria may be estimated as follows:

$$\left|\frac{u-u_{\text{old}}}{u_{\text{old}}}\right|_{\max} < 1.0\times 10^{-5},$$

$$\left|\frac{v-v_{\text{old}}}{v_{\text{old}}}\right|_{\max} < 1.0\times 10^{-5},$$

$$\left|\frac{T-T_{\text{old}}}{T_{\text{old}}}\right|_{\max} < 1.0\times 10^{-5},$$

where the subscript old denotes the previous iteration and the subscript max means the maximum value of the absolute value. The residual of each governing equation is smaller than 1.0×10^{-7}.

To simulate the typical process of the semiconductor crystal growth, the parameters are adopted as $\Gamma = 1.0$, $\text{Re} = 5000$, $\text{Ma} = 50$. The case of the designed magnetic field produced by two coils is studied at first. In order to gain the best magnetic damping effects on the flow near the free surface, the horizontal plane of purely radial magnetic field is located around the "key point" which relates to the maximum flow velocity on the free surface in the case without magnetic field. Changing the distance between the two coils, the magnetic damping effects on the flow near the free surface which are represented by the profiles of the reduced flow velocity on the free surface are compared with the case without magnetic field and with the longitudinal magnetic field (Fig. 3). In the case of two coils, when the distance is small, the flow velocity on the free surface near the cold end is reduced greatly and the reduced flow intensity is relatively more uniform compared with the case of without magnetic field and the case of the longitudinal magnetic field. For the part near the hot end, the damping effect is not so efficient

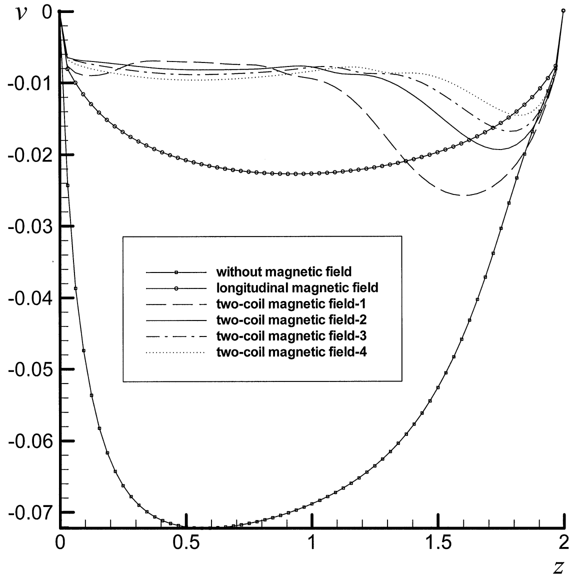

Fig. 3. The profiles of flow velocity on the free surface velocity v in the cases of the designed magnetic field produced by two coils when the coils are located at (1) $z = 0.2$ and $z = 0.9$; (2) $z = 0.0$ and $z = 1.1$; (3) $z = -0.1$ and $z = 1.2$; (4) $z = -0.2$ and $z = 1.3$, respectively for $\text{Pr} = 0.01$, $\text{Ma} = 50$ and $\Gamma = 1.0$.

due to the strong cancel between the magnetic fields produced by each coil which narrows the damping range. With increasing distance, the maximum reduction of the flow velocity on the free surface decreases to some extent, but compared with the case of the longitudinal magnetic field, the overall damping effects of the case of two coils on the flow velocity on the free surface is still obvious and much more uniform. It can be seen that the distance between the coils is an important parameter for the magnetic field design.

Compromising the maximum magnetic damping effects and the uniformity of the reduced flow velocity on the free surface, the case when the two coils are located at $z = 0.0$ and $z = 1.1$ (the solid line in Fig. 3), is chosen to represent the designed magnetic field produced by two coils. The effect of three types of magnetic fields on reducing the flow velocity and temperature distribution non-uniformity are compared in Fig. 4. For the case without magnetic field, the strong convective recirculation occupied the whole melt zone and the temperature distributions are obviously non-linear. When the

