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The Coriolis force effect on molten silicon convection in a rotating crucible

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Abstract—Silicon single crystals are usually grown from melt in a rotating crucible by the Czochralski method. The purpose of the present paper is to make the velocity profile in the azimuthal direction clear. The flow velocity profile has been obtained from numerical simulation and flow visualization by X-ray radiography. Numerical simulation and experimental flow visualization have made it clear that the flow in the azimuthal direction is modulated by the Coriolis force because the radial flow velocity is relatively high. The azimuthal flow velocity near a crucible wall has a smaller (or negative) value compared with the angular velocity of the crucible, while the flow with a larger azimuthal velocity exists in the center of the crucible.

1. INTRODUCTION

MOST SILICON single crystals for VLSIs are grown by the Czochralski (Cz) method. Generally, a crucible containing molten silicon is rotated during crystal growth to homogenize and/or to control the oxygen concentration in the grown crystals [1–3]. Since the oxygen concentration is affected by a flow field, the flow field should be clearly understood to obtain an exact oxygen concentration in the grown crystal. However, the flow velocity, especially the azimuthal component of the flow, has scarcely been discussed [4]. The reason may be as follows: the flow fields have been discussed only on the meridional plane since the Cz system has almost axisymmetric geometry.

From the above view points, we will discuss the azimuthal velocity of molten silicon convection in the Cz system in the present paper. Using the individually designed furnace with a double beam X-ray radiography system, we have obtained a three-dimensional flow pattern for the axisymmetric flow case in a crucible [5]. We also performed numerical simulation by a local model which contains convection in an axisymmetric geometry. Subsequently, we will discuss the characteristics of molten silicon convection, especially the Coriolis effect on the azimuthal velocity in the Cz system.

2. CORIOLIS AND CENTRIFUGAL FORCES

Let us consider the cylindrical coordinates as shown in Fig. 1. **i**, **j**, **k** are the unit vectors along the main axes in the cylindrical coordinates. The momentum equation (the Navier–Stokes equation) of rotating fluid contains terms of the Coriolis and the centrifugal forces as shown in equation (1) in a rotating coordinate system

$$\partial\mathbf{u}/\partial t = -\mathbf{u}\nabla\mathbf{u} - 2(\Omega\mathbf{k})\times\mathbf{u} = (\Omega\mathbf{k})\times(\Omega\mathbf{k})\times\mathbf{r} - 1/\rho\nabla p + \mu/\rho\Delta\mathbf{u} + \mathbf{g}\beta(T-T_0) \quad (1)$$

where **u** and **r** are the vectors of relative velocity on a rotational basis and position, respectively, Ω denotes the crucible rotation rate, p and μ represent pressure and viscosity of the fluid, **g**, β and T_0 are the vector of gravitational acceleration, the volume expansion coefficient, and the reference temperature corresponding to specific mass, respectively. The second and third terms of the right-hand side of equation (1) express the Coriolis and the centrifugal accelerations, respectively. The notation of velocities in the radial (r), azimuthal (θ), axial (z) components are v_1, v_2 and v_3, respectively. The vector of the crucible rotation is identical with the z direction as shown in Fig. 1. The Coriolis acceleration vector ($\mathbf{a}_{\mathrm{cor}}$) along the azimuthal

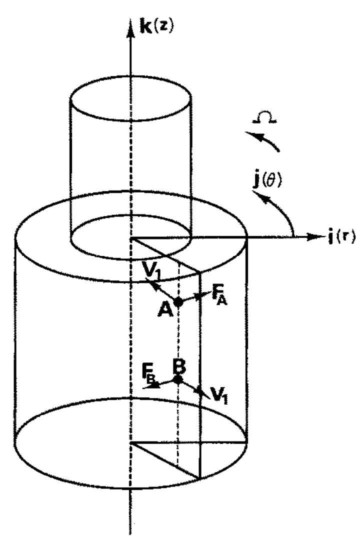

FIG. 1. Cylindrical coordinates in the Cz system.

