3D Numerical analysis of free surface shape in the floating zone (FZ) silicon growth with induction coil

Han, Xue-Feng
Research Institute for Applied Mechanics, Kyushu University

Liu, Xin
Research Institute for Applied Mechanics, Kyushu University

Nakano, Satoshi
Research Institute for Applied Mechanics, Kyushu University

Harada, Hirofumi
Research Institute for Applied Mechanics, Kyushu University

他

https://doi.org/10.15017/1928653

出版情報：九州大学応用力学研究所所報. 154, pp.1-5, 2018-03. Research Institute for Applied Mechanics, Kyushu University

Reports of Research Institute for Applied Mechanics, Kyushu University No.154 (1-5) March 2018

3D Numerical analysis of free surface shape in the floating zone (FZ) silicon growth with induction coil

Xue-Feng HAN[*1], Xin LIU[*1], Satoshi NAKANO[*1],
Hirofumi HARADA[*1] , Yoshiji MIYAMURA[*1] and Koichi KAKIMOTO[*1]
E-mail of corresponding author: *han0459@riam.kyushu-u.ac.jp*

(Received January 26, 2018)

Abstract

The floating zone process includes a molten silicon zone between the feed rod of poly crystalline silicon above and single crystalline silicon below. The molten silicon zone is maintained by the high frequency induction coil. The stability of the molten silicon zone is crucial for the growth process. The shape of the molten silicon zone is determined by the surface tension force, electromagnetic force and hydrostatic pressure in the melt. Since the induction coil is not symmetric, 3D numerical model has been developed for asymmetric shape of the free surface. In this model, 3D Young-Laplacian equations have been solving using volume of fluid (VOF) model. The effect of electromagnetic force has been considered. Concentric and eccentric cases have been calculated. The calculation results are validated by the experimental results.

Keywords：*Floating zone, Silicon, Computational fluid dynamics*

1. Introduction

FZ silicon is widely used for power devices for its high purity and low concentration of oxygen. The molten silicon is heated by the induction coil in the FZ crystal growth. The needle-eye inductor is developed for single crystal growth with large diameters. The high surface tension force and electromagnetic force stabilize the molten silicon above the single crystal silicon. The shape of free surface has an effect on the heat transfer and fluid flow. During the crystal growth in the experiment, the crystal and induction coil block the view of the full free surface. In particular, the interface shape is difficult to predict if the diameter of crystal is large.

The heat is generated by high-frequency currents at thin layer adjacent to the free surface. The currents and magnetic field also generate an inward electromagnetic force at the free surface. The layer is small enough that the force is assumed to be applied at the free surface. The high surface tension, strong electromagnetic force and hydrostatic pressure determine the shape of the free surface.

*1 Research Institute for Applied Mechanics, Kyushu Univ.

Coreill et al. presented the calculation for the shape of the free surface 40 years ago [1]. They suggested a 2D model to solve Young-Laplace equation by cylindrical coordinate system. Wünscher used this method to calculate the free surface with the effect of EM pressure and compared to the experimental results [2]. However, 2D axis-symmetric calculation results could not explain the asymmetric effect in the experiment. In the industrial process, to improve the homogeneity of distribution of impurities, the eccentric growth mode is employed [3]. In the eccentric growth mode, the feed rod and crystal are not co-axial. The free surface should not be assumed as 2D axis–symmetric for eccentric growth. Additionally, there is a main slit in the induction coil. The asymmetric shape of inductor induces asymmetric electromagnetic field at the free surface. The force applied at the free surface is also not symmetric.

Therefore, in this study, 3D numerical model is developed to calculate the shape of free surface. VOF model is used to solve 3D Young-Laplace equations. The inductor is also included in the model to obtain the 3D electromagnetic field. The 3D electromagnetic force has been coupled with the shape of free surface. The contact angle of silicon is considered when the boudanry conditions of internal triple point (ITP) and external triple point (ETP) are corrected. The calculation results have been validated by comparison with the experimental results from Wünscher [2].

