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Numerical simulation of thermal and solutal Marangoni convection in a half floating zone with radiation effects under zero gravity

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1. Introduction

Marangoni convection is the flow along the interface between two fluids due to the variation of surface tension, which is mainly caused by the temperature and/or concentration gradients, namely thermal and/or solutal Marangoni convection. In a crystal growth system such as the floating-zone system, Marangoni convection occurs along the free surface of the melt, becomes unstable, and leads to the growth striations, whose instabilities have negative effects on the crystal quality. Therefore, it is important to know the mechanism of Marangoni convection during crystal growth. In order to shed light on Marangoni convection only, it is necessary to set the whole system under zero gravity to eliminate the natural convection caused by the gravity effect. In the previous study, Minakuchi *et al.*[1-2] investigated the mixed thermal and solutal Marangoni convection in the same direction in a half-zone system and found the augmented effects with the *m*-fold symmetry under large Marangoni numbers. Jin *et al.*[3] investigated the combined thermal and solutal Marangoni convection in the opposite direction in a half-zone system and defined the flow modes and critical transitions. These half-zone studies are based on the adiabatic free surface of a half floating zone.

However, in a real floating-zone system, the heating coils are placed outside the melt part, moving together with the growing crystal and providing the temperature distribution to the free surface of a full floating zone. Based on it, Jin *et al.*[4] investigated thermal and solutal Marangoni convection in a full floating zone to focus on the radiative effects on flow patterns and flow characteristics along the free surface. From this point of view, the radiation can affect the induced Marangoni flow and may change the flow mode correspondingly, especially in a half floating zone. Therefore, the radiation effects are investigated in a half floating zone at the given thermal and solutal Marangoni numbers with a series of ambient temperature in this research, considering both thermal and solutal Marangoni convections in the same and opposite direction.

2. Numerical methods

In a floating-zone system of Si_xGe_{1-x}, the floating zone is simplified as the liquid bridge, which is in a cylindrical shape with the assumption of the molten zone being an incompressible and Newtonian fluid. **Figure 1** shows the floating-zone system and the numerical model of a liquid bridge. The blue and yellow arrows in the melt stand for the direction of thermal and solutal Marangoni flows, respectively. The governing equations are the well-known continuity, momentum, energy, and mass transfer equations, which are solved by the PISO algorithm in the OpenFOAM. The mesh number applied in simulation is 40, 160, and 60 in the r, θ, and z-direction, respectively, with a total mesh number of 384,000. Thermal and solutal Marangoni numbers are defined as follows,

$$Ma_{\mathrm{T}} = \left|\frac{\partial\sigma}{\partial T}\right| \cdot \frac{\Delta T L}{\mu\nu} \quad (1) \qquad Ma_{\mathrm{C}} = \left|\frac{\partial\sigma}{\partial C}\right| \cdot \frac{\Delta C L}{\mu\nu} \quad (2)$$

where $\frac{\partial\sigma}{\partial T}$ and $\frac{\partial\sigma}{\partial C}$ are the surface tension coefficients of temperature and concentration, respectively. ΔT and ΔC are the temperature difference and Si concentration difference between the top and bottom plane, respectively. The temperature on the plane is considered at 1680K and 1720K. L(=0.005m) is the length of liquid bridge. μ is viscosity and ν is kinematic viscosity of the melt.

The Marangoni boundary conditions in the r, θ, and z-direction on the free surface are shown as (3)-(5).

$$v_r = 0 \tag{3}$$

$$\mu\left[r\frac{\partial}{\partial r}\left(\frac{v_\theta}{r}\right)\right] = \frac{1}{r}\left(\frac{\partial\sigma}{\partial T}\frac{\partial T}{\partial\theta} + \frac{\partial\sigma}{\partial C}\frac{\partial C}{\partial\theta}\right) \tag{4}$$

$$\mu\frac{\partial v_z}{\partial r} = \frac{\partial\sigma}{\partial T}\frac{\partial T}{\partial z} + \frac{\partial\sigma}{\partial C}\frac{\partial C}{\partial z} \tag{5}$$

