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Numerical Simulation of Thermal and Solutal Marangoni Convection in a Full Floating Zone with Radiative Heat Transfer 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.

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. Given this situation, the radiative heat transfer induces the main flow. Meanwhile, the consideration of ambient temperature is necessary for creating the real surroundings of the liquid bridge. There are several heating models outside the floating-zone around the equatorial plane, among which the Gaussian profile is suitable for the assumption of heating coils in this research. In this profile, the equatorial plane receives the highest heat from the surroundings and the free surface receives less heat near the top and bottom plane. The objective of this research is to investigate thermal and solutal Marangoni convection in a full floating-zone with radiative heat transfer under zero gravity by numerical simulation.

2. Numerical methods

In a floating-zone system of Si_xGe_{1-x}, the floating-zone can be simplified as the liquid bridge, which is in a cylindrical shape with the assumption of incompressible and Newtonian fluid inside the zone. **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 thermal and solutal Marangoni flow, 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 120 in the r, θ, and z-direction, respectively, with a total mesh number of 784,000. 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 ΔT is the temperature difference between the maximum temperature on the free surface and plane temperature and ΔC is the Si concentration difference between the top and bottom plane.

The temperature boundary condition on the free surface is shown below,

$$-k\frac{\partial T}{\partial r} = \varepsilon\sigma_{\mathrm{SB}}(T^4 - T_{\mathrm{a}}^4) \quad (3)$$

where k is the thermal conductivity of melt, ε is the emissivity, σ_{SB} is the Stefan-Boltzmann constant, and T_a is the ambient temperature. As for the ambient temperature, the Gaussian profile regarded as a heat source is assumed outside the floating-zone system in the vertical direction, which is considered to be

$$T_a = T_C + (T_H - T_C)exp\left[-\left(\frac{z-L/2}{a}\right)^2\right] \quad (4)$$

where T_C is the melting point temperature, T_H is the maximum temperature on the free surface, L is the length of the liquid bridge, and a is the typical width of the distribution (a = 0.003m). Due to the extension of the liquid bridge, the aspect ratio (A_s=L/R) increases to 1. Prandtl number and Schmidt number are 6.37×10^{-3} and 14.0, respectively.

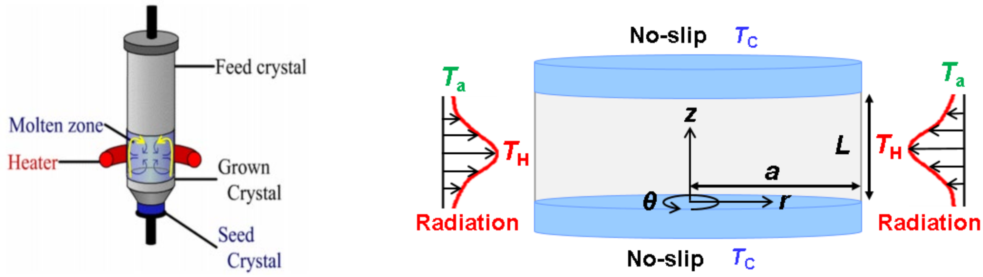


Fig. 1 The floating-zone system(Left) and simplified liquid bridge(Right).

3. Results and discussion

Figure 2 shows the temperature distributions on the free surface at different Ma_T, which are in the Gaussian profile. The temperature differences between the maximum and minimum value are 20K, 40K, and 60K at Ma_T=700, 1400, and 2100 respectively. In this profile, the heat is concentrated on the equatorial plane of the liquid bridge. These temperature differences on the free surface give rise to the thermal Marangoni convection.

Figure 3 shows the vertical velocity on the free surface at Ma_C=1072 and Ma_T=700, 1400, and 2100, which are in a smooth line. Higher velocity appears around the height of 0~0.2L and 0.8L~L, where strong vortexes form in these regions. Vertical velocity fluctuates around zero when the sampling point comes to the middle height of the liquid bridge (z/L=0.5). Therefore, from the bottom to the top plane, the vertical velocity undergoes a sharp increase to the peak then reduces to zero, and a reverse increase to the peak appears again near the top plane.

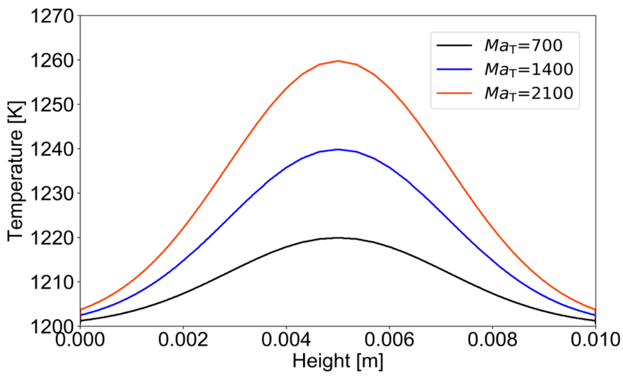


Fig. 2 Temperature distribution on the free surface.