NOMENCLATURE

$\mathbf{a}_{cor}$ acceleration by the Coriolis force [m s^{-2}]
$\mathbf{a}_{cen}$ acceleration by the centrifugal force [m s^{-2}]
c_p heat capacity [J kg^{-1} K^{-1}]
$\mathbf{g}$ gravitational acceleration [m s^{-2}]
Ra Raleigh number ($\mathbf{g}\beta\Delta T L^3\rho^2 c_p/\mu k$)
$\mathbf{i}$ unit vector along radial direction
$\mathbf{j}$ unit vector along azimuthal direction
$\mathbf{k}$ unit vector along axial direction
k thermal conductivity [W m^{-1} K^{-1}]
L angular momentum
l characteristic length [m]
p pressure [kg m^{-2}]
r radial position [m]
T temperature [K]
$\mathbf{u}$ relative velocity vector in the rotating basis [m s^{-1}]
v_1 relative radial velocity in the rotating basis [m s^{-1}]
v_2 relative azimuthal velocity in the rotating basis [m s^{-1}]
v_3 relative axial velocity in the rotating basis [m s^{-1}]
V_2 absolute azimuthal velocity in a inertial basis [m s^{-1}]
z axial position [m].

Greek symbols
β volume expansion coefficient [K^{-1}]
μ viscosity [kg m^{-1} s^{-1}]
ρ density [kg m^{-3}]
Ω rotation rate [rad s^{-1}].

direction in the cylindrical coordinates can be transformed as shown in equation (2)

$$\mathbf{a}_{cor} = -2\{(\Omega\mathbf{k})\times\mathbf{u}\} = -2(\Omega v_1\mathbf{j}-\Omega v_2\mathbf{i}). \quad (2)$$

First, let us consider the azimuthal component, $\mathbf{j}$ component, at point A in Fig.1 for simplification. The radial component of the flow has a negative value ($v_1 < 0$) at point A. The negative value is attributed to natural convection since the melt is heated from the side wall of a crucible by a resistor and cooled at the center of the melt surface. Therefore, the Coriolis force shown in equation (2) acts positively along the azimuthal direction on account of the positive Ω and negative v_1. Consequently, we can understand that the azimuthal flow velocity becomes large. Subsequently, let us consider point B in Fig. 1. The radial component of the flow has a positive value ($v_1 > 0$). Therefore, the Coriolis force acts in the negative direction which is opposite to the directional force at point A. This means that the azimuthal flow velocity becomes small or may be negative. Thus, the Coriolis force becomes large when the radial component of flow velocity is large, because the origin of the force is attributed to the coupling of the radial and azimuthal velocity components. The effect of the Coriolis force in the Cz system will be discussed in the next section.

Subsequently, we will consider the centrifugal force shown in the third term on the right-hand side of equation (1). The centrifugal acceleration vector ($\mathbf{a}_{cen}$) can be transformed as equation (3)

$$\mathbf{a}_{cen} = \Omega^2 r\mathbf{i} = L^2/r^3\mathbf{i}, \quad (3)$$

where $L(ru)$ is the angular momentum. When a small volume element moves instantaneously from the position r to r' ($=r+\Delta r$), excess force

$$\Delta\mathbf{a}_{cen} = L^2(1/r'^3-1/r^3)\mathbf{i}, \quad (4)$$

is caused by the conservation of angular momentum. Consequently, the centrifugal force always acts in the opposite direction as shown in equation (4). This means that the melt motion along the radial direction is suppressed by the crucible rotation. In the next section, we will discuss which force is more dominant in the Cz system, the Coriolis or the centrifugal force from the point of view of both experimental and numerical analysis.