2. Computation method

In this study, as shown in Fig. 1, we have constructed a simulation model for FZ silicon crystals with a diameter of 50 mm (2 inch), taking into account the argon gas and the silicon melt. The size of the model is according to the experiment from Wünscher et al. [2]. The positions of ETP, melting front and solid-liquid interface are fixed in the model. A 3D finite volume mesh is constructed using the mesh tool (snappyHexMesh [4]). The hexahedral mesh is used because the hexahedral mesh shows better stability than the tetrahedral mesh in OpenFOAM. Silicon melt and gases are considered as incompressible fluids to improve computational stability.

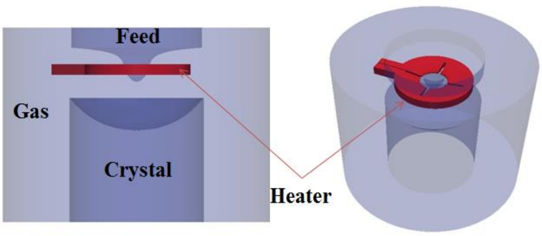

Fig.1 Concentric model of FZ for 50 mm (2 inch) diameter single crystal silicon. (red part is inductor)

The model includes gas and melt. To calculate the interface between tow fluids, VOF model in OpenFOAM was used coupling with continuity equation (1) and Navier–Stokes equations (2):

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

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

Here ρ, U, t, τ, p, and S are density, velocity vector, time, stress tensor, pressure, and source term, respectively. Surface tension force F_σ and gravity ρg are included in the source term:

$$S = F_\sigma + \rho g = C_k \nabla a + \rho g \quad (3)$$

where a is liquid fraction, C_k is surface tension coefficient. Surface tension force can be calculated by $C_k \nabla a$. The density is given by the following equation:

$$\rho = a\rho_1 + (1 - a)\rho_2 \quad (4)$$

Here, ρ_1 and ρ_2 are the density of argon gas and silicon melt, respectively. The compressibility of fluid is ignored. The divergence of velocity in the volume is zero:

$$\nabla \cdot \boldsymbol{U} = 0 \quad (5)$$

Combining the continuity equation, we can derive the following equations:

$$\nabla \cdot \boldsymbol{U} = -\frac{1}{\rho}\frac{D\rho}{Dt} \quad (6)$$

$$\begin{aligned} -\frac{1}{\rho}\frac{D\rho}{Dt} &= -\frac{1}{\rho}\frac{D(a(\rho_1 - \rho_2) + \rho_2)}{Dt} \\ &= -\frac{\rho_1 - \rho_2}{\rho}\frac{Da}{Dt} = 0 \end{aligned} \quad (7)$$

The volume fraction can be given in the equation as follows:

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

Electromagnetic force at thin layer pushes the shape of the free surface inwardly. So the calculation of high-frequency electromagnetic field is essential to investigate the shape of free surface. Due to the asymmetric distribution of the current density in the inductor, three-dimensional electromagnetic field needs to be considered. Since the electromagnetic field is caused by the induced current, three-dimensional inductor mesh is also constructed. The current density distribution in the inductor is calculated. For high-frequency electromagnetic field, the heat power is adjusted by changing the voltage between the electrodes. Therefore, it is considered that the electric potential difference between the electrodes is known. Under the electric potential boundary conditions, the electric field can be calculated:

$$\boldsymbol{E} = -grad(\varphi) \quad (9)$$

here $\boldsymbol{E}$ is electric field, and φ is electric potential. From Ohm's law, the current density $\boldsymbol{J}$ can be calculated from electric fields:

$$\boldsymbol{J} = \sigma \boldsymbol{E} \quad (10)$$

where σ is conductivity of inductor. Magnetic vector potential $\boldsymbol{A}$ can be derived by the following equation:

$$\nabla^2 \boldsymbol{A} = -\mu \boldsymbol{J} \quad (11)$$

μ is the permeability for the copper. The magnetic field can be calculated by the curl of magnetic vector potential $\boldsymbol{A}$:

$$\boldsymbol{B} = \nabla \times \boldsymbol{A} \tag{12}$$

Under the effect of magnetic field and current at the free surface, the electromagnetic force forms at the free surface. The force is given by the equation:

