JASMAC
Conference of the Japan Society of Microgravity Application

P04

HZ 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マランゴニ数の時間変化の影響

Effect of time dependency of Marangoni number on Marangoni convection due to temperature and concentration differences in a HZ

島袋史栄 [1], 水口尚 [2], 岡野康則 [3],
Shiei SHIMABUKURO[1], 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

One of the production methods Si/Ge bulk single crystals is a Floating Zone (FZ) method, which is performed in a microgravity environment. In the FZ method, the polycrystalline raw material is fed from the top and passed through a heater to create a melt section with the seed crystal, and the melt section is cooled to obtain the desired single crystal. However, the FZ method has the problem that Marangoni convection generated in the melt adversely affects crystal growth. Marangoni convection is a flow generated by surface tension differences due to temperature and concentration differences. Therefore, controlling Marangoni convection leads to quality crystal growth. This study uses the half-zone model, which is frequently used in studies of Marangoni convection (see, for instance, Refs1-2)). The strength of convection is expressed in terms of a dimensionless number called the Marangoni number , and the critical value of the Marangoni number is treated as the critical Marangoni number3). The Marangoni number is defined by the physical properties of the melt, the temperature difference.

There have been many analyses of Marangoni convection caused by temperature differences. However, in the growth of alloys such as Si_xGe_{1-x}, 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. Therefore, in order to shed light on the relative contributions of thermal and solutal Marangoni convections occurring in the melt of a half-zone of the FZ system, we have carried out three-dimensional numerical simulations4-5). Especially analysis was performed considering time dependency of temperature and concentration differences in the present study.

2.Analysis Method

In this study, Figure 1 was used as the model for the analysis. The sides are free surface, with the top surface hot and the bottom surface cold. The analysis area was the melt only, the free surface height [L] was 5 mm radius [a] was 10 mm, and As = a/L = 0.5 was used. In addition to assuming a microgravity environment, the gas-liquid and solid-liquid surface shapes were flat. The sampling point is (r,θ,z)=(0.99a,0,0.5L). The basic analytical equations are the continuous equation (1), the Navier-Stokes equation (2), the energy equation (3), and the diffusion equation (4), which are 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 differences was considered for the side surfaces. Thermal and solutal Marangoni numbers and sum of thermal and solutal Marangoni numbers, which indicates the intensity of convection, are then given below.

$$Ma_T = -\frac{\partial \sigma}{\partial T}\frac{\Delta TL}{\mu \upsilon},\ Ma_C = \frac{\partial \sigma}{\partial C}\frac{\Delta CL}{\mu \upsilon},\ Ma = Ma_T + Ma_C \tag{5~7}$$

The thermal and solutal Marangoni numbers were changed with time considering the time dependency of temperature and concentration differences. Using the three routes shown in Figure 2. Ma_C and Ma_T are increased between 20000s. Route I is increased to Ma_C=0~1786 and then to Ma_T=0~3572. Route II is increased Ma_C=0~1786 and Ma_T=0~3572 simultaneously. Route Ⅲ is increased to Ma_T=0~3572 and then to Ma_T=0~1786.

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 $\boldsymbol{\upsilon}$	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 [-]

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.

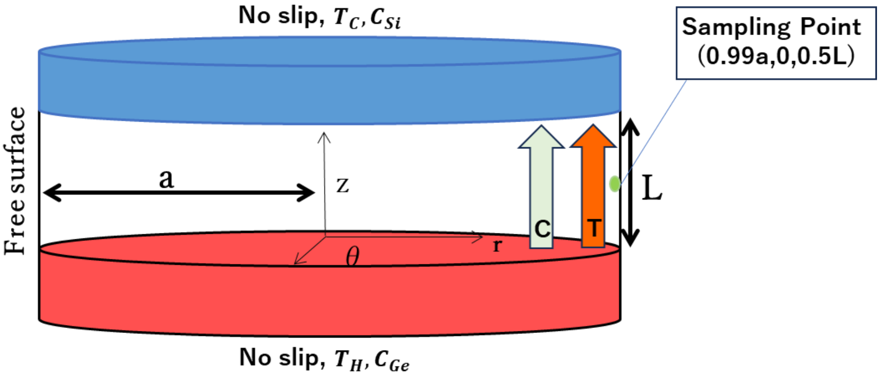


Figure 1. Geometry of the analytical liquid bridge.

