Magnetic Damping of Axisymmetric Thermocapillary Convection in Float Zones in Microgravity

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Introduction

IN the floating-zone process, surface tension holds a small body of liquid between a melting polycrystalline feed rod and a coaxial growing crystal. On Earth, the size of the single crystal is limited by the balance between the hydrostatic pressure and surface tension of the melt, whereas, in space, the size of the crystals that can be grown is much larger. With the residual acceleration as low as 10^{-3}–10^{-4} g, buoyant convection is negligible, and thermocapillary convection is dominant and causes two cells of circulation with flow along the free surface from the hotter middle circumference of the free surface to the colder circumferences at the feed rod and crystal.

Numerical simulations of thermocapillary convection in the floating-zone process were performed by Chang and Wilcox,[1] who reported unsteady thermocapillary convections in their calculations for small temperature differences along the free surface. In commercial applications, temperature differences along the free surface are large and cause unsteady conditions in the melt that produce undesirable dopant striations in the single crystal.

Robertson et al.[2] and Cröll et al.[3] grew nearly striation-free crystals using a strong, uniform, axial magnetic field in their float zone experiments. Müller and Rupp[4] presented numerical simulations that verified these experimental findings, and they attributed the improved crystal quality to the magnetic suppression of the unsteady thermocapillary convection. Series and Hurle[5] reviewed the benefits of magnetic fields in semiconductor crystal growth.

We present numerical and asymptotic solutions of the thermocapillary convection in floating zones with a strong axial magnetic field under axisymmetric conditions. Comparisons of the numerical and asymptotic solutions are made and asymptotic behaviors are discussed.

Problem Formulation

We consider the axisymmetric thermocapillary convection in a cylindrical liquid floating zone that has a height and diameter of $2L$, and that lies between the coaxial feed rod and crystal. The cylindrical coordinates, r and z, have been normalized by L, and are positioned at the center of the cylinder. The feed rod and crystal are treated as electrical insulators, the temperature at both liquid–solid interfaces is the solidification temperature T_s^*, and there is a heat flux into the fixed free surface at $r = 1$, which varies parabolically with z, which has been used to model optically heated float zones.[4] There is a uniform dc magnetic field B, which is parallel to the z axis.

The magnetic Reynolds number $R_m = \mu_p\sigma UL$ is the characteristic ratio of the induced to the applied magnetic field strengths that is much less than one for semiconductors. Hence, we neglect the induced magnetic field. Here, μ_p and σ are the magnetic permeability and electrical conductivity of the liquid. Khine and Walker[6] present the appropriate characteristic velocity for magnetically damped thermocapillary convection, $U = (-\mathrm{d}\Gamma/\mathrm{d}T^*)\Delta T^*/BL(\sigma\mu)^{1/2}$. Here, the surface tension Γ, is a linearly decreasing function of increasing dimensional temperature.* For optical heating in the mirror furnace, the maximum heat flux q^* occurs near the center of the free surface at $r = 1$, $z = 0$. Following Müller *et al.*,[4] we define our characteristic temperature difference as $\Delta T^* = q^*L/k$. Here, k and μ are the thermal conductivity and viscosity of the liquid. For a typical GaAs floating zone process with $\Delta T^* = 15$ K and $B = 0.5$ T, $U = 5$ mm/s. For molten GaAs, $\sigma = 6.5E5(\Omega m)^{-1}$, $\rho = 5.71E3$ kg/m^3, $\mu = 2.78E-3$ kg/ms, $\mathrm{d}\Gamma/\mathrm{d}T^* = -1.8E-4$ N/mK, and $k = 14$ W/mK. We have taken $L = 0.0254$ m.

The governing nondimensional equations are the incompressible continuity, the Navier–Stokes equations with a magnetic body force $(-\hat{\boldsymbol{e}}_r v_r)$, and the energy equation:

$$\nabla\cdot\boldsymbol{v} = 0 \tag{1a}$$

$$N^{-1}\frac{\mathrm{D}\boldsymbol{v}}{\mathrm{D}t} = -\nabla P - \hat{\boldsymbol{e}}_r v_r + Ha^{-2}\nabla^2\boldsymbol{v} \tag{1b}$$

$$Pe\frac{\mathrm{D}T}{\mathrm{D}t} = \nabla^2 T \tag{1c}$$

Here, the velocity vector $\boldsymbol{v} = (v_r, v_z)$ is normalized by U, the pressure P is normalized by σUB^2L, the temperature $T = (T^* - T_s^*)/\Delta T^*$, and t is time normalized by L/U. The interaction parameter $N = \sigma B^2L/\rho U$, the Hartmann number $Ha = BL(\sigma/\mu)^{1/2}$, and the Péclet number $Pe = UL/\kappa$. The parameters ρ and κ are the density and thermal diffusivity of the liquid, respectively. With the Prandtl number $Pr = 0.0675$ for GaAs, $Pe = Ha^2Pr/N$.