3. EFFECT OF THE CORIOLIS AND CENTRIFUGAL FORCES IN THE Cz SYSTEM

As reported in previous work, the flow pattern is sensitive to the melt geometry in the silicon Cz system [6]. If the aspect ratio R (= melt radius/melt depth) is large, the flow pattern becomes axisymmetric, i.e. a torus-like pattern, although the flow becomes non-axisymmetric for small R. We will focus on the axisymmetric flow pattern in the present paper. The radial velocity component for the silicon melt becomes large because of the large Grashof number [7] to satisfy the continuity equation. Therefore, the Coriolis force effect becomes large for molten silicon in the Cz system. This is also the case for molten semiconductors with similar thermophysical properties to those of molten silicon. From the above viewpoint, the Coriolis force affects and modulates the azimuthal component of the flow in the Cz system by considering equation (2) because the fluid is usually rotating.

Figure 2(a) shows the plane view of particle path during 60 s observation obtained from the double X-ray beam radiography system and Fig. 2(b) shows the time-dependent velocity of the V_2 component. V_2 represents the absolute velocity of the azimuthal component on an inertial basis. The axes direction in Fig. 2 is different from that in Fig. 1. The rotation rates of the crucible and crystal are $+1$ ($+0.105$ rad s^{-1}) and -1 rpm (-0.105 rad s^{-1}), respectively. The flow direction is identical to the crucible rotation, as shown in Fig. 2(a). A sharp tooth-like path near the crucible wall, indicated by an open arrow, can be found, while a dull tooth-like path in the center of the crucible, indicated by a closed arrow, was also found in the same figure. The moments marked by the open and closed arrows in Fig. 2(b) correspond to those in Fig. 2(a). Consequently, we can estimate from the above results that the azimuthal velocity near the crucible wall is smaller than the azimuthal velocity in the center of the crucible. To make the variation of the azimuthal velocity (V_2) in the azimuthal direction clear, the time dependence of the V_2 velocity for 90 s is shown in Fig. 2(b). We find that the angular velocity (V_2) oscillates drastically on account of variation of the tracer position by the natural convection in the meridional plane. Flow with a smaller or negative azimuthal velocity exists near the periphery of the crucible while a flow with a velocity larger than that at a periphery of the crucible exists at the center of the crucible. The above experimental result is qualitatively identical to the phenomena explained in the previous section. If the centrifugal force is dominant in the crucible, the force acts in the opposite direction

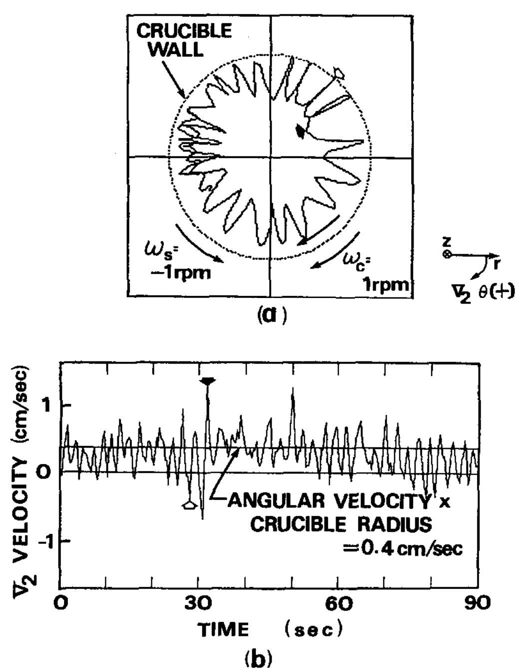

FIG. 2. (a) Plane view of the particle path with crucible and crystal rotation rates as $+1$ and -1 rpm, respectively, obtained by X-ray radiography experiment. (b) Time dependence of the azimuthal velocity component for 90 s.

as shown in equations (3) and (4) [1]. Therefore, the flow velocity, especially the radial velocity, will be decreased by the force. Consequently, the Coriolis effect which couples with the radial velocity becomes smaller. From the above consideration, we can confirm that the Coriolis force is more dominant than the centrifugal force for the silicon Cz case.