$$\boldsymbol{F_{EM}} = j \times \boldsymbol{B} \tag{13}$$

where $\boldsymbol{F_{EM}}$ is electromagnetic force volume density. If the magnetic field is known, the electromagnetic force can be solved by using the following equation:

$$\boldsymbol{F_{EM}} = -\frac{1}{2\mu} grad(\boldsymbol{B}^2) \tag{14}$$

Since the skin layer is so thin that the EM force $\boldsymbol{F_{EM}}$ is imposed at the interface between the argon gas and the silicon melt. Finally, the source term in the Navier-Stokes equation is revised as following form:

$$S = \boldsymbol{F_\sigma} + \rho g + \boldsymbol{F_{EM}} \tag{15}$$

3. Results and Discussion

We performed transient calculations using the model described above. In the first case, we assume that the feed rod and the crystal are coaxial. And both the feed rods and the crystals are stationary (Fig. 1). In the initial stage, the space between the feed rod and the crystal is filled with silicon melt (Fig. 2a). Since single crystal can not support too much melt, excessive melt drops due to gravity. This phenomenon has also been experimentally studied [5], especially when the crystal diameter is large. After transient calculation, the melt is stable (Fig. 2b), showing a stable interface between the gas and the melt. A stable free surface starts with ETP and ends with ITP. ETP is determined by the shape of the crystal, its diameter is 50 mm. However, ITP is calculated by VOF model that takes into account the contact angle between the melt and the feed rod. In Fig. 2b, at the top of the model, the rest of the melt does not flow down due to the contact angle boundary conditions. The amount of remaining melt is exactly the upper limit that the crystal can support. The interface coordinates are extracted to form a three-dimensional free surface, as shown in Fig. 3. The shape is symmetric despite the deviations at the periphery.

Due to the surface tension of silicon and the inward force from electromagnetic field, the shape of the free surface is stable even if the diameter of the FZ silicon is

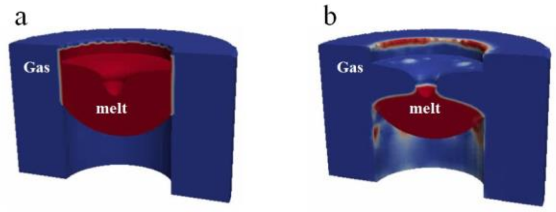

Fig.2 Silicon melt fraction (red part) and gas fraction (blue part) distribution: (a) initial condition; (b) final result after 1 s transient calculation

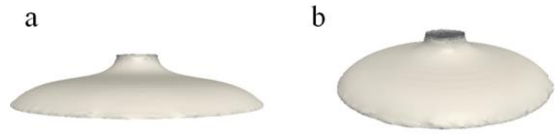

Fig.3 3D interface shape in concentric mode: (a) front view; (b) perspective view

large. Electromagnetic pressure distribution is determined by the magnetic field distribution, mainly by the geometric design of the inductor coil. The geometry of the inductor in this study is according to the experimental results obtained by Wunscher et al. [6]. There are three side slits and one main slit in the inductor (Fig. 4a). This design makes electromagnetic heating more uniform. The electric potential difference between the electrodes is 1 volt. The potential distribution is shown in Fig. 4a. The potential drops evenly from the positive electrode to the negative electrode. Fig. 4b shows the current density vector distribution. The maximum current density occurs at the tip of the side slit and at the contact part between the electrodes and the inductor. This phenomenon is described in previous calculations due to the concentration of current [6].

