Special Anniversary Issue: Professor Jan Czochralski Year 2013 — Invited Paper

Development of Crystal Growth Technique of Silicon by the Czochralski Method

K. Kakimoto*

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

We report on the Czochralski method for single silicon crystal growth and discuss heat and mass transfer and defect formation in the crystal. A reflector was used for separation of the heating and cooling areas in the furnace enabling us to speed up crystal growth. The melt flow to stabilize the temperature distribution in a crucible was controlled using transverse magnetic fields in a large-scale silicon Czochralski furnace. The setup allows for changes in important parameters of point defect formation to be made, such as vacancies and interstitials, by changing temperature and flow fields in the furnace. A numerical calculation was developed to predict the tendency for growth of a vacancy rich or interstitial rich crystal by estimating the value of the ratio between the growth rate and temperature gradient in the crystals.

DOI: 10.12693/APhysPolA.124.227

PACS: 68.08.−p, 81.10.Dn, 47.27.te

1. Introduction

Single silicon crystals are used widely in applications such as the microelectronics, solar cells, and inverter power devices. Continuous developments in devices such as large scale integrated circuits (LSIs), solar cells, and inverters are required to improve the quality of life derived from the information, energy production and energy saving fields. To realize these improvements, we need to be able to grow silicon crystals without dislocations and point defects. Growing crystals remain in contact with the quartz crucible in which the melt is set, thereby making it easy to introduce defects during crystal growth and cooling from melting point to room temperature. Study of growth velocity which affects defect formation was performed by Dr. Czochralski [1].

The dislocation free growth method developed by Teal and Little [2] allows for single silicon crystal growth without dislocations. This development allowed crystal growth researchers and engineers to increase crystal production yield, simultaneously with high crystal growth velocities and rapid cooling [3]. The growth and cooling rates of crystals without dislocation can be increased compared with those with dislocation, as the deformation is elastic and final residual stresses in the crystals are reduced at room temperature to non-existent.

Another important point of the development is the control of point defects such as vacancies and interstitials in the crystals during crystal growth. The point defects form voids and/or dislocation loops during cooling after solidification of the crystals, which degrade oxide layer properties in the LSIs [4]. Advances in information technology cannot be achieved without a reduction in void and/or dislocation loop formation. Therefore, the distribution and concentration of point defects should be controlled during crystal cooling.

The Czochralski method is a key technology to achieving advances in information technology in sustainable energy production. In this paper, we report on the development of the Czochralski method of silicon crystals related to growth rate and temperature distribution and its influence on point defect formation.

2. Growth conditions

Conditions should be selected to produce crystals of high quality and yield during crystal growth. Yield is an important production cost parameter, and is affected directly by crystal growth rate. The left half of Fig. 1 shows the simple setup during the early stages of Czochralski growth of silicon, in which a purge tube is located at the top of the furnace. The furnace consists of the melt, a crystal, crucibles, a heater and insulators. The argon gas purge tube is used to control the argon gas flow in the furnace as shown in the left half of Fig. 1. The growing crystal diameter is monitored by a camera located at the top window, with data fed back to the heating system based on a resistive heater. During crystal growth, the power distribution of the heat flux from the heater to the melt was adjusted through the crucible in the furnace. The crucible was raised during crystal growth to allow for the monitoring of the meniscus position by the camera at a fixed position [5].

Crystal growth requires a difference in chemical potential between the solid and the melt to promote crystallization. The driving force is equal to the temperature gradient in the furnace used in the Czochralski method. The use of a metal reflector located between the hot and cold parts in the furnace as shown in the right half of Fig. 1 was proposed to establish a temperature gradient in the furnace [6]. The reflector should reflect the heat flux from the hot part of the furnace including the heater and crucible to the melt. This should reduce the heat transfer