Subsequently, the flow pattern will be discussed from the numerical simulation. We have also performed the numerical simulation by the finite difference method with an assumption of axisymmetric flow as the experimental result was axisymmetric. The calculation was performed only within the melt using a commercially available code of FLUENT prepared by Creare Corp. [8]. This means that the calculation was not performed with a global model which contained the heat balance calculation in a whole furnace but a local model in which a thermal boundary condition was imposed. The simultaneously solved equations are the continuity, momentum (Navier–Stokes), and energy equations shown in the following equations for the cylindrical coordinate.

$$1/r\,\partial(rv_1)/\partial r+\partial v_3/\partial z = 0, \tag{5a}$$

$$v_1\,\partial v_1/\partial r+v_3\,\partial v_1/\partial z-v_2^2/r = -1/\rho\,\partial p/\partial r+\mu/\rho(\Delta v_1-v_1/r^2), \tag{5b}$$

$$v_1\,\partial v_2/\partial r+v_3\,\partial v_2/\partial z+v_1v_2/r = \mu/\rho(\Delta v_2-v_2/r^2), \tag{5c}$$

$$v_1\,\partial v_3/\partial r+v_3\,\partial v_3/\partial z = -1/\rho\,\partial p/\partial z+\mu/\rho\,\Delta v_3+\mathbf{g}\beta(T-T_0), \tag{5d}$$

$$\rho c_p(v_1\,\partial T/\partial r+v_3\,\partial T/\partial z) = k\,\Delta T, \tag{5e}$$

where

$$\Delta = \partial^2/\partial r^2+1/r\,\partial/\partial r+\partial^2/\partial z^2,$$

c_p and k are the specific heat and thermal conductivity, respectively. The Boussinesq approximation has been applied in the present work. The analytical conditions and thermophysical properties used in the calculation are shown in Tables 1 and 2, respectively. The *Ra*

Table 1. Analytical conditions

Parameters	Values
Crystal radius (m)	0.0188
Crucible radius (m)	0.0375
Crystal rotation rate (rpm)	−1
Crucible rotation rate (rpm)	+1
Aspect rotation (melt radius/melt depth)	1
Crucible temperature (K)	1705
Solid–liquid interface temperature (K)	1686
Free surface temperature	Linearly interpolated between 1685 and 1705 K
Free surface velocity	Free slip
Velocity boundary condition at the crucible and solid–liquid interface	Non-slip

Table 2. Thermophysical properties of molten silicon

Thermal conductivity (W m^{-1} K^{-1})	42.9
Volume expansion coefficient (K^{-1})	1.43×10^{-4}
Density (kg m^{-3})	2520
Viscosity (kg m^{-1} s^{-1})	0.7×10^{-3}
Specific heat (J kg^{-1} K^{-1})	9.683×10^{2}

number of the present system is 2.87×10^7 where the radius of the crucible was adopted as the characteristic length (l) in the Ra number: 0.0375 m. Figure 3 shows the finite different mesh of 40×40. The smaller mesh was set near the boundaries, such as the crucible wall and the solid–liquid interface. Figures 4(a) and (b) show the contours of the calculated temperature distribution and stream function, respectively. We found that the temperature distribution in the molten silicon is modulated by the buoyancy convection, as shown in Fig. 4(a), and that the buoyancy convection is dominant in the stream function, as shown in Fig. 4(b). Figure 5 shows the contours of the relative azimuthal velocity component (v_2) on a rotating basis. The upper part of the figure shows the velocity profile along A–A'. We identified that flow with larger azimuthal velocity exists at the center of the crucible while flow with smaller azimuthal velocity exists near the periphery of the crucible.