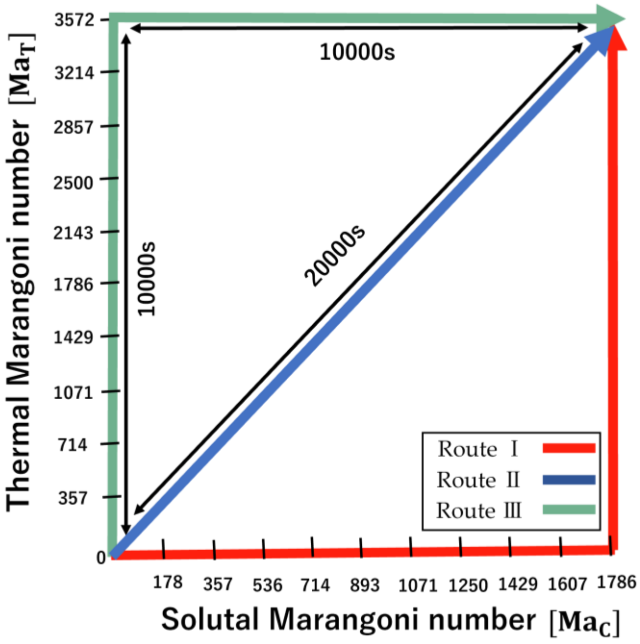
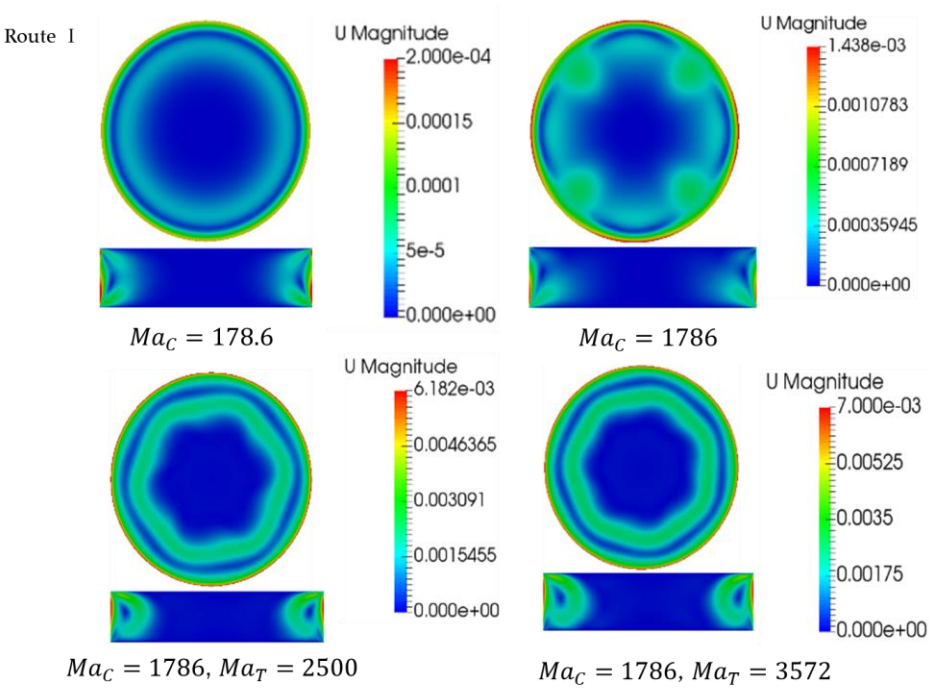


Figure2. Route diagram.

3.Results and discussion

Figures 3(a), (b) and (c) show the convective structure changes at each route. The wave number (m) was m = 0→4→6→7 at route I. It was m = 0→4→5→7 at route II. It was m = 0→3→3′ at route III. Figure 4 shows the time dependency of the heightwise velocity at a sampling point (r, θ, z)=(0.99a, 0, 0.5L). As the Marangoni number (time) increased, the velocity of each route increased. However, results at routes I and II transitioned to oscillating flow, while it at route III remained steady flow. Figure 5 shows the relationship between sum of thermal and solutal Marangoni numbers and wave number. Even with the same Ma number, the final wave number was depended on the route. Comparing routes I and II, the critical Marangoni number at route I was Ma_C=1250 and Ma_T=0. At route II, the critical Marangoni number was