The convective heat transfer in the ambience is negligible, and the temperature boundary condition on the free surface follows radiative heat transfer and is shown as,

$$-k\frac{\partial T}{\partial r} = \varepsilon\sigma_{\mathrm{SB}}(T^4 - T_{\mathrm{a}}^4) \tag{6}$$

where k(=64W/m·K) is the thermal conductivity of melt, ε(=0.3) is the emissivity, σ_{SB} is the Stefan-Boltzmann constant, and T_a is the ambient temperature. The ambient temperature can be either lower or higher than the plane temperature to focus on the conditions of heat loss and heat gain. Prandtl number and Schmidt number are 6.37×10^{-3} and 14.0, respectively. The governing equations and associated boundary conditions were solved by the PISO algorithm in the OpenFOAM.

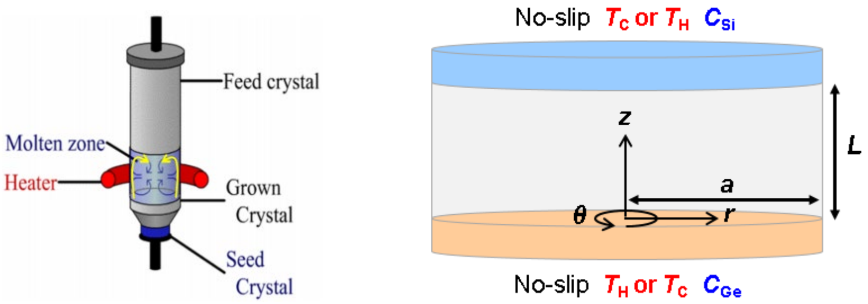

Fig. 1 The floating-zone system (Left) and simplified liquid bridge (Right).

3. Results and discussion

Figure 2 shows the snapshots of Si concentration distribution in the central r-θ plane from the top view at the height of 0.5L at Ma_C=1250 and Ma_T=2800 with different ambient temperature. When thermal and solutal Marangoni convections are in the same direction (a-f), the 3D rotating oscillatory flow is observed with symmetric azimuthal wave with m=7 at a low ambient temperature (T_a). The lower T_a gives rise to the indistinct azimuthal wave due to the strong heat loss (T_a=500K). However, the flow pattern remains 2D axisymmetric at a higher T_a. With the increase of T_a from 1500K to 2000K, there is a transition of the flow mode from oscillatory rotating flow to axisymmetric flow when the heat gain overwhelms the heat loss.

When thermal and solutal Marangoni convections are in the opposite direction (g-l), although the flow pattern behaves chaotic, the flow mode is slightly different under the conditions of heat loss and heat gain. Compared to the flow pattern with heat loss (g-i), the exterior outline of azimuthal wave becomes distinct at a higher T_a, especially the quasi-symmetric azimuthal wave with m=4 at T_a=3000K under the condition of heat gain.

Figure 3(a) shows the vertical velocity with time at the sampling point of (0.99a, 0, 0.50L), which is the middle point on the free surface, at Ma_C=1250 and Ma_T=2800 with thermal and solutal Marangoni convection in the same direction. Corresponding to **Figure 2(a-f)**, the flow becomes periodic in the oscillatory rotating flow at a lower T_a (no more than 1500K) after t=500s, while it remains constant at a higher T_a (no less than 2000K). **Figure 3(b)** shows the vertical velocity where thermal and solutal Marangoni convections are in the opposite direction. Under the condition of heat loss, the fluctuation is much stronger and more complicated than that of heat gain. On the whole, the magnitude of vertical velocity tends to decrease with the increase of T_a under the condition of heat gain for both thermal and solutal Marangoni convection in the same and opposite direction.

