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HZ内の温度差と濃度差マランゴニ対流の回転印加による非定常制御

Unsteady control of thermo-solutal Marangoni convection in a half-zone liquid bridge by applying rotation

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Abstract: The Floating Zone (FZ) method conducted under microgravity is a key technique for the growth of high-purity single crystals, playing an important role in semiconductor material production. During the fabrication of bulk SiGe single crystals using the FZ method, unstable Marangoni convection driven by temperature and concentration gradients can hinder uniform single crystal growth. In order to achieve a detailed understanding of the Marangoni convection structure and establish effective control strategies, this study analyzed the control of Marangoni convection by external forces, particularly through rotational control. It was found that applying rotation simultaneously with an increasing Marangoni number from zero (no flow) is more effective at suppressing Marangoni convection than applying rotation at a fixed Marangoni number (unsteady flow). The critical Marangoni number was observed to increase with increasing rotation speed. Furthermore, the transition from steady to unsteady flow can exhibit faster changes in wave number when rotation is applied, compared to the case without rotation.

Keywords: Floating Zone method, Marangoni convection, rotational control

1. Introduction

The Floating Zone (FZ) method conducted under microgravity is a key technology for the growth of high-purity single crystals and plays an important role, particularly in the production of semiconductor materials. During the fabrication of bulk Si/Ge single crystals by the FZ method, unstable Marangoni convection induced by temperature and concentration differences is known to hinder uniform single crystal growth. Therefore, for the successful production of Si/Ge single crystals, it is essential to understand and control the structure of Marangoni convection in the melt. The application of disc rotation and magnetic fields is found to be effective to suppress unsteady thermal Marangoni convection[1-2].

In this study, the half-zone (HZ) model, which is widely employed in Marangoni convection research, was adopted (see, for instance, Refs[3-4]. In this study, the half-zone (HZ) model, which is widely employed in Marangoni convection research, was adopted (see, for instance, Refs3-4). In order to control the thermal and solutal Marangoni convections occurring in the melt of a float-zone system, we have carried out numerical simulations to investigate the effects of disc rotation on thermo-solutal Marangoni convection in a liquid bridge under zero-gravity.

2. Analysis Method

In this study, Figure 1 was used as the analytical model. The sides are free surfaces, with the top disk set to a low temperature and the bottom disk set to a high temperature. Both the top and bottom disks were rotated at the same rotation speeds [ω] under steady rotation, with the rotation axis aligned with the z-axis. The rotation speeds were set to 1, 0.25, 0.1, and 0.05 rpm. The free surface height L was set to 5 mm and the radius a to 10 mm, giving an aspect ratio of $As=a/L=0.5$. In addition, a microgravity environment was assumed, and both the gas–liquid and solid–liquid interfaces were considered flat. The sampling pointis (r,θ,z)=(0.99a,0,0.5L). The basic analytical equations are the continuity equation (1), the Navier–Stokes equation (2), the energy equation (3), and the diffusion equation (4), all of which were discretized using the finite volume method. The equations are shown below.

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

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla u} = -\frac{1}{\rho}\nabla p + \nu \nabla^2 \boldsymbol{u} \tag{2}$$

$$\frac{\partial T}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} T = \alpha \nabla^2 T, \tag{3}$$

$$\frac{\partial C}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} C = D \nabla^2 C \tag{4}$$

The boundary condition for temperature was set constant at the lowest temperature on the top surface and the highest temperature on the bottom surface, and adiabatic at the free interface on the side boundary condition. The boundary condition for concentration was the same as the boundary condition for temperature. The boundary condition for velocity was the no slip condition for the top and bottom surfaces, while the Marangoni convection caused by the temperature and concentration difference was considered for the side surfaces. Marangoni number, which indicates the intensity of convection, is then given below.

$$\boldsymbol{Ma_T} = -\frac{\boldsymbol{\partial \sigma}}{\boldsymbol{\partial T}}\frac{\boldsymbol{\Delta T L}}{\boldsymbol{\mu v}}, \ \boldsymbol{Ma_C} = \frac{\boldsymbol{\partial \sigma}}{\boldsymbol{\partial C}}\frac{\boldsymbol{\Delta C L}}{\boldsymbol{\mu v}} \tag{5)-(6}$$

The physical properties of Si/Ge (Si_xGe_{1-x}) used in this study are listed in Table 1.

