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HZ 液柱内の温度差と濃度差に起因するマランゴニ対流に及ぼすアスペクト比の影響

Effect of aspect ratio on Marangoni convection due to temperature and concentration differences in a HZ liquid bridge

原田和晃 [1], 美里碧 [2], 水口尚 [2], 岡野泰則 [3] ,
Kazuaki HARADA[1], Aoki MISATO[2], Hisashi MINAKUCHI[2] and Yasunori OKANO[3]
[1] 琉球大学大学院理工学研究科,Graduate School of Engineering and Science, University of the Ryukyus, Okinawa ,Japan,
[2] 琉球大学工学部, Faculty of Engineering, University of the Ryukyus, Okinawa, Japan,
[3] 大阪大学大学院基礎工学研究科 Graduate School of Engineering Science, Osaka University, Osaka, Japan,

1. Introduction

In a floating zone (FZ) method under microgravity, which is considered as one of the production methods for bulk single crystals that are expected to have higher performance than conventional semiconductor materials, Marangoni convection is generated due to temperature difference. This convection is known to adversely affect crystal growth. It is therefore essential for the growth of high quality crystals by FZ to have a better understanding for the Marangoni convection in the melt, and the precise control of it is necessary. Therefore, a large number of literature has contributed to the study of thermal Marangoni convection in FZ systems (see, for instance, Refs. [1-2]). For simplicity and to reduce computational cost, a half-zone (HZ) model as in Figure 1[a] is often used [3-4]. The HZ model is considered as a liquid bridge between two hot and cold discs by establishing a temperature gradient along the free surface of the liquid bridge. For small thermal Marangoni numbers, the Marangoni convection in the half-zone is steady and axisymmetric. However, at high thermal Marangoni numbers the flow in the melt becomes 3-D and asymmetric. The 3-D flows have m-fold symmetry of the flow pattern. The symmetry number m (azimuthal wave number) depends strongly on the aspect ratio, As (As = height/radius), of the half-zone. In addition, in the growth of alloys such as Si_xGe_{1-x}, it was shown that it is necessary to consider not only the thermal Marangoni convection but also the solutal Marangoni convection due to surface tension differences of the components of the alloy [5-9].

In order to elucidate the convective structure and mechanism of thermo-solutal Marangoni convection occurring in the melt of the half-zone of the FZ method. We analyzed models with different aspect ratios by setting temperature and concentration differences.

2. Numerical Methods

In this study, we use the half-zone model with radius *a* and liquid column height *L*, assuming the upper part of the melt in the FZ method, as shown in Figure 1[a]. The arrows represent the direction of Marangoni forces by the temperature and concentration gradients along the surface. The half zone model is considered as a liquid bridge between the cold and hot discs as shown in Figure 1[a] assuming that (1) the fluid is incompressible and Newtonian, (2) the solid/liquid interfaces are flat and (3) the system is under zero gravity. The governing equations obtained by the mass, momentum, energy and concentration are:

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

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

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

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

The boundary conditions at the free surface, upper disc, and lower disc are：

Free surface (r=a):

$$u_r = 0 \tag{5}$$

$$\mu\left\{r\frac{\partial}{\partial r}\left(\frac{u_\theta}{r}\right)\right\} = \frac{1}{r}\left(\frac{\partial \sigma}{\partial T}\right)\frac{\partial T}{\partial \theta} + \frac{1}{r}\left(\frac{\partial \sigma}{\partial C}\right)\frac{\partial C}{\partial \theta} \tag{6}$$

$$\mu\frac{\partial u_z}{\partial r} = \left(\frac{\partial \sigma}{\partial T}\right)\frac{\partial T}{\partial z} + \left(\frac{\partial \sigma}{\partial C}\right)\frac{\partial C}{\partial z} \tag{7}$$

$$\frac{\partial T}{\partial r} = 0 \tag{8}$$

$$\frac{\partial C}{\partial r} = 0 \tag{9}$$

Upper cold disc (z=L):

$$u_r = 0, u_\theta = 0, u_z = 0, T = T_C, C = C_{Si} \qquad (10)\text{~}(14)$$

Lower hot disc (z=0):

$$u_r = 0, u_\theta = 0, u_z = 0, T = T_h, C = C_{Ge} \qquad (15)\text{~}(19)$$

where, $\boldsymbol{u}$ ($u_r\ u_\theta\ u_z$) is the velocity vector, *t* is the time, *p* is the pressure, *T* is the temperature, and *C* is the silicon concentration. ρ is the density, $\upsilon(=\mu/\rho)$ is the kinematic viscosity, α is the thermal diffusion coefficient, and *D* is the diffusion coefficient. Non-dimensional numbers are:

$$Ma_T = -\frac{\partial\sigma}{\partial T}\frac{\Delta TL}{\mu\upsilon},\ Ma_C = \frac{\partial\sigma}{\partial C}\frac{\Delta CL}{\mu\upsilon}, Sc = \frac{\upsilon}{D}, Pr = \frac{\upsilon}{\alpha}, As = \frac{a}{L} \qquad (20)\sim(24)$$