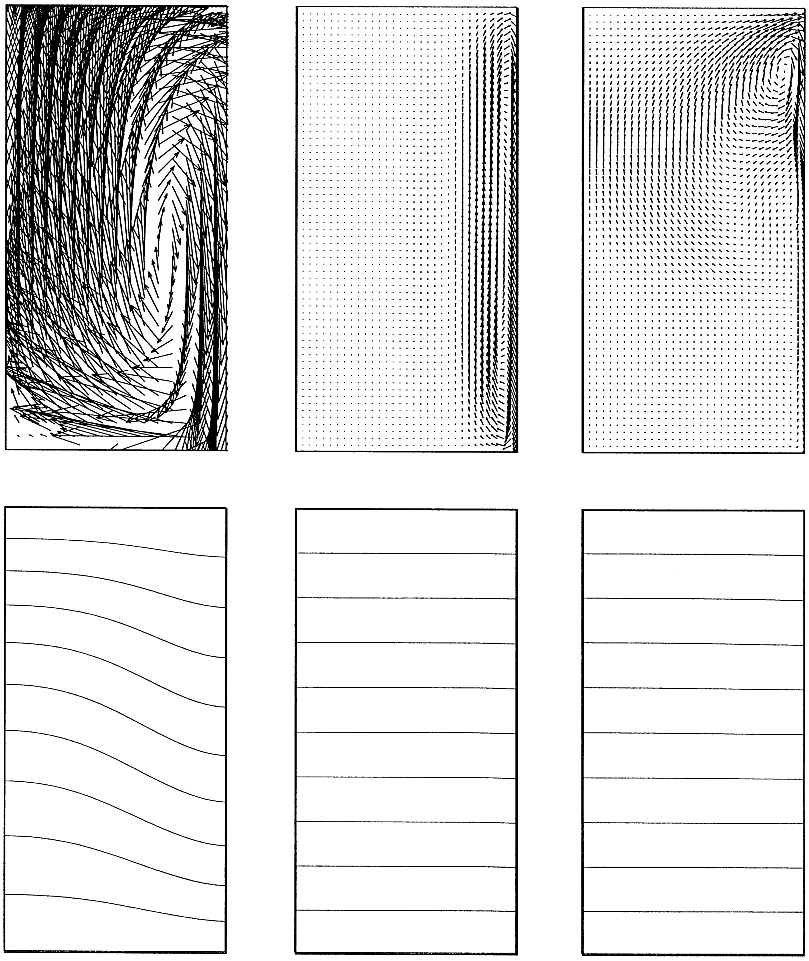

Fig. 4. The flow velocity (upper) and temperature distributions (lower) in the case of the designed magnetic field produced by two coils (right) compared with the case without magnetic field (left) and the case of the longitudinal magnetic field (middle) for $\mathrm{Pr}=0.01$, $\mathrm{Ma}=50$ and $\Gamma=1.0$. The space of dimensionless iso-temperature lines is $\Delta T=0.1$.

strong longitudinal magnetic field is applied, the flow intensity is reduced to a great extent, but the relatively strong convective recirculation still persists along the free surface. The difference between the flow intensity in the core region and the one near the free surface is obvious. It can also be proved by the distortion of the temperature distribution near the free surface. In the case of the designed magnetic field produced by two coils, the reduced weak and uniform flow on most part of the free surface can only drive a weak convective recirculation at the corner near the hot end. It may be expected to result in a better impurity mixture in the body of the melt zone compared with the case of the longitudinal magnetic field. Moreover, the flow intensity in front of the cold end is weak and relatively more uniform as shown in Fig. 5 which results in the linear temperature distribution there. In other words, the damped flow field structure is more suitable compared with the case of the longitudinal magnetic field.