Table 1. Physical properties of Si_xGe_{1-x}

Kinematic viscosity $\boldsymbol{v}$	1.4×10^{-7} [m²/s]
Thermal Diffusion Coefficient $\boldsymbol{\alpha}$	2.2×10^{-5} [m²/s]
Diffusion coefficient $\boldsymbol{D}$	1.0×10^{-8} [m²/s]
Prandtl number $\boldsymbol{Pr}$	6.37×10^{-3} [-]
Schmidt number $\boldsymbol{Sc}$	14.0 [-]

The open source CFD software OpenFOAM is used. The governing equations (eq. 1-4) are discretized using the finite volume method, and the unsteady algorithm, PISO method, is used.

In this analysis, three cases are considered: without rotation while increasing the Marangoni number over time, with rotation at a fixed Marangoni number, and with rotation while increasing the Marangoni number over time. For the cases in which the Marangoni number increased over time without rotation, as well as those with rotation, the simulation time was set to 10,000s. In both cases, the Marangoni number increased Ma_C=0~1786 and Ma_T=0~3572 simultaneously. For the case with rotation at a fixed Marangoni number, the simulation time was set to 1000s. The Marangoni numbers were fixed at Ma_C=1696 and Ma_T=3394.

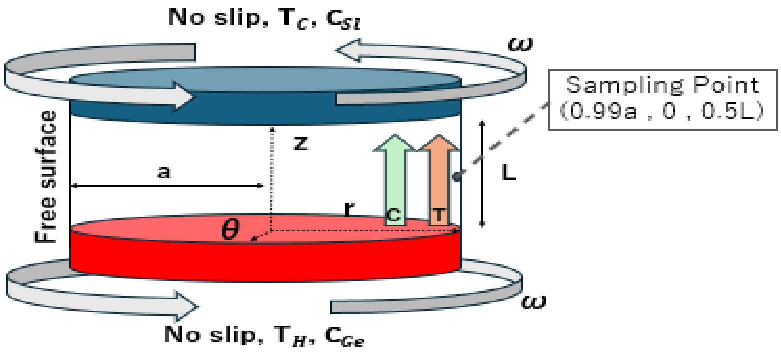

Figure 1. Geometry of the analytical liquid bridge.

3. Results and discussion

3.1 Comparison between cases without rotation and with rotation under a time-dependent increase in the Marangoni number

Figures 2 and 3 show the heightwise flow velocity and concentration distribution for the case without rotation. Figures 4 and 5 show the heightwise flow velocity and concentration distribution for the case with rotation (1rpm). As seen from Figure 3, as the Marangoni number increases, the convective structure in the melt changes from m = 5 → 6 → 7 (where m is the azimuthal wavenumber). In contrast, Figure 5 shows an axisymmetric convective structure throughout. This indicates that applying rotation suppresses Marangoni convection within the HZ.

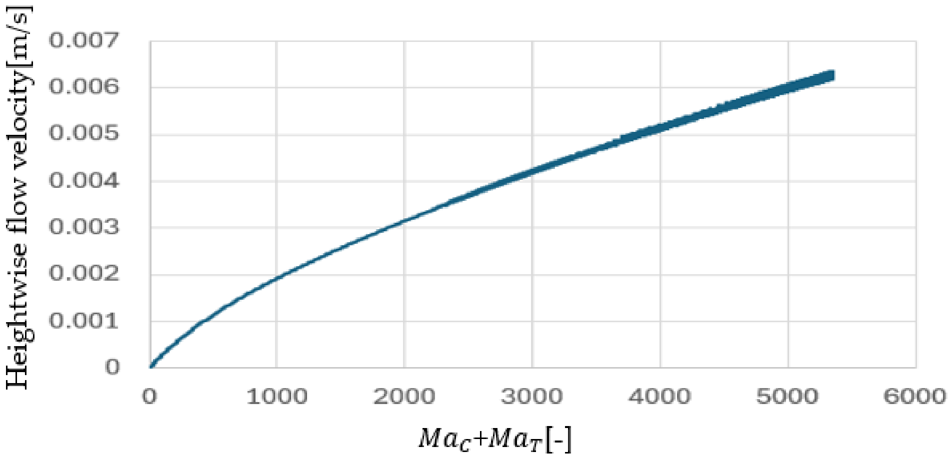

Figure 2. Heightwise flow velocity without rotation.