The physical properties of Si/Ge (Si_xGe_{1-x}) used in this study are listed in Table 1. In addition, As (aspect ratio) = 0.417, 0.500, and 0.625 are used as analytical models. Models with arbitrary numbers of radius, circumference, and height, as shown in Figure 1[b], are used for the analysis, and the total number of meshes is denoted by the number of meshes n. The number of meshes within this study is n=144000 for As=0.417 and 0.500, and n=115200 for As=0.625. OpenFOAM, a free and open source CFD software, is used. The governing equations (eq. 1-4) are discretized using the finite volume method, and the unsteady algorithm, PISO method, is used.

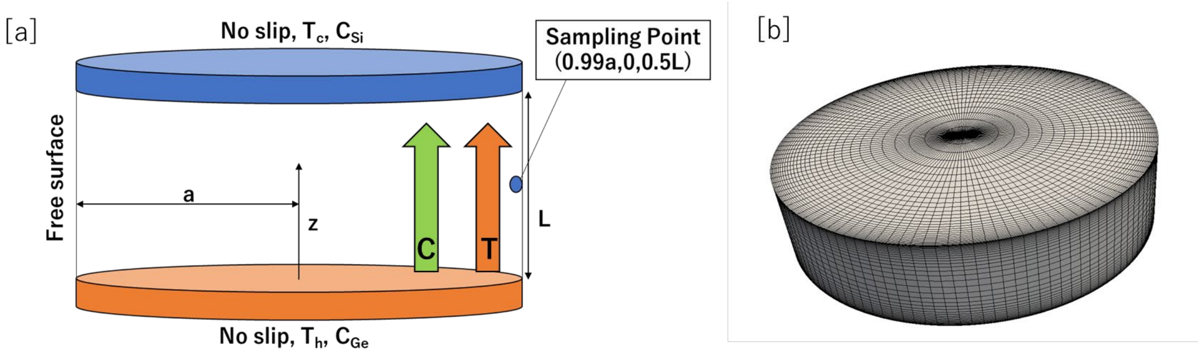

Figure 1. Geometry of the analytical liquid bridge[a] and mesh geometry of the analytical model at As=0.5[b].

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

Kinematic viscosity $\boldsymbol{\upsilon}$	1.4×10^{-7} [m^2/s]
Thermal Diffusion Coefficient $\boldsymbol{\alpha}$	2.2×10^{-5} [m^2/s]
Diffusion coefficient $\boldsymbol{D}$	1.0×10^{-8} [m^2/s]
Prandtl number $\boldsymbol{Pr}$	6.37×10^{-3} [-]
Schmidt number $\boldsymbol{Sc}$	14.0 [-]

3. Results and discussion

Figure 2 shows the heightwise flow velocity at the sampling point when the temperature difference between the top and bottom surfaces is set to 0 (Ma_T=0) and the concentration difference is increased by ΔMa_C=0.1786/s for the model with As=0.5. Figure 3 shows the transition from a two-dimensional axisymmetric steady flow at low solutal Marangoni number (Ma_C=893) to a three-dimensional unsteady flow with azimuthal wave number m=4 at high Ma_C (=1429,1473 and 1518). This indicates that the As=0.5 model reaches a critical value for the concentration difference around Ma_C=1250, and the flow transitions from the axisymmetric steady flow to the unsteady flow. The value of Ma_C=1250 is set as the critical value of the solutal Marangoni number. Under the same conditions, for As=0.417 and 0.625, the flow transitions are observed at Ma_C=1350 and 1400.