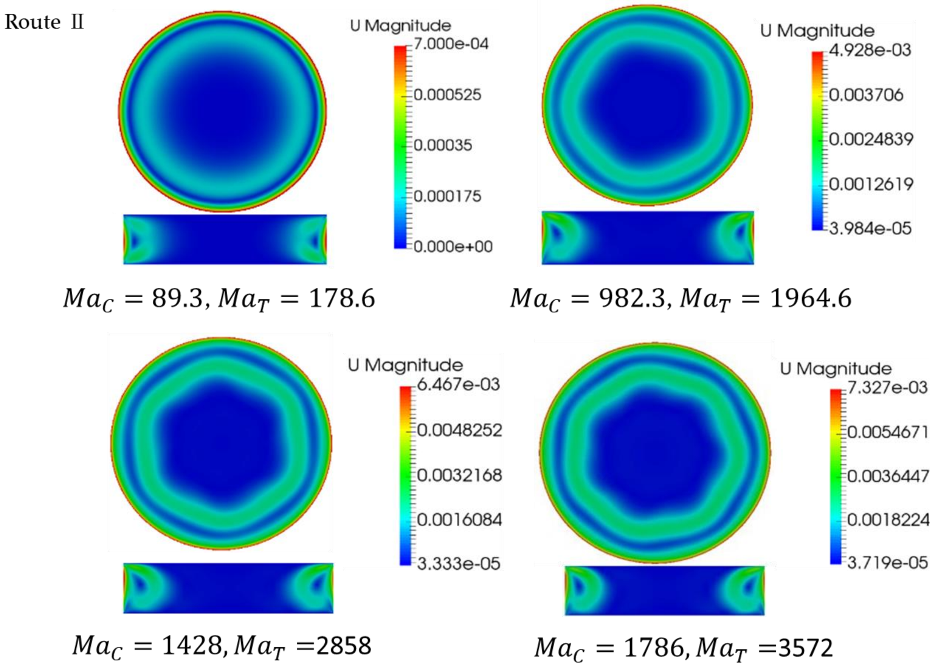
Ma_C=696 and Ma_T=1393. Therefore, the critical solutal Marangoni number of thermo-solutal Marangoni convection was smaller than that of only solutal Marangoni convection.



$Ma_C = 178.6$ $Ma_C = 1786$

$Ma_C = 1786, Ma_T = 2500$ $Ma_C = 1786, Ma_T = 3572$

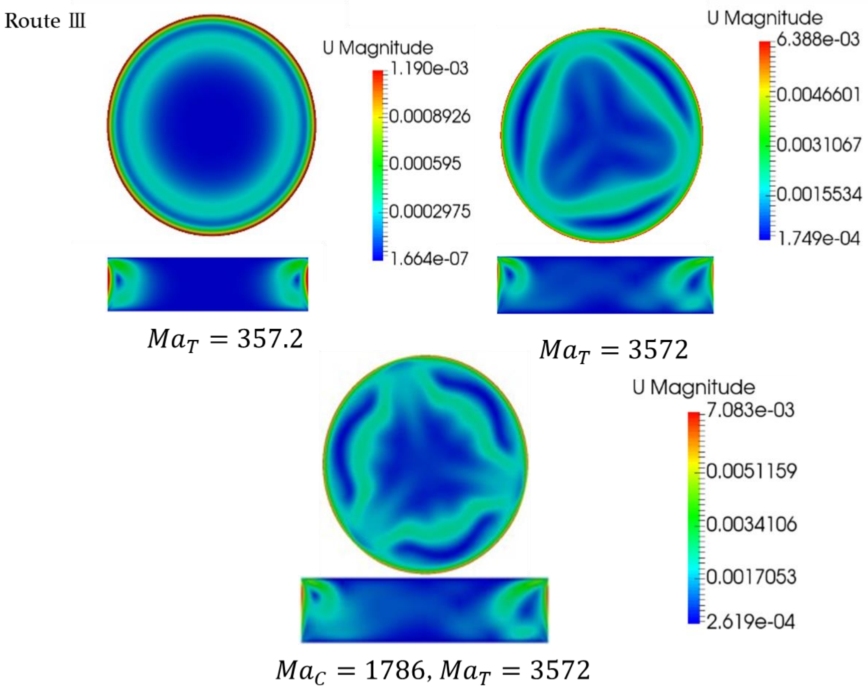
Figure 3(a). Convective structure changes at route Ⅰ.