From both experimental and numerical results, we are able to conclude that the angular momentum obtained at the periphery of a crucible is conserved even at as low a rotation rate as 1 rpm when the low Prandtl number melt, such as silicon, rotates under high Grashof number conditions. Consequently, flow at the center of a crucible has a larger velocity. In the present work, we compared experimental and numerical results quantitatively because the thermal boundary condition on a crucible wall was not calculated using a global model but imposed. The previously reported flow pattern [9], especially the azimuthal velocity component, has not been modulated by the Coriolis force because one order of magnitude smaller value of the volume expansion coefficient ($\beta = 1.43 \times 10^{-5}$ K^{-1}) was adopted. The calculated flow velocity was about one order of magnitude smaller than the experimentally obtained one owing to the smaller

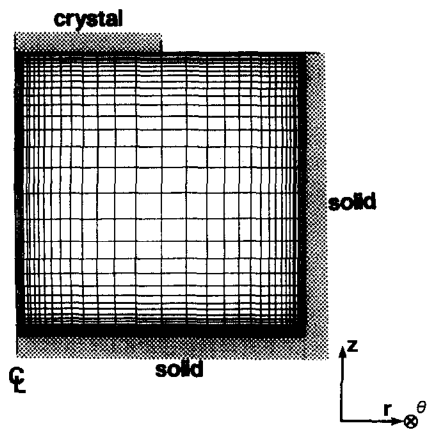

FIG. 3. The finite difference mesh (axisymmetric view).

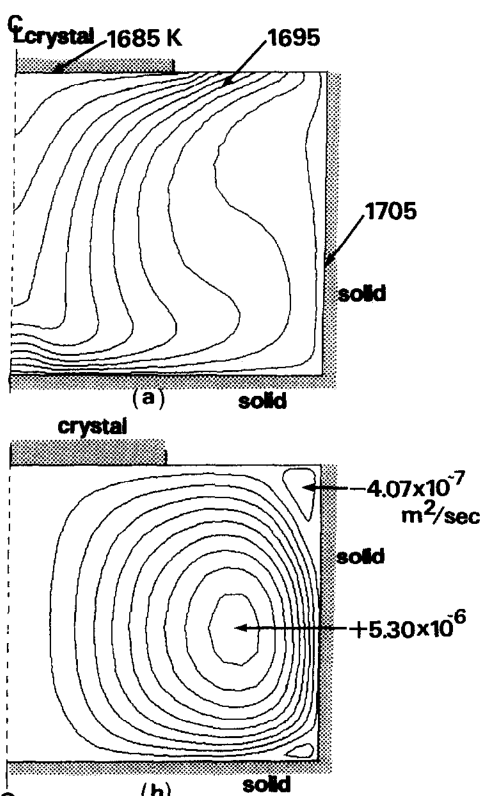

FIG. 4. (a) Calculated temperature distribution. (b) Calculated stream function.

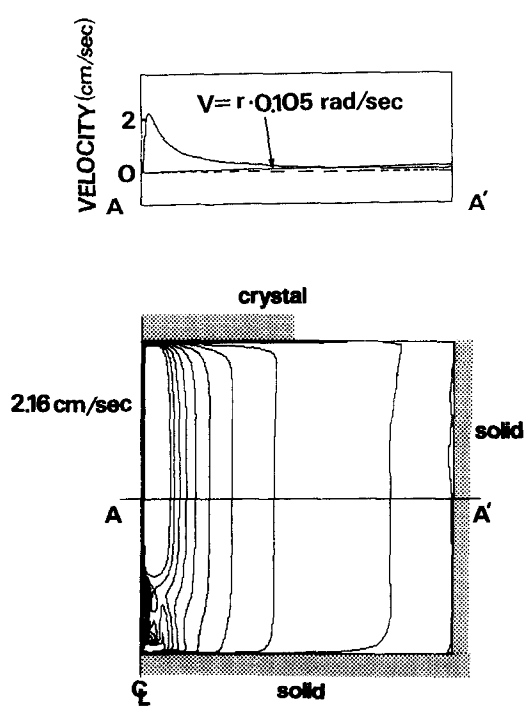

FIG. 5. Contours of the azimuthal velocity component. Velocity distribution along A–A' (upper).