We introduce the stream function $\psi(r, z, t)$ with $v_r = r^{-1}\partial\psi/\partial z$ and $v_z = -r^{-1}\partial\psi/\partial r$, to satisfy Eq. (1a), and we eliminate the pressure by cross-differentiating and subtracting Eqs. (1b), the momentum equations, which gives a fourth-order, nonlinear, transient equation in $\psi(r, z, t)$. The boundary conditions are

$$\psi = 0 \tag{2a}$$

$$\frac{\partial^2\psi}{\partial r^2} - \frac{\partial\psi}{\partial r} = Ha\frac{\partial T}{\partial z} \tag{2b}$$

$$\frac{\partial T}{\partial r} = 1 - z^2 \quad \text{at} \quad r = 1 \tag{2c}$$

$$\psi = 0 \tag{2d}$$

$$\frac{\partial\psi}{\partial z} = 0 \tag{2e}$$

$$T = 0 \quad \text{at} \quad z = \pm 1 \tag{2f}$$

$T(r, z, t)$ and $\psi(r, z, t)$ were computed numerically by the Chebyshev spectral collocation method by integrating forward in time with a third-order-accurate semi-implicit Adams–Moulton scheme.

One of our objectives was to investigate the possibility of an instability with transition from steady to periodic axisymmetric thermocapillary convection. For each value of Ha, we first set N to a large value, so that the nonlinear terms in Eqs. (1b) and (1c) had negligible effects. The interaction parameter N was gradually reduced with $Pe = Ha^2Pr/N$ for each simulation starting from an initially perturbed condition. Fixing the values of Ha corresponds to fixing the applied magnetic flux

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density, and gradually decreasing the value of N corresponds to increasing q^* and U, thus increasing the nonlinear contributions of inertia and heat convection. No axisymmetric periodic thermocapillary convection was found for any value of Ha. We found that there was a critical value of N for each value of Ha below which the disturbed flow would not decay to a steady state and the disturbance would grow exponentially.

Asymptotic Formulation

In a former paper,[7] we presented the asymptotic formulation of a planar domain with a fixed free-surface temperature difference. Here, we consider the cylindrical domain with a prescribed parabolic heat flux and present the steady-state asymptotic solutions of Eqs. (1) in $0 \le r \le 1$ and $0 \le z \le 1$.

We assume that B is sufficiently large that $Ha >> 1$ and $N >> 1$. The subregions are the inviscid, inertialess core c, the Hartmann layer h with an $\mathcal{O}(Ha^{-1})$ thickness at $z = 1$, the parallel layer p with an $\mathcal{O}(Ha^{-1/2})$ thickness adjacent to the free surface at $r = 1$, and the intersection region I with $\mathcal{O}(Ha^{-1/2}) \times \mathcal{O}(Ha^{-1})$ dimensions at $r = 1$, $z = 1$.

The temperature in the core is governed by $\nabla^2 T_{ck}(r, z) = 0$, where the subscript c denotes the core and k is the kth term in the asymptotic expansion. The leading-order temperature ($k = 0$) is

$$T_{c0}(r, z) = \sum_{n=0}^{\infty} A_n \frac{I_0[(n + 1/2)\pi r]}{I_0[(n + 1/2)\pi]} \cos[(n + 1/2)\pi z] \qquad (3)$$

where I_0 is the modified Bessel function of zero order. The coefficients A_n are determined by matching the core temperature with the temperature in the parallel layer T_p.

We assume that $N = \alpha^{-1} Ha^{3/2}$, where α is a magnetic Marangoni number and is an $\mathcal{O}(1)$ parameter, so that viscous and inertial effects are comparable for the thermocapillary convection in the parallel layer. Analysis of the momentum equations gives the following boundary-layer equation:

$$\alpha \left(\frac{\partial^2 F}{\partial \xi^2} \frac{\partial^3 F}{\partial \xi^2 \partial z} - \frac{\partial^2 F}{\partial \xi \partial z} \frac{\partial^3 F}{\partial \xi^3} \right) = \frac{\partial^2 F}{\partial z^2} - \frac{\partial^4 F}{\partial \xi^4} \qquad (4)$$

where $F(\xi, z)$ is an integration function and the stretched coordinate $\xi = (r - 1)Ha^{1/2}$. Note that