In the case of the designed magnetic field produced by two coils, the merits of the magnetic damped flow structure are obvious, but the flow intensity near the hot end is not reduced enough, so the magnetic field produced by three coils is

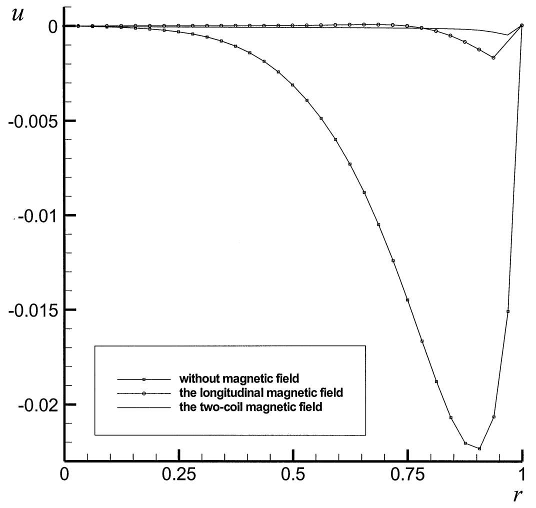

Fig. 5. The profiles of the radial flow velocity at $z = 0.015625$, which is very close to the cold melt-rod interface, for the cases without magnetic field, with the longitudinal magnetic field and with the designed magnetic field produced by two coils.

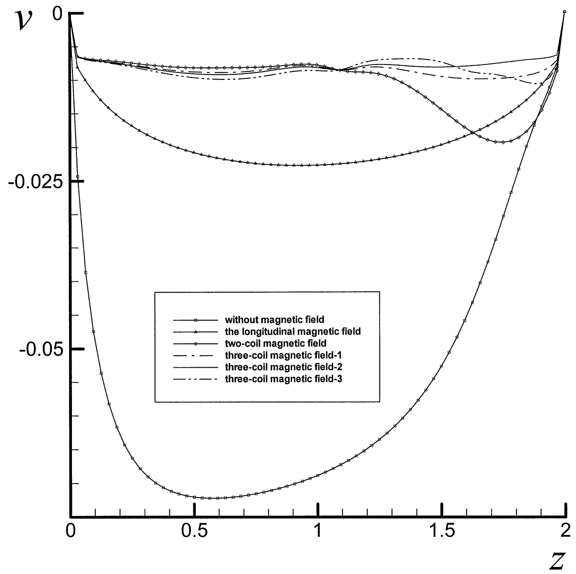

Fig. 6. The profiles of the flow velocity on the free surface velocity v in the cases of the designed magnetic field produced by three coils when the coils are located at $z = 0.0$, $z = 1.1$ and $z = 2.4$; (2) $z = 0.0$, $z = 1.1$ and $z = 2.0$ (3) $z = 0.0$, $z = 1.1$ and $z = 1.6$, respectively for $\mathrm{Pr} = 0.01$, $\mathrm{Ma} = 50$ and $\Gamma = 1.0$.

designed based on the previous study. It can be seen that the relative position of the third coil is also important for the overall magnetic damping effects (Fig. 6) on the flow near the free surface, especially the part near the hot end. The magnetic damping effects on the flow velocity on the free surface are adjusted best when the coils are located at $z = 0.0$, 1.1 and 2.0 respectively (the solid line in Fig. 6). In this case, the profile of the reduced flow velocity on the free surface is almost straight by the further reduction near the hot end. It results in a weaker and more uniform damped flow field and a linear temperature distribution which is close to a pure thermal conduction case (Fig. 7).

To check the validity of the designed magnetic field in the case of the large Marangoni number, the effects of the designed magnetic fields on reducing the flow velocity and temperature distribution non-uniformity, when $\mathrm{Ma} = 0.5 \times 10^3$, are simulated as shown in Fig. 8. The results show that the variation principles of the flow velocity and temperature distribution under the magnetic fields are similar to the case of the relatively small Marangoni number.

From the study above, it can be seen that to gain the suitable flow structure which helps to reduce the radial macro-segregation while damping the thermocapillary convection, the application of the designed magnetic fields produced by electrical coils to reduce the flow near the free surface is really attractive.