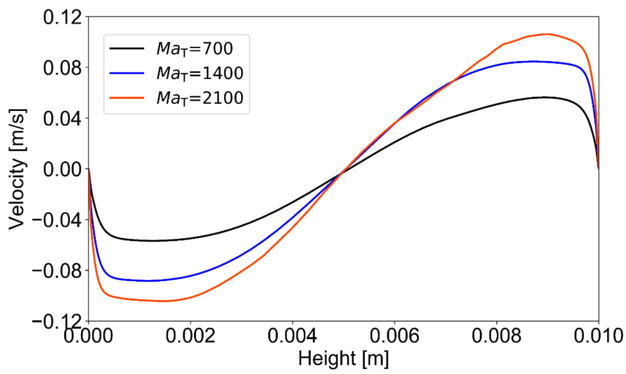
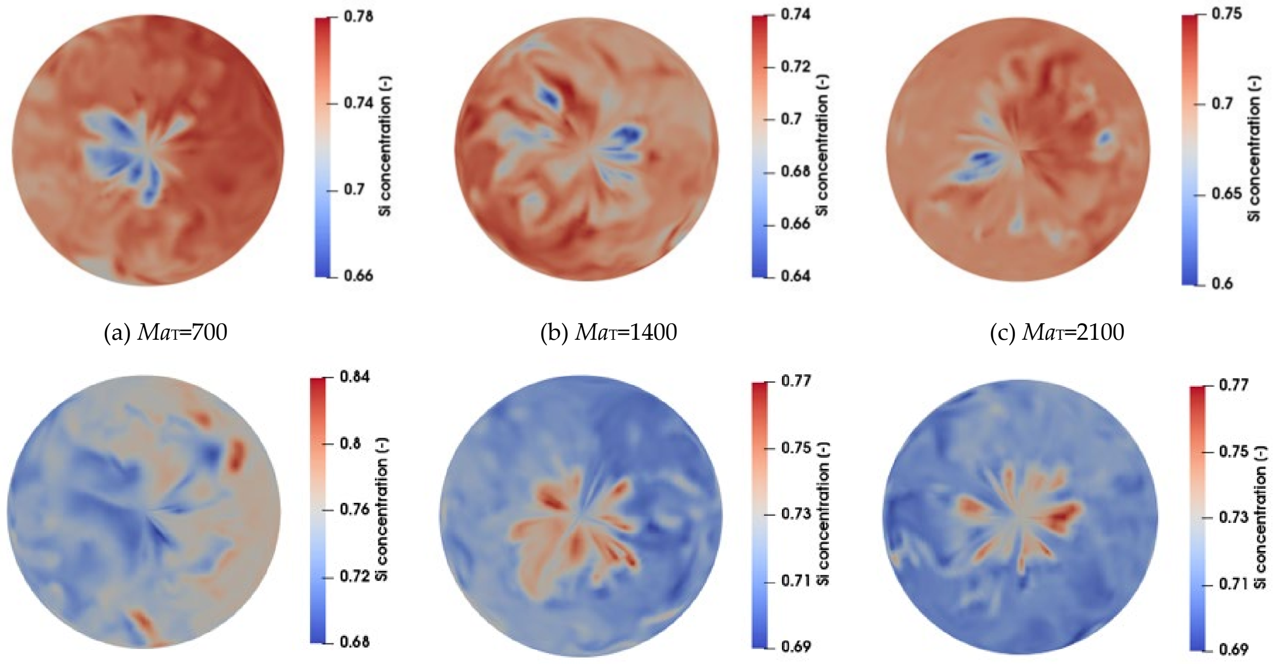


Fig. 3 Vertical velocity on the free surface at Ma_C=1072.

Figure 4 shows the snapshots of concentration distribution along the cutting r-θ plane from the top view at the height of 0.25L and 0.75L at Ma_C=1072 and Ma_T=700, 1400, and 2100. **Figure 4(a)-(c)** are taken from the height of 0.25L, where thermal and solutal Marangoni convections flow in the opposite direction in this region (Lower part of the liquid bridge). Slight flow pattern can be observed at a smaller Ma_T (Ma_T=700). However, the flow pattern behaves chaotically at Ma_T=1400 or 2100. In view of the flow patterns, we may guess in this region the flow pattern varies due to different Marangoni numbers. Meanwhile, **Figure 4(d)-(f)** is taken from the height of 0.75L, where thermal and solutal Marangoni convections flow in the same direction (Upper part of the liquid bridge). In this region, at a larger Ma_T (Ma_T=1400 or 2100), the azimuthal wave pattern can be observed, which means the augmented effect of thermal and solutal Marangoni convection gives rise to the flow instability. However, in order to make a clear definition of the flow mode, longer-time calculation and more cases (i.e. different Ma_C and Ma_T) are required for further investigation.



(a) Ma_T=700 (b) Ma_T=1400 (c) Ma_T=2100

(d) Ma_T=700 (e) Ma_T=1400 (f) Ma_T=2100

Fig. 4 Snapshots of Si concentration distribution at Ma_C=1072 and different Ma_T at the r-θ cutting plane from the top view at the height of 0.25L (a-c) and 0.75L (d-f).

4. Conclusions

Numerical simulation of thermal and solutal Marangoni convection in a full floating-zone was conducted and the cases of Ma_C=1072 and Ma_T=700, 1400, and 2100 were investigated.

(1) The temperature distribution on the free surface shows the Gaussian profile, with the equatorial plane receiving the most heat, which is the generation of thermal Marangoni convection on the free surface in this system.

(2) The vertical velocity on the free surface increases to the peak then decreases to 0 at the middle height of the liquid bridge and reversely increases to the peak again with the increase of height on the free surface.

(3) The characteristics of concentration pattern vary due to the different regions and the relationship of Ma_C and Ma_T, and longer-time calculation is necessary for the mode definition in further investigation.

Acknowledgments

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