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3D numerical simulation of free surface shape during the crystal growth of floating zone (FZ) silicon

Xue-Feng Han *, Xin Liu, Satoshi Nakano, Hirofumi Harada, Yoshiji Miyamura, Koichi Kakimoto

Research Institute for Applied Mechanics, Kyushu University, 6-1 Kasuga-koen, Kasuga, Fukuoka 816-8580, Japan

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ABSTRACT

In FZ growth processes, the stability of the free surface is important in the production of single crystal silicon with high quality. To investigate the shape of the free surface in the FZ silicon crystal growth, a 3D numerical model that included gas and liquid phases was developed. In this present study, 3D Young-Laplacian equations have been solved using the Volume of Fluid (VOF) Model. Using this new model, we predicted the 3D shape of the free surface in FZ silicon crystal growth. The effect of magnetic pressure on shape of free surface has been considered. In particular, the free surface of the eccentric growth model, which could not be previously solved using the 2D Young-Laplacian equations, was solved using the VOF model. The calculation results are validated by the experimental results.

1. Introduction

The FZ method is mainly used to produce the silicon, which is employed in power electronics due to its high purity. Over the past decades, the diameter of the FZ silicon crystal has been increased from 2 to 8 in. [1]. The successful increase in the diameter of the FZ silicon gives the credit to the excellent physical properties of silicon, such as high surface tension and low density of molten silicon. The electromagnetic supporting force also plays an important role in stabilizing the shape of the molten silicon. One of the limitations of large-diameter crystal growth is gravity [2]. Its negative influence can cause obvious distortions during the growth of the large-diameter crystals. In the experiments, melt spillage, which caused the formation of bulges in the crystal, was observed.

To investigate and solve the problems of free surface, the numerical analysis dating back to 1970s has been extensively employed. For example, S.R. Coriell and M.R. Cordes solved the 2D Young-Laplace equation for a cylindrical coordinate system [3]. Following this, Riahi and K.H. Lie calculated the free surface using a high frequency induction coil [4,5]. This method was widely used in numerical simulations, and the results agreed well with experiment results [6]. Using the accurate results of the free surface shape, the induction heating power of the free surface was calculated [7]. In the industrial production of the FZ silicon, the feed rod is usually not coaxial with the crystal to help improve the homogeneity of the radial resistivity [2]. This eccentric crystal growth results in an asymmetrical shape of the free surface. Therefore, the 2D Young-Laplace equations do not apply to this phenomenon. Until now, there has been no report of a solution for 3D free surface shapes for the FZ silicon. The free surface shape is crucial for further study of heat transfer, resistivity distribution, and thermal stress in eccentric crystal growth.

In this study, a 3D numerical model has been developed using the VOF model to solve the 3D Young-Laplace equations. The contact angle of silicon was imposed at internal triple point (ITP) and external triple point (ETP). Additionally, a 3D Electromagnetic (EM) model was developed. The results of these calculations were compared with the experimental results of Wünscher et al. [6]; the results were found to be in agreement with each other. The shape of the eccentric crystal growth was also investigated.

2. Numerical models

2.1. Model of silicon melt and gas

In this study, as shown in Fig. 1, we have constructed a simulation model of an FZ silicon crystal of 50 mm diameter, considering the gas and silicon melt. The dimensions of the model are based on the experiments performed by Wünscher et al. [6]. A 3D finite volume mesh was constructed using the OpenFOAM mesh tool (snappyHexMesh [8]). A hexahedron mesh was used because, in comparison with the tetrahedron mesh in OpenFOAM, the

* Corresponding author.
E-mail address: han0459@riam.kyushu-u.ac.jp (X.-F. Han).

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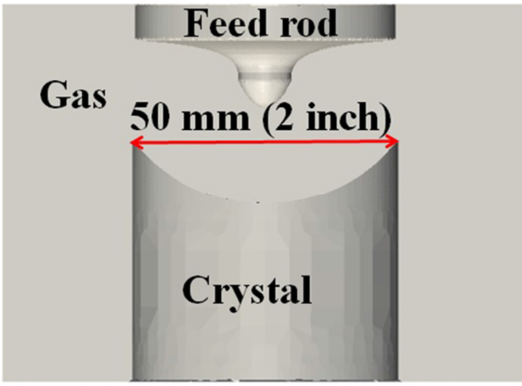

Fig. 1. Cross section of numerical model of FZ for 50 mm (2 in.) single crystal silicon in concentric growth mode.

hexahedron mesh exhibited better stability. Both the silicon melt and gas were designated as incompressible fluids to increase the stability of the calculations.

