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The relative contributions of thermo-solutal Marangoni convections on flow patterns in a liquid bridge

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ABSTRACT

A numerical simulation study was carried out to investigate the relative contributions of thermal and solutal Marangoni convections on transport structures in a liquid bridge under zero gravity. The liquid bridge in the model represents a three dimensional half-zone configuration of the Floating Zone (FZ) growth system. Three dimensional field equations of the liquid zone, i.e. continuity, momentum, energy, and diffusion equations, were solved by the PISO algorithm. Computations were performed using the open source software OpenFOAM. The numerical simulation results show that the flow field becomes three-dimensional and time-depended when the solutal Marangoni number is larger than the critical value. It was also shown that not only flow patterns but also the azimuthal wave number (m) changes due to the competing contributions of thermal and solutal Marangoni convective flows.

1. Introduction

When there is a free surface in a melt, the variation in the surface tension drives a convective flow along the free surface in the melt. This flow is known as Marangoni convection, and may be produced by temperature (thermal Marangoni convection) and/or concentration gradients (solutal Marangoni convection) in the melt. It is known that such Marangoni convective flows may become unstable much easier than the buoyancy driven natural convection. When a free surface exists in a crystal growth technique such as the Floating-zone (FZ) technique, unstable Marangoni flows that develop in the melt (liquid bridge) may induce undesirable growth striations in the grown crystals. FZ crystal growth being a containerless technique (in which the melt is solidified through a liquid bridge with a free surface) has the advantage of producing crystals free from crucible contamination. However, when larger liquid bridges are selected in order to grow large crystals, or/and when temperature and concentration gradients are steeper, Marangoni convection may become stronger and lead to flow instabilities in the melt.

In the growth of Si_xGe_{1-x} single crystals, a concentration gradient in the melt leads to further segregation. Such a concentration gradient gives rise to a strong solutal Marangoni convection in the melt compared with thermal Marangoni convection. It is important to know the relative contributions of these convections in the growth of Si_xGe_{1-x} crystals by FZ [1,2]. From this point of view, the present study investigates the role of thermal and solutal Marangoni convections in the Floating Zone system numerically. Most modeling studies in literature have considered thermal Marangoni convection only [3–7]. Those considering solutal Marangoni convection were few [8], including an experimental work on the Si–Ge crystal growth that has reported the adverse effect of solutal Marangoni convection in crystal growth [9].

To this end, a numerical simulation study would be very handy to shed light on the relative contributions of such convective flows. In this study, this is done through three-dimensional numerical simulations for the thermal and solutal Marangoni convections in the melt of the Si–Ge FZ growth system, and their effects on transport structures of the melt are examined. In order to make the relative contributions of thermo-solutal Marangoni convections distinguishable, and not to involve the contribution of natural convection, the gravity level was taken zero ($g=0$) in the model.

2. Mathematical model

In FZ growth of single crystals, various factors such as growth rate, interface deformation, the concentration condition at the liquid–solid interface and the temperature condition at the free interface may play roles as described in [10]. However, since the objective of the present study is to shed light on the relative contributions of thermo-solutal Marangoni convection on flow structures of the melt under zero gravity, we have simplified the

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Nomenclature

a	radius of liquid bridge [m]
Asp	aspect ratio ($=L/a$)
C	molar fraction of Si [–]
D	diffusion coefficient of Si_xGe_{1-x} [m^2/s]
L	length of free surface [m]
m	azimuthal wave number
Ma	Marangoni number
N	mesh number
p	pressure [Pa]
Pr	Prandtl number
r	radial coordinate [m]
Sc	Schmidt number
t	time [s]
T	temperature [K]
$\vec{V}$	velocity vector [m/s]
z	axial coordinate [m]
α	thermal diffusivity [m^2/s]
θ	azimuthal coordinate [rad]
ΔC	concentration difference [–]
ΔT	temperature difference [K]
θ	azimuthal coordinate [rad]
μ	viscosity [Pa s]
ν	kinematic viscosity [m^2/s]
ρ	density [kg/m^3]
σ	surface tension [N/m]

Subscripts

0	initial
c	cold
C	solutal
h	hot
p	period
T	thermal
R	R-direction
Z	Z-direction
θ	θ-direction

model as much as possible by not taking into account some of these factors to remove their possible influences.