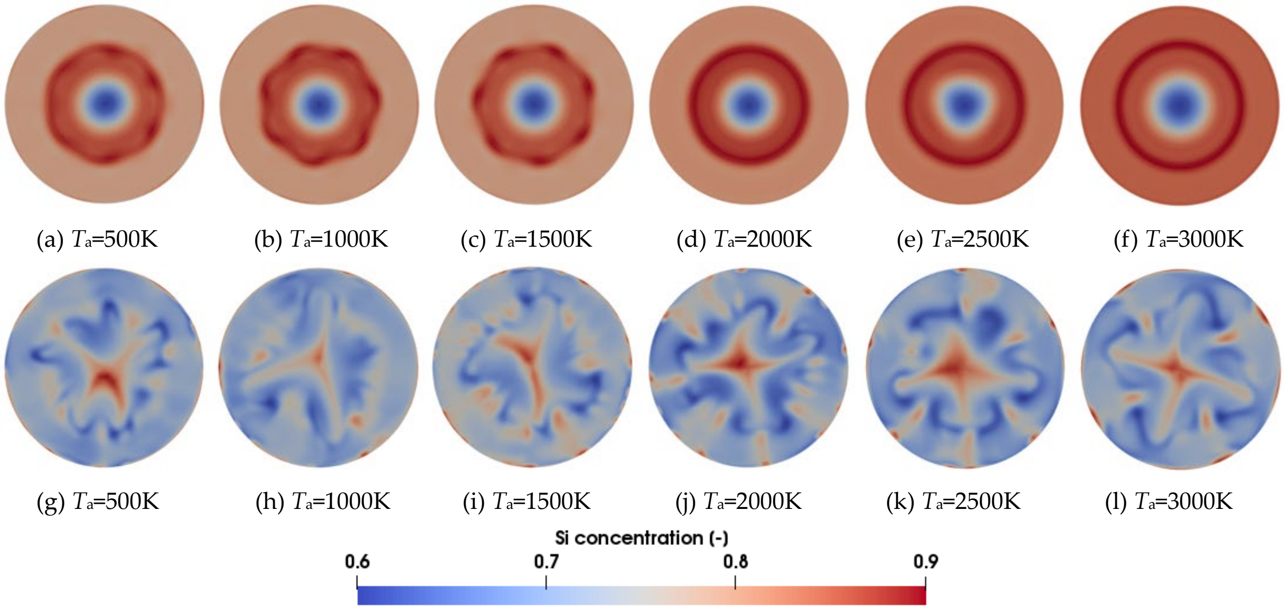

Fig. 2 Snapshots of Si concentration distribution in the central r-θ plane at the height of 0.5L at Ma_C=1250 and Ma_T=2800 with different ambient temperature. Thermal and solutal Marangoni convection are in the same direction in (a)-(f), and in the opposite direction in (g)-(l).

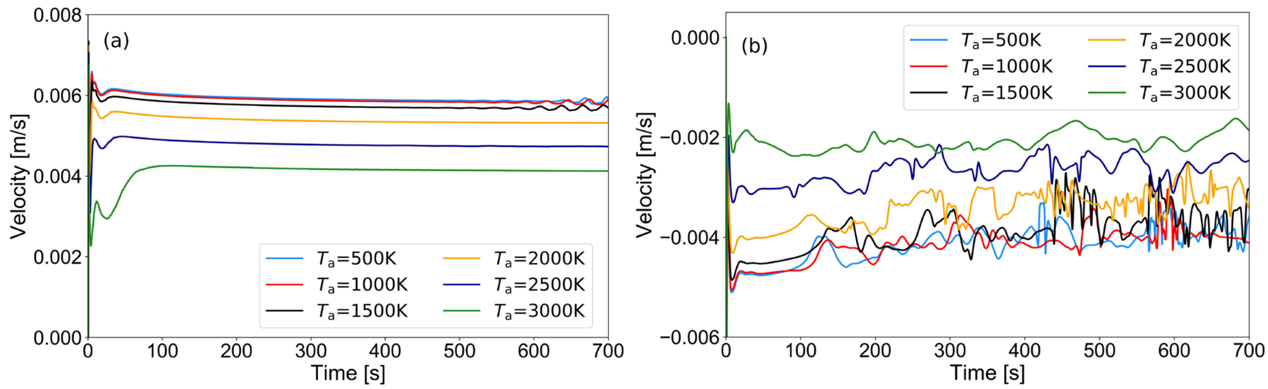

Fig. 3 Vertical velocity with time at the sampling point of (0.99a, 0, 0.50L) at Ma_C=1250 and Ma_T=2800 with different ambient temperature. (a) Thermal and solutal Marangoni flows are in the same direction. (b) Thermal and solutal Marangoni flows are in the opposite direction.