4. Discussion

In the present paper, the magnetic fields produced by electrical coils are designed for damping the thermocapillary convection in a floating half-zone in microgravity. The fields are designed specially to reduced the flow near the free surface and then in the melt zone by adjusting the longitudinal coil positions close to the melt zone. The effects of the designed magnetic fields on reducing the flow velocity and temperature distribution non-uniformity are stronger than those of the case of uniform longitudinal magnetic field obtained by numerical simulation, particularly at the melt–rod interface. It gives the fundamental insights into the heat and mass transfer control at

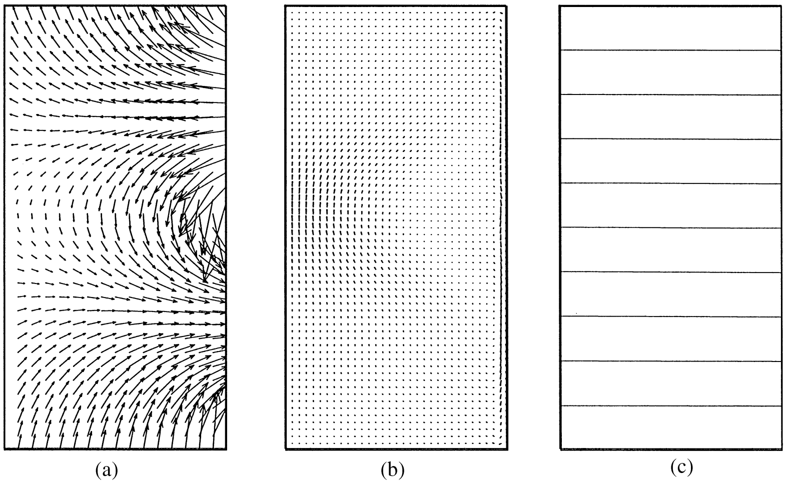

Fig. 7. (a) The magnetic field schematic diagram, (b) the flow velocity and (c) temperature distribution in the case of the designed magnetic field produced by three coils for $\mathrm{Pr}=0.01$, $\mathrm{Ma}=50$ and $\Gamma=1.0$. The space of dimensionless iso-temperature lines is $\Delta T=0.1$.

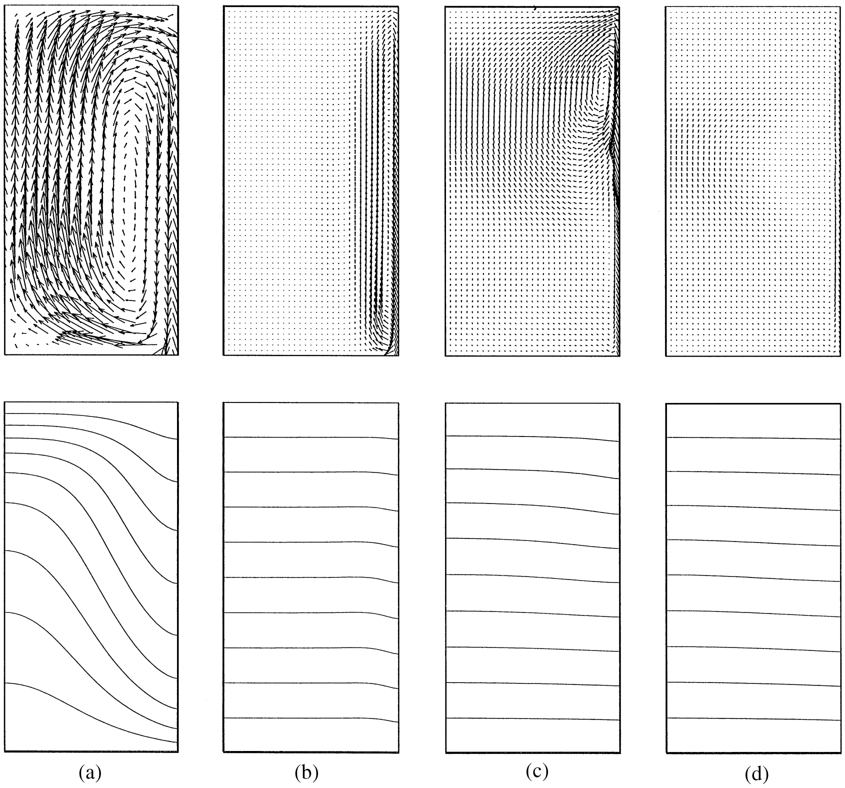

Fig. 8. The flow velocity (upper) and temperature distributions (lower) in the case of the designed magnetic fields produced by two coils (c) and three coils (d) compared with the case without magnetic field (a) and the case of the longitudinal magnetic field (b) for $\mathrm{Pr}=0.01$, $\mathrm{Ma}=0.5\times10^3$ and $\Gamma=1.0$. The space of dimensionless iso-temperature lines is $\Delta T=0.1$.

the solidification interface by the magnetic field design for crystal growth by the floating zone method.