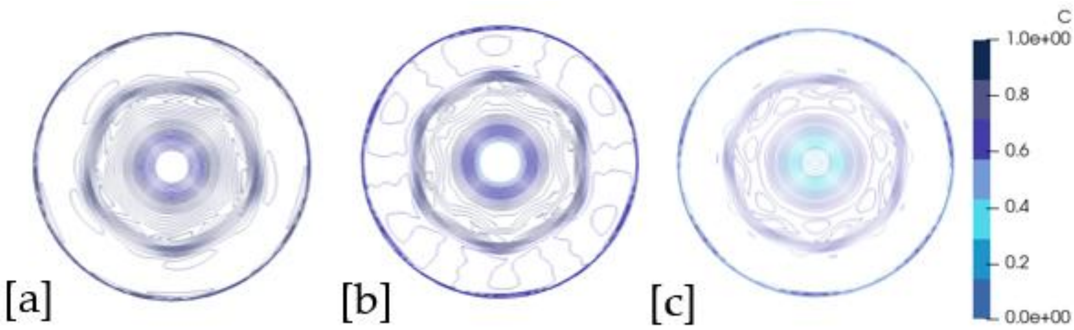

Figure 3. Convective structures at specific Marangoni numbers Ma_C+Ma_T=2151,m=5[a],Ma_C+Ma_T=3698,m=6[b],Ma_C+Ma_T=5090,m=7[c].

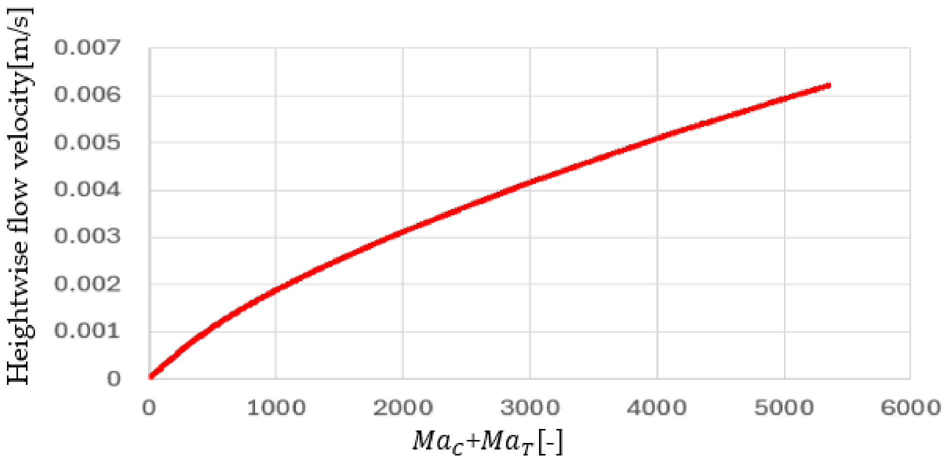

Figure 4. Heightwise flow velocity with rotation.

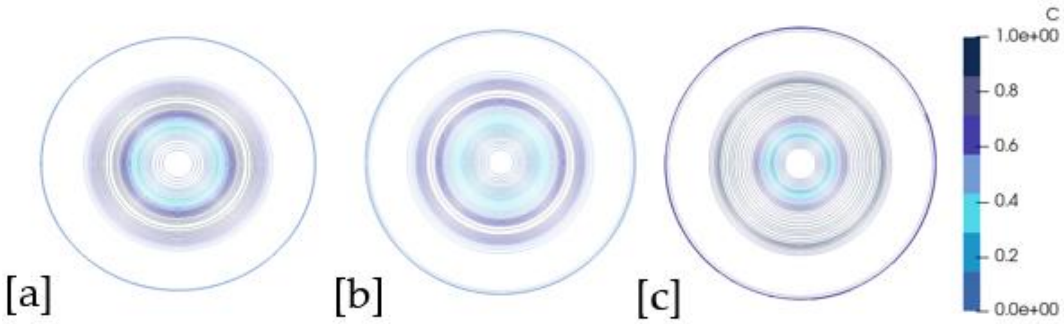

Figure 5. Convective structures at specific Marangoni numbers Ma_C+Ma_T=2151,m=5[a],Ma_C+Ma_T=3698,m=6[b],Ma_C+Ma_T=5090,m=7[c].