$Ma_C = 89.3, Ma_T = 178.6$ $Ma_C = 982.3, Ma_T = 1964.6$

$Ma_C = 1428, Ma_T = 2858$ $Ma_C = 1786, Ma_T = 3572$

Figure 3(b). Convective structure changes at route II.



$Ma_T = 357.2$

$Ma_T = 3572$

$Ma_C = 1786, Ma_T = 3572$

Figure 3(c). Convective structure changes at route III.

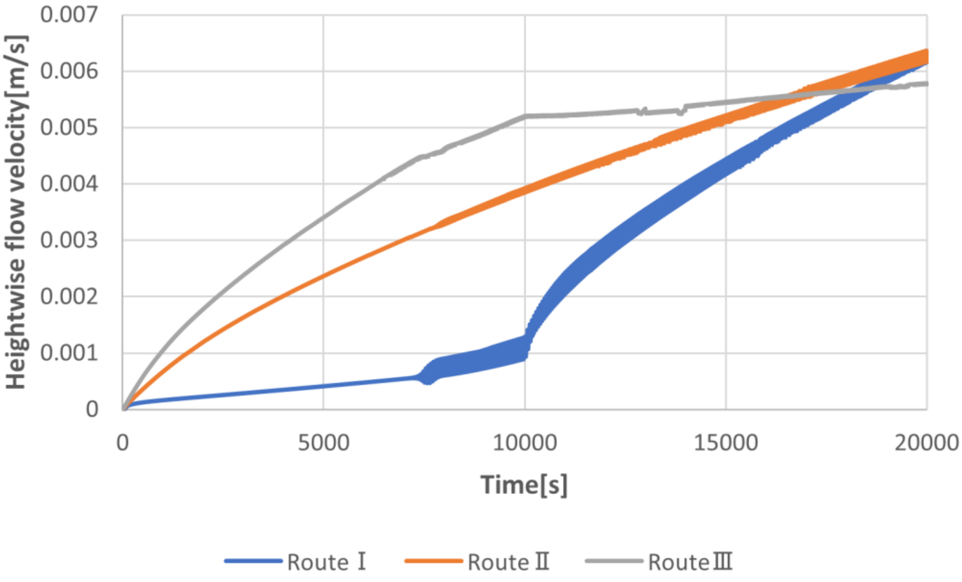


Figure 4. Tiem dependency of the heightwise velocity at a sampling point.

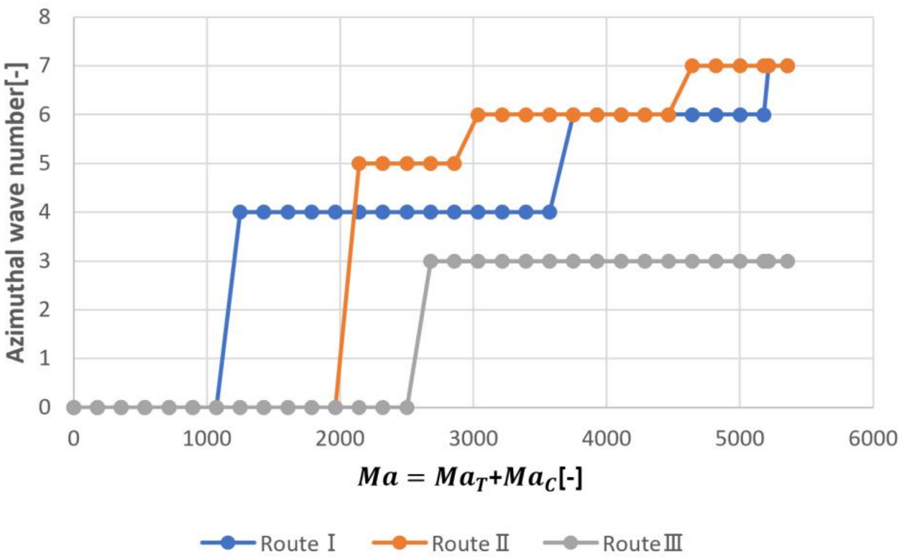


Figure 5. Relationship between sum of Marangoni numbers and wave number.

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