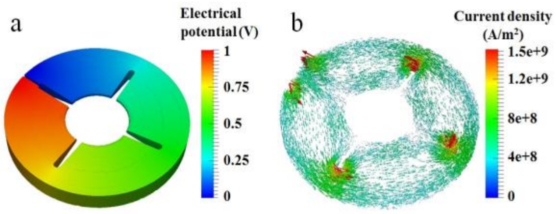

Fig.4 (a) Electric potential distribution of inductor under 1 V condition; (b) current density vector distribution in the inductor

Since the current density distribution inside the heater has been calculated above, the magnetic field distribution can be calculated. The results shown in Fig. 5a confirm that the magnetic vector is in the same direction as the current in the inductor. Since the furnace wall is electrically conductive, we assume that the value of the magnetic vector is zero at the furnace wall, which is considered to be the boundary of the computational domain. So the magnetic vector potential drops from the inductor to the furnace wall. Fig. 5b shows the magnetic field around the heater. The magnetic vector rotates around the inductor. Under applied current conditions, the maximum value is 2 Tesla. The purpose of the side slit is to distribute the magnetic field more widely.

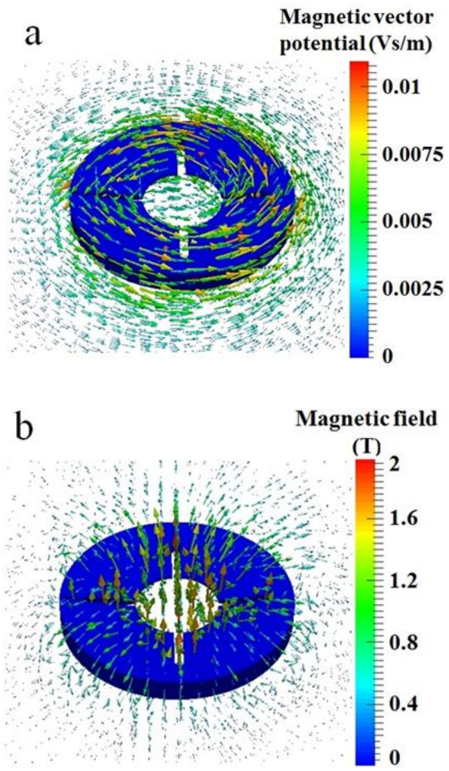

Fig.6 (a) Magnetic vector potential distribution; (b) magnetic field distribution

Because the three-dimensional calculation method is different from the two-dimensional calculation method, it is necessary to discuss the validation of this method by comparing the simulation results with the existed experimental data. Fig. 6 shows the comparison of experimental and calculation results. The experiment, conducted by Wunscher et al. [2], used a camera system to capture the image during the 2-inch FZ silicon crystal growth [6]. In Fig. 6a, the white dashed line shows the result of a two-dimensional assumption without the electromagnetic force calculated by Wunscher et al. [6]. The red line is the 3D calculation from the VOF model without electromagnetic force. It can be seen that the 3D results of the VOF model are in good agreement with the 2D results of the previous study. Since the inductor block the view of ITP, the calculation line is longer than the experimental free surface. Without the influence of electromagnetic force, the two-dimensional and three-dimensional calculations show a higher position than the experimental results. Though VOF model and 2D assumption do not consider the rotation effect and temperature, they are both credible to predict the shape of the interface by solving Young-Laplace equations.

Because the free surface is three-dimensional, three-dimensional electromagnetic field calculations are also applied to the model. In order to consider the effect of the electromagnetic field on the free surface, electromagnetic pressure is incorporated into the VOF model. We assume that the frequency of the electromagnetic field is a constant value of 3 MHz. Fig. 6b shows the comparison of the calculated results of 2D and 3D free surfaces and experimental results. Compared with Fig. 6a, the electromagnetic field calculation results fit better with the experimental results because the magnetic pressure significantly pushes the free surface to the inside. This also indicates that under high-frequency magnetic field, the silicon melt is more stable.