3.2 Comparison of rotating cases between a fixed Marangoni number and a time-dependent increase in the Marangoni number

Figure 6 shows the heightwise flow velocity and the convective structures at specific Marangoni numbers for the case with a fixed Marangoni number under rotation. The fixed Marangoni numbers are $\boldsymbol{Ma_C}$=1696 and $\boldsymbol{Ma_T}$=3394 , and the rotation speed is set to 1 rpm. In Figure 6, rotation was applied to unsteady Marangoni convection, so it was not possible to control it to steady state at a rotation speed of 1 rpm. This shows that even if rotation is applied to an unsteady flow, the effect of rotation in suppressing convection is small.

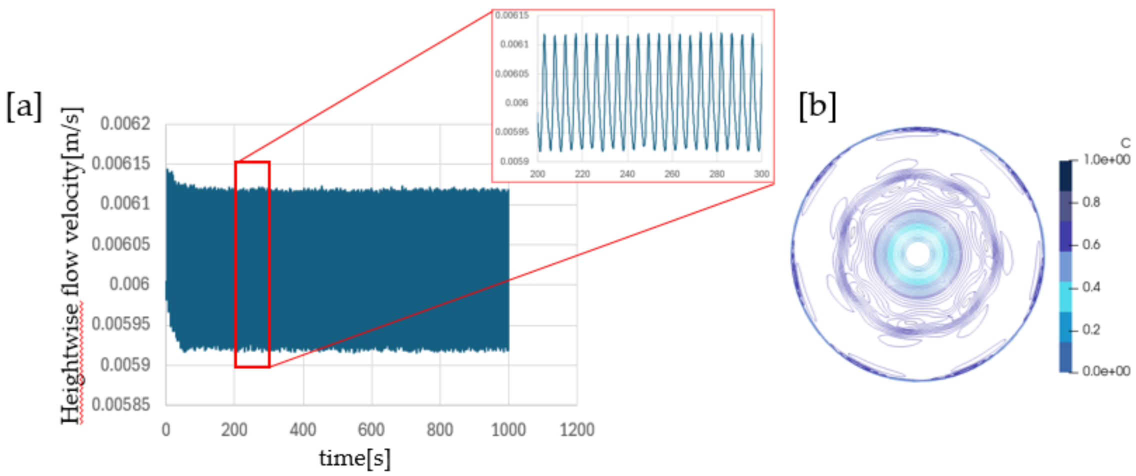

Figure 6. Heightwise flow velocity[a] and the convective structures(time=1000[s]) at specific Marangoni numbers[b] for the case with a fixed Marangoni number under rotation.

3.3 Variation of critical Marangoni number and wavenumber at each rotation speeds

Figures 7-9 show the azimuthal flow velocity [a] and convection structure when the Marangoni number is larger than the critical Marangoni number [b]. Figure 10 presents the relationship between the total Marangoni numbers and the wavenumber. In Figures 7-9 when an axisymmetric steady flow occurs in the melt, the azimuthal velocity remains nearly constant. However, when the critical Marangoni number is exceeded and unsteady flow occurs, the circumferential velocity begins to oscillate. The critical Marangoni number gradually increases with increasing rotation speed. Furthermore, Figure 10 indicates that the wavenumber at which Marangoni convection first appears also differs, and in some cases, the transition from steady to unsteady flow occurs earlier.