Grashof number. Consequently, the calculated Coriolis force was smaller than that obtained from a larger value of volume expansion ($\beta = 1.43 \times 10^{-4}$ K^{-1}). When the diameter of the crucible becomes larger the flow velocity increases owing to the high Grashof number which contains a characteristic length, such as the crucible radius. Moreover, since the generally used rotation rate of a crucible is as large as 5–10 rpm, the Coriolis force modulates the azimuthal velocity component drastically in an industrially used system.

4. SUMMARY

The flow velocity along the azimuthal direction has been analyzed from the points of view of experiment and numerical calculation. It has become clear that the rotating molten silicon has velocity modulation in the azimuthal direction. The velocity modulation can be explained by the Coriolis force. It has also been made clear that the Coriolis force is more dominant than the centrifugal force.

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EFFET DE CORIOLIS SUR LA CONVECTION DE SILICE FONDUE DANS UN CREUSET TOURNANT

Résumé—Des cristaux uniques de silice croissent à partir d'un bain dans un creuset tournant, selon la méthode de Czochralski. On veut ici connaître le profil de vitesse dans la direction azimutale. Le profil de vitesse est obtenu par simulation numérique et la visualisation de l'écoulement par radiographie X. La simulation numérique et la visualisation montrent clairement que l'écoulement dans la direction azimutale est modulée par la force de Coriolis parce que la vitesse radiale de l'écoulement est relativement élevée. La vitesse azimutale près de la paroi du creuset a une valeur plus faible (ou négative) comparée à la vitesse angulaire du creuset, tandis qu'un écoulement à grande vitesse azimutale existe au centre du creuset.

EINFLUSS DER CORIOLIS-KRAFT AUF DIE KONVEKTION VON GESCHMOLZENEM SILIZIUM IN EINEM ROTIERENDEN TIEGEL

Zusammenfassung—Silizium-Einkristalle werden im allgemeinen nach der Czochralski-Methode in einem rotierenden Tiegel gezüchtet. In der vorliegenden Arbeit werden die Geschwindigkeitsprofile in azimutaler Richtung dargestellt. Das Profil der Strömungsgeschwindigkeit wird durch numerische Simulation ermittelt und durch Radiografie in der Strömung sichtbar gemacht. Sowohl die numerische Simulation als auch das Experiment machen deutlich, daß die Strömung in azimutaler Richtung von der Coriolis-Kraft beeinflußt wird, da die Radialgeschwindigkeit relativ groß ist. Die azimutale Strömungsgeschwindigkeit nimmt nahe der Tiegelwand im Vergleich zur Drehgeschwindigkeit des Tiegels kleinere (oder negative) Werte an. In der Mitte des Tiegels weist die Strömung dagegen eine größere Azimutalgeschwindigkeit auf.

ВЛИЯНИЕ КОРИОЛИСОВЫХ СИЛ НА КОНВЕКЦИЮ В РАСПЛАВЕ КРЕМНИЯ, ПОМЕЩЕННОМ ВО ВРАЩАЮЩИЙСЯ ТИГЕЛЬ

Аннотация—Монокристаллы кремния обычно выращиваются методом Чохральского из расплава, находящегося во вращающемся тигле. Целью настоящего исследования является определение профиля скоростей течения в азимутальном направлении. Профиль скоростей получен посредством численного моделирования и визуализации с использованием рентгенографии. При этом показано, что течение в азимутальном направлении модулируется кориолисовой силой, поскольку радиальная скорость течения сравнительно высока. Азимутальная скорость течения вблизи стенки тигля имеет малую (или отрицательную) величину по сравнению с угловой скоростью тигля, в то время как в центре тигля осуществляется течение с высокой азимутальной скоростью.