Figure 4 shows the heightwise flow velocity and frequency when the critical value of Ma_C obtained is fixed and the temperature difference is varied with time (ΔMa_T=0.357/s). Figure 4[b] shows that the frequency increases as Ma_T increases for all aspect ratios. Figure 5 shows the azimuthal wave number at each thermal Marangoni number (Ma_T). In the coexistence of thermal and solutal Marangoni convections, the azimuthal number increases when the thermal Marangoni number increases. The flow structure transitions show that the values of Ma_T at which the azimuthal wave number changes are close to each other for each aspect ratio. Figure 6 shows a plot of the relationship between aspect ratio times azimuthal wave number and frequency of flow. The correlation shown in the red box in the figure indicates that there is a certain law for Marangoni convection mixed with temperature and concentration differences in the aspect ratio change.

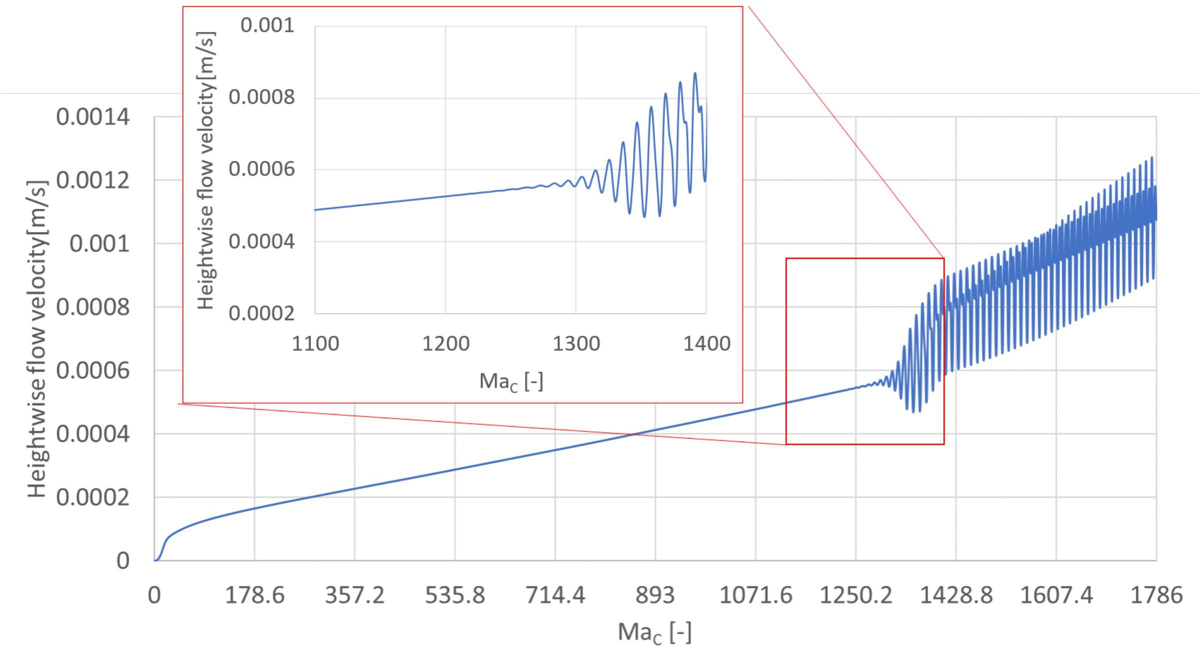

Figure 2. The heightwise flow velocity at each the solutal Marangoni number and the sampling point (As=0.5).