Figure 4 shows the vertical velocity along the free surface at Ma_C=1250 and Ma_T=2800. **Figure 4(a)** describes thermal and solutal Marangoni convections are in the same direction at different ambient temperature. When T_a is ranged from 500K to 2000K, the profiles of vertical velocity are similar, and velocity increases with the height and reaches at the maximum at around 0.003m to 0.004m, and then decreases to zero near the top plane. As T_a increases to 2500K, the maximum moves to 0.045m, which means the flow strength is enhanced near the top plane. Contrary to the others, as T_a further reaches 3000K, there is a reverse flow near the bottom plane because the highest temperature point on the free surface is slightly higher than the bottom plane. Higher than the point, the velocity increases upwards with a maximum value at around 0.045m. Meanwhile, at the height of 0.025m (z/L=0.50), it is obvious that with the increase of T_a, the flow strength decreases, especially under the condition of heat gain, which is in agreement with **Figure 3(a)**. **Figure 4(b)** describes thermal and solutal Marangoni convections are in the opposite direction. Compared to the combined flows in the same direction, the profiles become slightly complicated in the opposite direction. Although the velocity profile owns similar tendency with the increase of height on the free surface, the maximum value occurs closer to the bottom plane as T_a increases gradually. At T_a equals 3000K, due to a second weak vortex appears near the top plane, there is a reverse increase in vertical velocity around 0.035m to 0.045m.

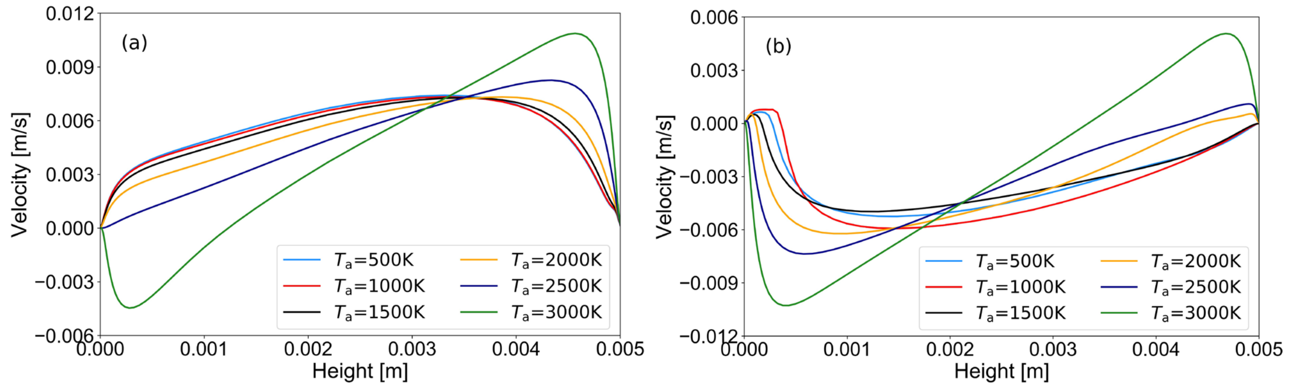

Fig. 4 Vertical velocity along the free surface at Ma_C=1250 and Ma_T=2800 with different ambient temperature. (a) Thermal and solutal Marangoni flows are in the same direction. (b) Thermal and solutal Marangoni flows are in the opposite direction.

4. Conclusions

Numerical simulation of thermal and solutal Marangoni convection in a half floating zone at Ma_C=1250 and Ma_T=2800 with radiation effects of heat loss and heat gain under zero gravity was investigated.

(1) In the same-direction thermal and solutal Marangoni flows, there is a transition of flow pattern from oscillatory rotating flow to axisymmetric flow with the increase of T_a.

(2) In the opposite-direction thermal and solutal Marangoni flows, the flow pattern is less chaotic and complicated under the condition of heat gain.

(3) Under the condition of heat gain, the vertical velocity tends to decrease with the increase of T_a. Although in the opposite-direction flow, the flow becomes chaotic, it also follows this tendency.

(4) At a higher T_a, there is a reverse flow near the plane area, which means a second vortex forms due to the temperature difference near the plane.

Acknowledgments

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