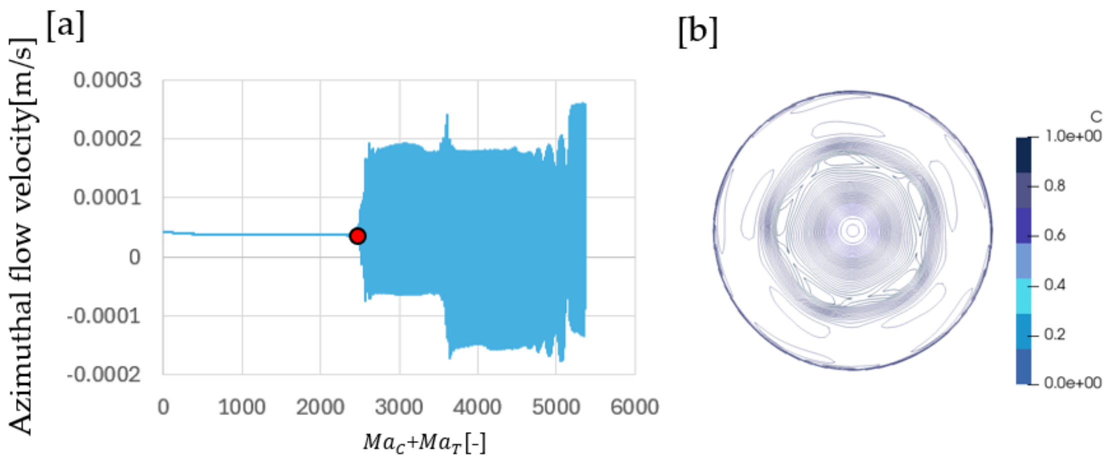

Figure 7. Azimuthal flow velocity[a] and convection structure at $\boldsymbol{Ma_C}$+$\boldsymbol{Ma_T}$=2412[b] at 0.05rpm.

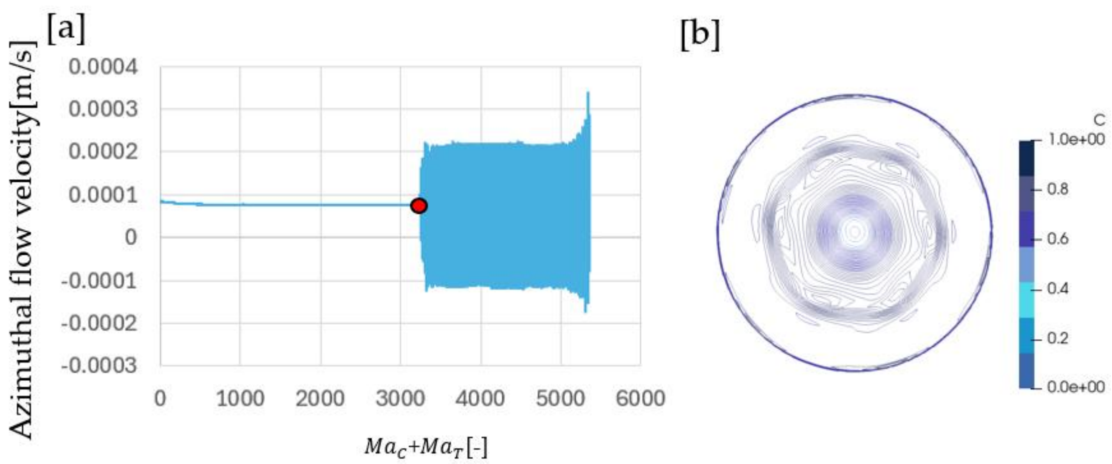

Figure 8. Azimuthal flow velocity[a] and convection structure at $\boldsymbol{Ma_C}$+$\boldsymbol{Ma_T}$=3269 [b] at 0.1rpm.