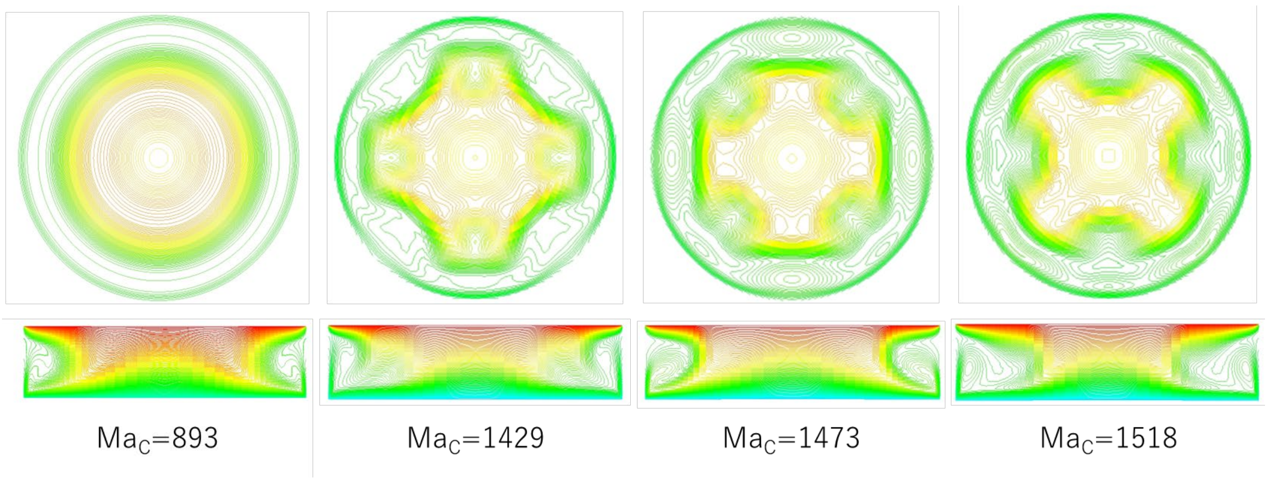

Figure 3. Transition in concentration distribution at steady to unsteady flow (As=0.5).

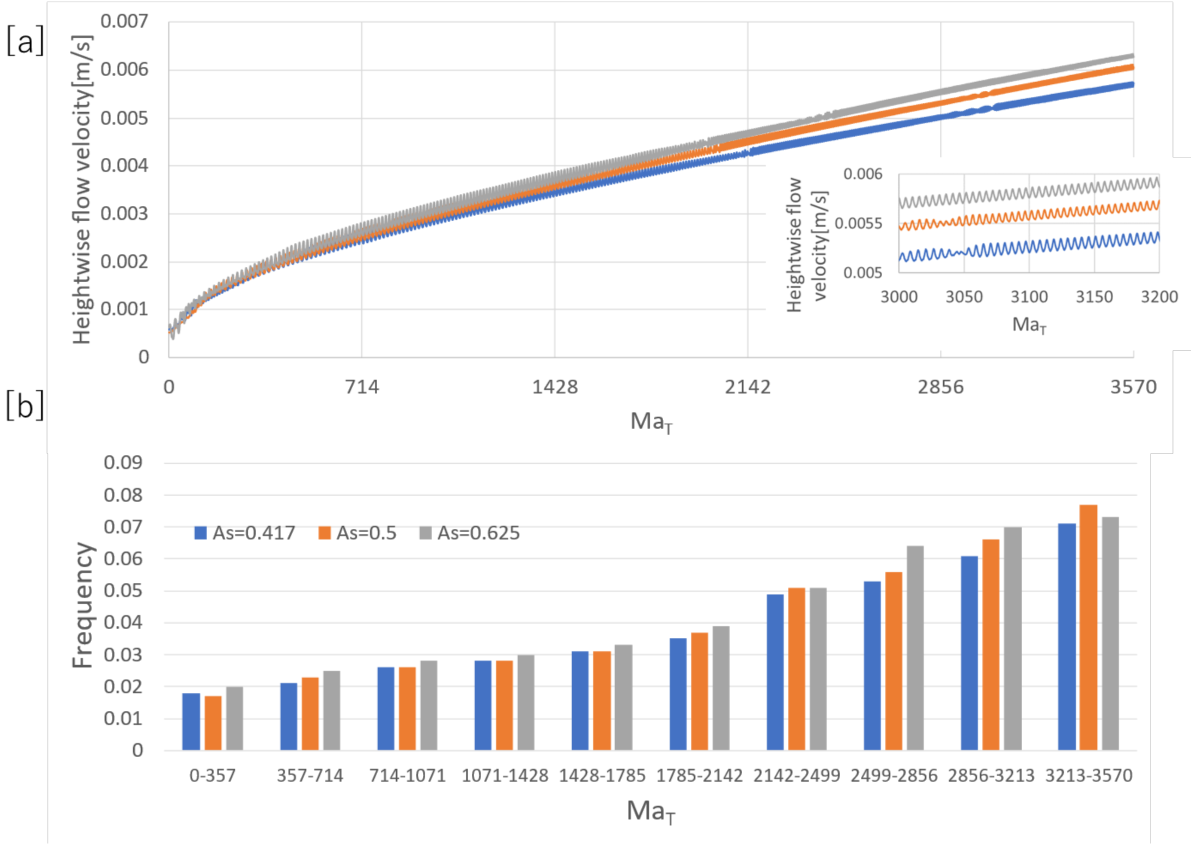

Figure 4. The heightwise flow velocity [a] and frequency [b] at each the thermal number

(Mac is fixed at each the critical value).