In order to track the interface between the silicon melt and the gas, a VOF model in OpenFOAM was used. In the VOF model, the continuity equation (1) and Navier–Stokes equations (2) were solved:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}) = 0, \tag{1}$$

$$\frac{\partial \rho \boldsymbol{U}}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}\boldsymbol{U}) - \nabla \cdot \tau = -\nabla p + S, \tag{2}$$

where ρ, U, t, τ, p, and S are density, velocity vector, time, stress tensor, pressure, and source term, respectively. The source term consists of surface tension force F_σ and gravity ρg:

$$S = F_\sigma + \rho g = C_k \nabla a + \rho g, \tag{3}$$

where C_k is surface tension coefficient. In Eq. (1), the density is solved as follows:

$$\rho = a\rho_1 + (1-a)\rho_2. \tag{4}$$

Here, ρ_1 and ρ_2 are the density of gas and liquid, respectively; a is the liquid fraction. Since the gas and liquid phase were regarded as incompressible fluids, the divergence of velocity should be zero:

$$\nabla \cdot \boldsymbol{U} = 0. \tag{5}$$

From Eq. (1), we can derive the following:

$$\nabla \cdot \boldsymbol{U} = -\frac{1}{\rho}\frac{D\rho}{Dt}. \tag{6}$$

Combining Eqs. (5) and (6), the equation is expressed as follows:

$$-\frac{1}{\rho}\frac{D\rho}{Dt} = -\frac{1}{\rho}\frac{D(a(\rho_1-\rho_2)+\rho_2)}{Dt} = -\frac{\rho_1-\rho_2}{\rho}\frac{Da}{Dt} = 0. \tag{7}$$

Then, we can derive the volume fraction equation as follows:

$$\frac{Da}{Dt} = \frac{\partial a}{\partial t} + \nabla \cdot (a\boldsymbol{U}) = 0. \tag{8}$$

The contact angle between silicon melt and silicon crystal is about 11° [3]. The constant contact angle θ_C is corrected in the boundary conditions when the interface had been solved:

$$\cos\theta_C = \frac{\sigma_{SG} - \sigma_{SL}}{\sigma_{LG}}, \tag{9}$$

where σ_{SG} is solid–gas interfacial energy, σ_{SL} is solid–liquid interfacial energy, and σ_{LG} is liquid–gas interfacial energy. The contact angle θ_C is determined by the highest (advancing) contact angle θ_A and lowest (receding) contact angle θ_R. The advancing contact angle is the contact angle when increasing the volume of the silicon. The receding contact angle is the contact angle when decreasing the volume of the silicon. The equilibrium contact angle is calculated in the following equation [9]:

$$\theta_C = \arccos\left(\frac{\gamma_A\cos(\theta_A) + \gamma_R\cos(\theta_R)}{\gamma_A + \gamma_R}\right), \tag{10}$$

where γ_A and γ_R are defined in the following equations:

$$r_A = \sqrt[3]{\frac{\sin^3(\theta_A)}{2 - 3\cos(\theta_A) + \cos^3(\theta_A)}}, \tag{11}$$

$$r_R = \sqrt[3]{\frac{\sin^3(\theta_R)}{2 - 3\cos(\theta_R) + \cos^3(\theta_R)}}. \tag{12}$$

More detailed calculation method can be referred in the OpenFOAM library code for multiphase solver.

2.2. Model of 3D electromagnetic force

Electromagnetic field also has an effect on the shape of the free surface. High frequency electromagnetic field in FZ is crucial to maintain the shape of the free surface. Because of the non-symmetrical distribution of current density in the inductor, the electromagnetic field in three dimensions should be taken into consideration. Since the electromagnetic field was induced by the inductor current, the current density of the inductor must be calculated. For high frequency systems, the current was adjusted by changing the voltage between the electrodes. So, a known electric potential difference between the electrodes was assumed. From the electric potential boundary condition, the electric field can be obtained by solving the following equation:

$$\boldsymbol{E} = -grad(\phi), \tag{13}$$

where E is electric field, and ϕ is electric potential. From Ohm's law for conductors, the current density J is given by

$$\boldsymbol{J} = \sigma\boldsymbol{E}, \tag{14}$$

where σ is conductivity of copper. To calculate the magnetic field, magnetic vector potential $\boldsymbol{A}$ is introduced. With appropriate gauge condition, the following equation can be derived [10]:

$$\nabla^2\boldsymbol{A} = -\mu\boldsymbol{J}, \tag{15}$$

where μ is the permeability. Since there is no magnetic material in the model, μ is same in all the domains. Magnetic vector potential $\boldsymbol{A}$ is defined such that the curl of $\boldsymbol{A}$ is the magnetic field $\boldsymbol{B}$:

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}. \tag{16}$$

The electromagnetic field could induce a potential force at the free surface. The equation for the force volume density is as follows:

$$\boldsymbol{F_{EM}} = j \times \boldsymbol{B}, \tag{17}$$

where $\boldsymbol{F_{EM}}$ is electromagnetic force volume density. It can be directly calculated using magnetic field $\boldsymbol{B}$ [11]:

$$\boldsymbol{F_{EM}} = -\frac{1}{2\mu}grad(\boldsymbol{B}^2). \tag{18}$$

The electromagnetic force $\boldsymbol{F_{EM}}$ is only applied at the interface between the gas and the melt. To take account of the electromagnetic pressure, $\boldsymbol{F_{EM}}$ is added in the Navier–Stokes equation as a source term:

$$S = \boldsymbol{F_\sigma} + \rho g + \boldsymbol{F_{EM}}. \tag{19}$$