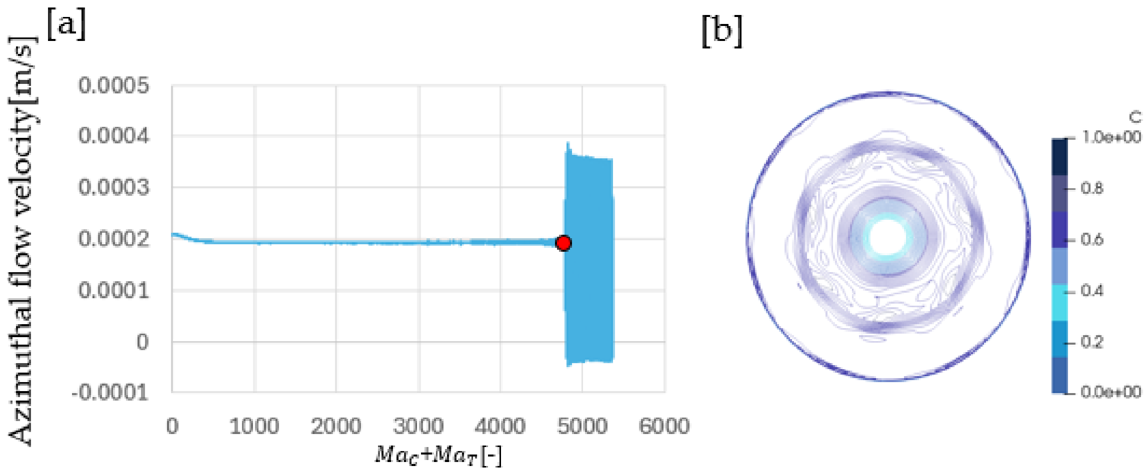

Figure 9. Azimuthal flow velocity[a] and convection structure at $\boldsymbol{Ma_C}$+$\boldsymbol{Ma_T}$=4825 [b] at 0.25rpm.

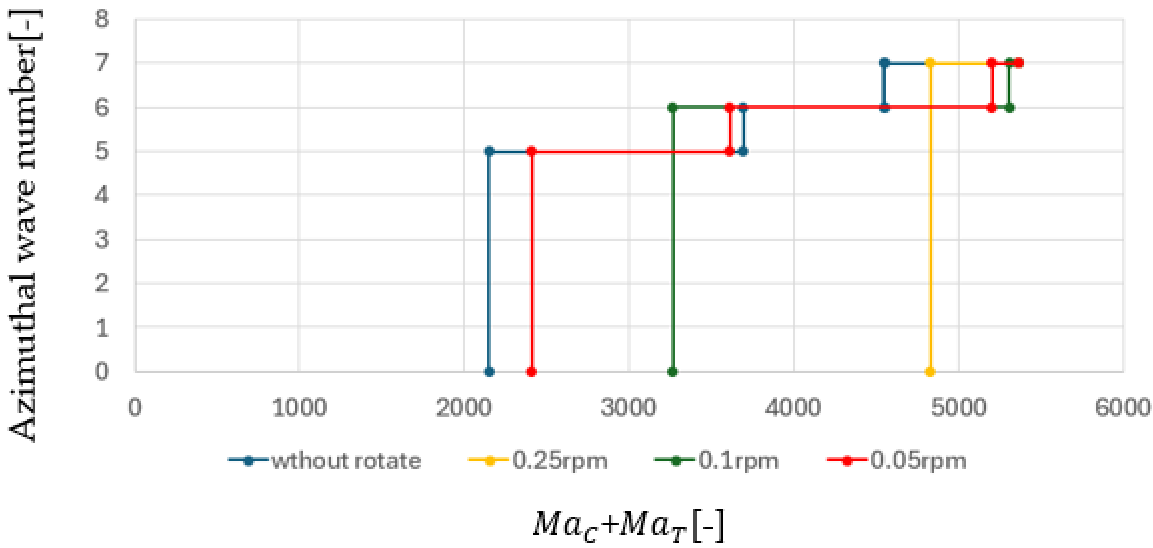

Figure 10. Relationship between Marangoni number and wave number at each rotation speeds.

4. Conclusions

In this study, numerical analyses on the rotational control of thermo-solutal Marangoni convection in a half-zone liquid bridge were conducted using OpenFOAM, leading to the following conclusion:

・Rotation control is more effective in suppressing Marangoni convection when rotation is applied simultaneously with the increase of the Marangoni number from zero (no flow), compared to the case of a fixed Marangoni number(unsteady flow).

・The critical Marangoni number also varies with the rotation rate, increasing as the rotation rate becomes higher.

・In some cases, applying rotation causes a faster change in wavenumber during the transition from steady to unsteady flow than without roatation.

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