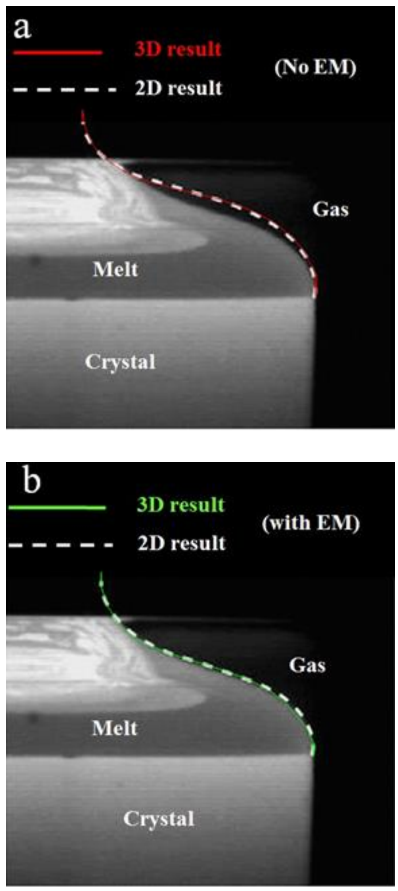

Fig.5 Comparison of free surface shape between 3D calculation results, 2D calculation results, and experimental results [2]: (a) no electromagnetic force in the calculation; (b) with electromagnetic force in the calculation

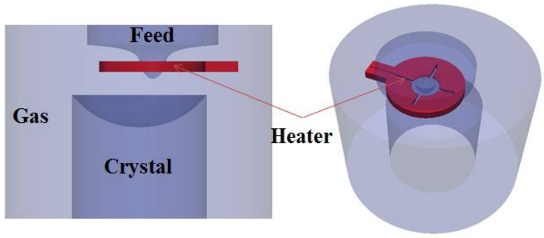

Fig.7 Eccentric model of FZ for 50 mm (2 inch) diameter single crystal silicon. (red part is inductor)

As shown in Figure 7, we also built an eccentric model to analyze the free surface. In this model, the relative positions of the feed rod and crystal are shifted by 5 mm. The other initial and boundary conditions are the same as the previous concentric calculation. In this new calculation, we assume that the ETP position remains unchanged even though the position of the feed rod and the inductor has changed. Through transient calculation results, a three-dimensional asymmetric free surface is obtained (Fig. 8). As can be seen from the side view of the free surface, the shape of the curve varies greatly in different directions, which can lead to different heating power distributions. The location of ITP also changed. In the actual growth process, if the inductor has changed, ETP and solid-liquid interface should be changed. This effect will be discussed in future research work. The successful calculation of three-dimensional asymmetric freeform surface will provide a good foundation for the future research on asymmetric induction heating.

Fig.8 3D interface shape in eccentric mode: (a) front view; (b) perspective view

4. Summary

By developing a combined model of transient VOF model and electromagnetic field model based on finite volume method, a three-dimensional free surface in the process of FZ grown single crystal silicon was obtained. In order to study the influence of the electromagnetic field, the current distribution of the inductor and the distribution of the electromagnetic field are calculated in three-dimension. The 3D electromagnetic results show a similar distribution with the previous study. It is confirmed that the magnetic pressure drives the free surface inward. By introducing the electromagnetic field into the VOF model, the 3D calculation results are in good agreement with the previous 2D and experimental results. We have successfully calculated the shape of free surface under both concentric and eccentric growth condition. The realization of an accurate free surface helps to increase the accuracy of study on the heat transfer, mass transfer and crystal quality in the future.

Acknowledgment

This work was partly supported by the New Energy and Industrial Technology Development Organization (NEDO) under the Ministry of Economy, Trade and Industry (METI).

References

1) S. Coriell, M. Cordes, Theory of molten zone shape and stability, Journal of Crystal Growth, 42 466-472, 1977
2) M. Wünscher, A. Lüdge, H. Riemann, Growth angle and melt meniscus of the RF-heated floating zone in silicon crystal growth, Journal of Crystal Growth, 314, 43-47, 2011
3) W. Dietze, W. Keller, A. Mühlbauer, Crystal Growth, Properties and Applications, in, Springer, Berlin, 1981.
4) https://openfoam.org/release/2-3-0/snappyhexmesh.
5) D.-I.R. Menzel, Growth Conditions for Large Diameter FZ Si Single Crystals, PhD thesis.
6) M. Wünscher, R. Menzel, H. Riemann, A. Lüdge, Combined 3D and 2.5D modeling of the floating zone process with Comsol Multiphysics, Journal of Crystal Growth, 385, 100-105, 2014.