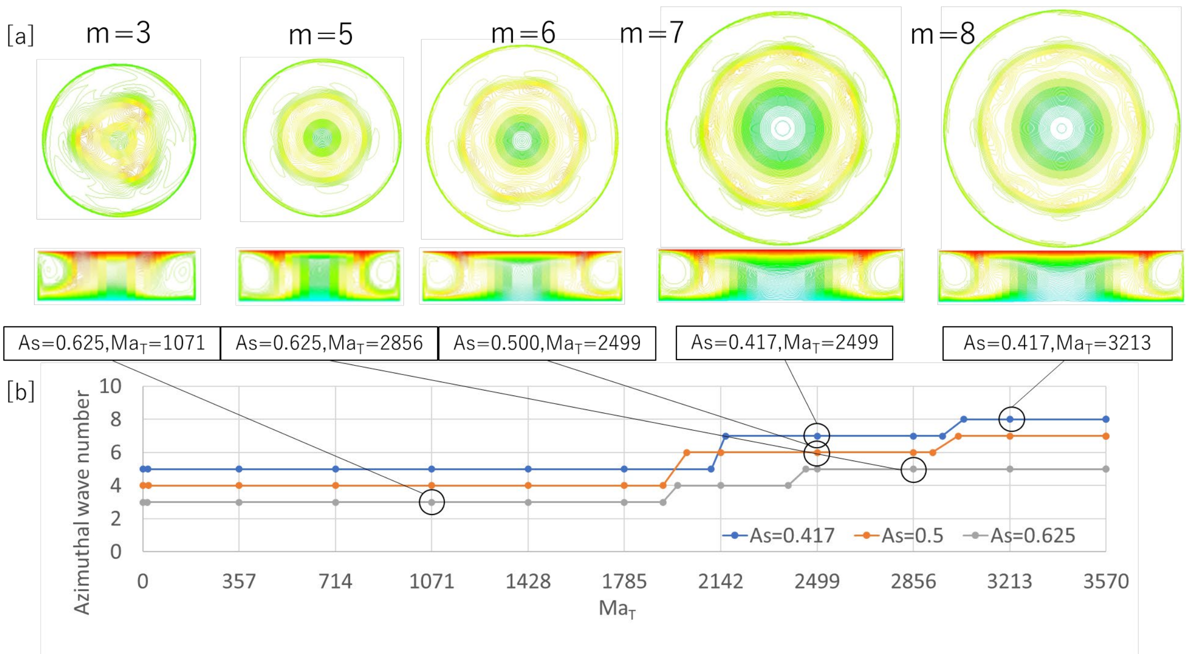

Figure 5. Concentration distribution [a] and azimuthal wave number [b] at each the thermal Marangoni number (Mac is fixed at each the critical value).

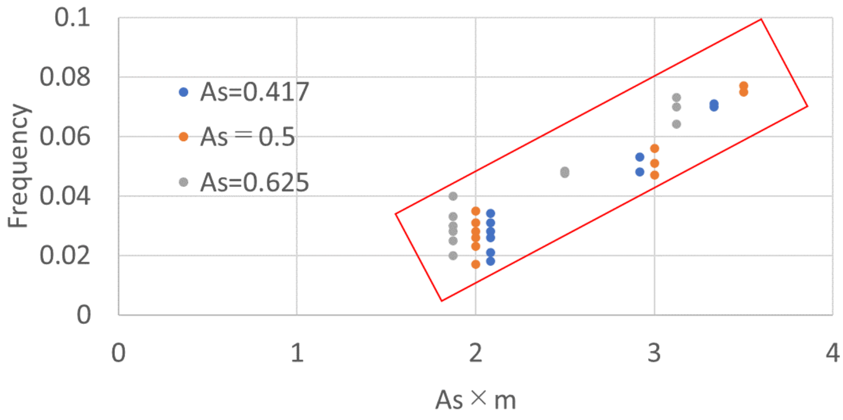

Figure 5. Correlation between As × m and frequency.

4. Conclusions

In this study, the effect of aspect ratio on the thermos-solutal Marangoni convection in the half-zone liquid bridge was examined using OpenFOAM led to the following conclusions:

- The azimuthal wave number m depends not only on the aspect ratio but also on the thermal Marangoni number due to the effect of thermo-solutal Marangoni convection on flow patterns.
- The azimuthal wave number increases almost only with the increase of the thermal Marangoni number.
- There is a correlation between aspect ratio times azimuthal wave number and frequency.

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