With this in mind, we have made the following assumptions in the model: (i) the Si–Ge melt is an incompressible, Newtonian fluid mixture, (ii) the solid/liquid interfaces are flat, and (iii) the system is under zero gravity. Since the gravity is taken zero, the liquid bridge remains cylindrical (and thus the liquid/gas interface is flat), and natural convection does not develop in the melt (due to the absence of the gravitational body force). The three-dimensional half-zone of the FZ liquid bridge is considered as the liquid phase of the model domain (its schematic description is given in Fig. 1).

Under these assumptions, the following governing equations of the liquid phase are obtained respectively from the overall mass conservation, the balance of momentum, the balance of energy and the conservation of mass of species:

Continuity

$$\nabla\cdot\vec{V}=0 \tag{1}$$

Momentum

$$\frac{\partial\vec{V}}{\partial t}+\vec{V}\cdot\nabla\vec{V}=-\frac{1}{\rho}\nabla p+\nu\Delta\vec{V} \tag{2}$$

Energy

$$\frac{\partial T}{\partial t}+\vec{V}\cdot\nabla T=\alpha\Delta T \tag{3}$$

Mass transport

$$\frac{\partial C}{\partial t}+\vec{V}\cdot\nabla C=D\Delta C \tag{4}$$

Boundary conditions:

We consider the following boundary conditions in the computational domain.

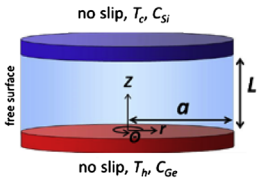

Fig. 1. Schematics of the liquid bridge.

Upper-disc ($z=L$): Along the upper boundary we consider the non-slip condition on the flow velocity field, and assumed that temperature is prescribed at $T=T_c$. The melt concentration is assumed as the pure silicon at this boundary:

$$C=1 \tag{5}$$

Lower-disc ($z=0$): Along the lower boundary, similarly we also use the non-slip condition on the flow velocity field, and assumed that temperature is prescribed at $T=T_h$. The melt concentration on this boundary is taken as the pure germanium

$$C=0 \tag{6}$$

The concentration boundary conditions imply that we assume the melt is in equilibrium with the discs (solids) concentrations during melting and growth.

Free surface ($r=a$): Along the free surface we use the following conditions. The contribution of Marangoni convection was taken into account using the following tangential force balance at the free surface:

$$V_r=0 \tag{7}$$

$$\mu\frac{\partial V_z}{\partial r}=-\left(\frac{\partial\sigma}{\partial T}\frac{\partial T}{\partial z}+\frac{\partial\sigma}{\partial C}\frac{\partial C}{\partial z}\right) \tag{8}$$

$$\mu\left\{r\frac{\partial}{\partial r}\left(\frac{V_\theta}{r}\right)\right\}=-\frac{1}{r}\left(\frac{\partial\sigma}{\partial T}\frac{\partial T}{\partial\theta}+\frac{\partial\sigma}{\partial C}\frac{\partial C}{\partial\theta}\right) \tag{9}$$

Table 1
Parameters and properties of the Si_xGe_{1-x} system [13].

Property	Symbol	Value
Temperature coefficient of surface tension	$\partial\sigma/\partial T$ [N/m K]	$(0,-2.20,-5.51)\times10^{-6}$
Concentration coefficient of surface tension	$\partial\sigma/\partial C$ [N/m]	$0-2.57\times10^{-5}$
Radius of liquid bridge	a [m]	1.00×10^{-2}
Length of liquid bridge	L [m]	5.00×10^{-3}
Aspect ratio	Asp	0.5
Thermal diffusivity	α [m^2/s]	2.20×10^{-5}
Kinematic viscosity	ν [m^2/s]	1.40×10^{-7}
Diffusion coefficient	D [m^2/s]	1.00×10^{-8}
Prandtl number	Pr	6.37×10^{-3}
Schmidt number	Sc	14.0