The main idea of the present paper is to locate the coil as closely to the free surface as possible, and the thermocapillary convection driven from the free surface can be reduced obviously near the source and then in the floating zone. The results of the calculation show that the approach of the magnetic field design can reduce the thermocapillary convection. On the other hand, from a practical viewpoint, the high temperature melt of the floating half-zone prevents the coils from being placed too closely to the free surface of the melt. A careful design should be applied in order to use the idea of magnetic field design in practice. The space experiment of semiconductor crystal growth has been performed for a rod of 2″ in diameter [15], so, as an example, we adopted the radius of semiconductor and then the free surface location at $R_0 = 4$ cm, and the radius of the electrical coils located at $1.5R_0 = 6$ cm for producing the designed magnetic field as discussed in the present paper. In this case, there is enough room to arrange the coils with enough current such as $I_0 = 10^4$ A.

The floating zone method is beneficial for high-quality semiconductor production on the ground, but the gravity limits the diameter of the sample and the buoyancy convection may induce the concentration distribution non-uniformity in the sample. The microgravity environment reduces greatly the buoyancy convection, and the thermocapillary convection may also be oscillatory in the case of larger temperature difference or the Marangoni number. Therefore, introducing a magnetic field to improve the velocity and concentration distributions of the sample is important even in microgravity environment. The conclusion of the present paper shows that the effect of a designed magnetic field will be better than that of the longitudinal magnetic field, which is usually adopted. It should be noted that a simplified model to proper the idea of designed magnetic field is discussed in the present paper, and more analyses to improve the simplified model to relate the practice are necessary, and will be discussed elsewhere. Moreover, further study on the effect of the designed magnetic field on the concentration distribution is necessary.

Acknowledgements

This research was supported by the project 95-yu-34 of the Ministry of Science and Technology of China and by grant (19789201) of the National Natural Science Foundation of China.

References

[1] N.de. Leon, J. Guldberg, J. Salling, J. Crystal Growth 55 (1981) 406.
[2] G.D. Robertson Jr., D.J. O'Connor, J. Crystal Growth 76 (1986) 111.
[3] A. Croll, P. Dold, K.W. Benz, J. Crystal Growth 137 (1994) 95.
[4] R.W. Series, D.T.J. Hurle, J. Crystal Growth 113 (1991) 305.
[5] C.E. Chang, W.R. Wilcox, J. Crystal Growth 28 (1975) 8.
[6] C.H. Chun, W. Wuest, Acta Astronautica 5 (1978) 681.
[7] D. Schwabe, A. Scharmann, J. Crystal Growth 46 (1979) 125.
[8] F. Preisser, D. Schwabe, A. Scharmann, J. Fluid Mech. 126 (1983) 545.
[9] Y. Kamotani, S. Ostrach, M. Vargas, J. Crystal Growth 66 (1984) 83.
[10] W.R. Hu, H.T. You, C.H. Cao, Science in China A 4 (1992) 383.
[11] W.R. Hu, J.Z. Shu, R. Zhou, Z.M. Tang, J. Crystal Growth 142 (1994) 379.
[12] C.W. Lan, J. Crystal Growth 169 (1996) 269.
[13] D.B. Spalding, Int. J. Numer. Meth. Eng. 4 (1972) 551.
[14] S.V. Patankar, in: Advanced Computational Heat Transfer and Fluid Flow, Graduate Student Course 8352 of Mechanical Engineering Department at University of Minnesota, USA.
[15] E.V. Markov, V.Yu. Antropov, V.M. Biryukov, V.A. Goncharov, Yu.N. Dyakov, V.A. Pilgoon, V.A. Pesikov, V.P. Chegnov, A.I. Ivanov, V.P. Nikitsky, in: V.S. Avduyevsky, V.I. Polezhaev (Eds.), Proceedings of the Joint X th European and VIth Russian Symposium on Physical Sciences in Microgravity, St. Petersburg, Russia, Vol. 2 (1997) 11.