$$\psi_p = \frac{\partial F}{\partial \xi} \qquad (5a)$$

$$P_p = -\frac{\partial F}{\partial z} \qquad (5b)$$

$$v_{rp} = \frac{\partial^2 F}{\partial \xi \partial z} \qquad (5c)$$

$$v_{zp} = -\frac{\partial^2 F}{\partial \xi^2} \qquad (5d)$$

When expanded, $\alpha = \rho(-\mathrm{d}\Gamma/\mathrm{d}T^*)\Delta T^*/B^{3/2}L^{1/2}\sigma^{3/4}\mu^{5/4}$, so that inertial effects are proportional to $B^{-3/2}$ or $Ha^{-3/2}$ and $L^{1/2}$ because $\Delta T^* = q^* L/k$.

The temperature and the flow problems are coupled in the boundary layer. Following the procedure discussed in our former paper,[7] we find the heat flux into the core is given by

$$\frac{\partial T_{c0}}{\partial r}(1, z) = (1 - z^2) + \gamma^2 \frac{\mathrm{d}}{\mathrm{d}z} \left\{ \frac{\partial T_{c0}}{\partial z}(1, z) \int_{-\infty}^{0} \left[\frac{\partial F_0}{\partial \xi}(\xi, z) \right]^2 \mathrm{d}\xi \right\} \qquad (6)$$

Here, we have introduced $Pe = \gamma Ha^{1/4}$, where γ is an $\mathcal{O}(1)$ parameter. Equation (6) represents the redistribution by the recirculating, parallel, boundary-layer flow of the parabolic heat flux that enters the free surface. The effects of curvature are evident once Eq. (3) is substituted into Eq. (6). The boundary conditions and matching conditions with the temperature in the stagnant core are

$$\frac{\partial F}{\partial \xi} = 0 \qquad (7a)$$

$$\frac{\partial^3 F}{\partial \xi^3} = \frac{\partial T_{c0}}{\partial z}(1, z) \quad \text{at} \quad \xi = 0 \qquad (7b)$$

$$F = 0 \quad \text{at} \quad z = 1 \qquad (7c)$$

$$F \to 0 \quad \text{as} \quad \xi \to -\infty \qquad (7d)$$

F is an odd function of z. We solve for F and A_n by the iterative method described in Ref. 7.

Results

The error in the asymptotic solution is $\mathcal{O}(Ha^{-1/2})$, so that the streamlines computed from the asymptotic analysis for $Ha = 200$, $N = 2000$, and $Pe = 1.35$ are virtually identical to the steady-state streamlines found by integrating the full equations (numerical), which are shown in Fig. 1. At $Ha = 200$, 100, and 50, the numerical $\psi_{max} = 0.14230$, 0.12652, 0.10525, and the asymptotic $\psi_{max} = 0.14102$, 0.13678, 0.11874, which correspond to errors of 0.9, 8.1, and 12.8 percent, respectively. The positions of ψ_{max} in the numerical and asymptotic analyses vary by less than a few percent.

Figure 2 compares the numerical and asymptotic nondimensional free-surface temperature distribution $T(1, z)$, and the nondimensional heat flux into the core evaluated at $r = r_0$, $\partial T/\partial r(r_0, z)$, for $Ha = 200$. Here, $r_0 = 1 - 3Ha^{-1/2}$, where $3Ha^{-1/2}$ is the radial width of the parallel layer that is between the core and the free surface. At $Ha = 200$, 100, and 50, $r_0 =$

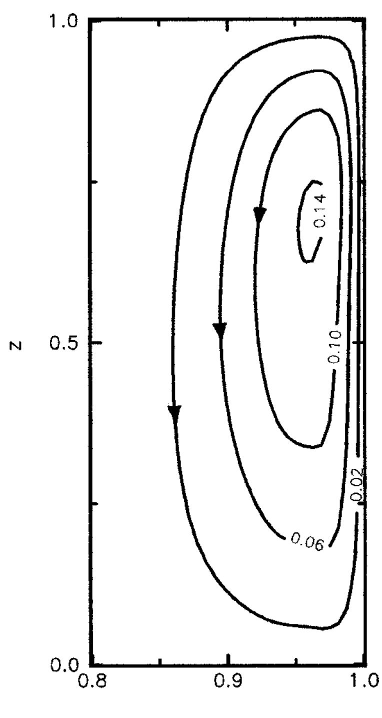

Fig. 1 Steady-state streamlines for $Ha = 200$, $N = 2000$, and $Pe = 1.35$ ($\alpha = 1.414$ and $\gamma = 0.359$).