*e-mail: kakimoto@riam.kyushu-u.ac.jp

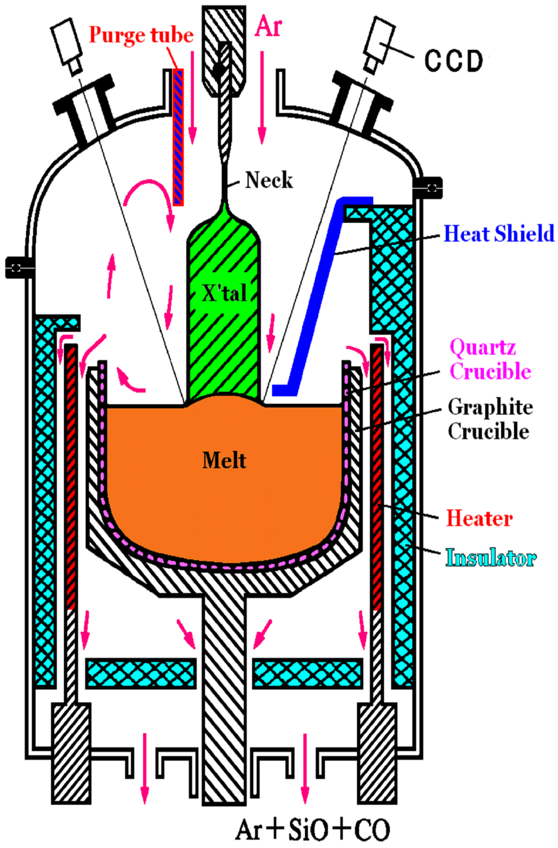

Fig. 1. Conventional and developed silicon Czochralski furnace (purge tube for controlling argon gas flow and reflector set between hot and cold portions of the furnace shown on the left and right, respectively).

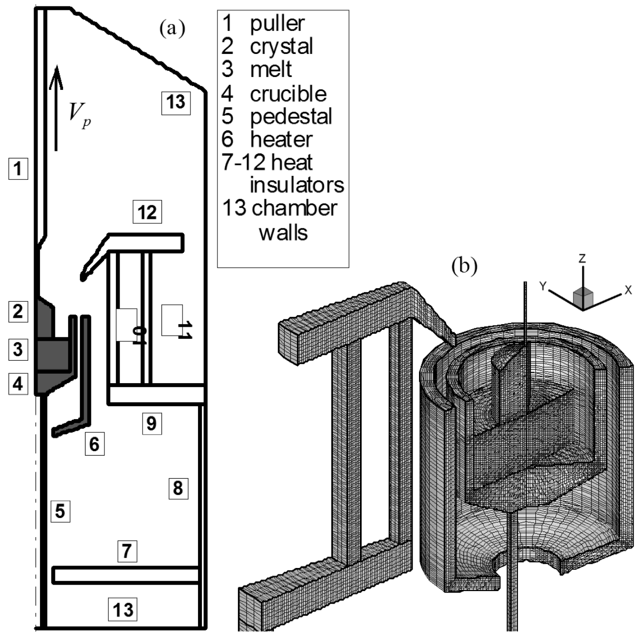

Fig. 2. Discrete system of a typical Czochralski growth furnace. (a) Configuration and domain partition: 3D domain (gray) and 2D domain (open). (b) Local view of computational grid at center domains.

from the hot to the cold part of the furnace by more effectively enhancing their separation. Heat transfer can be reduced by using a reflector with small thermal conductivity such as carbon felt. A material with small thermal conductivity reduces the heat flux from the heater to the growing crystal and increases the temperature gradient near the solid-liquid interface.

Nowadays, crystal diameters are being increased to reduce LSI production costs. A melt with large diameter is required to obtain large diameter crystals. However, melts with large diameter melt flows become unstable. The application of magnetic fields in the magnetic melts of silicon crystal growth is an effective method for controlling the shape of the melt–crystal interface and melt convection in a crucible and therefore for improving crystal quality. The method is effective for crystals with large diameter, since flow in a crucible becomes unstable and weakly turbulent because of the large mass of the melt in the crucible.

A transverse magnetic field applied to silicon CZ growth processes (TMCZ) can be used for controlling the melt flow in a large diameter crucible. The melt flow in a large diameter crucible and, hence, the global thermal field in the growth furnace is three-dimensional (3D) under the influence of a transverse magnetic field. Because the TMCZ growth furnace is a highly nonlinear and conjugated system, 3D global modeling is necessary.

Liu and Kakimoto [7] proposed a 3D global model which includes all convective and conductive heat transfer, radiative heat exchange between diffuse surfaces and the Navier–Stokes equations for the melt phase which are coupled and solved together with a finite volume method in a 3D configuration. In this study, the 3D domain (shown by the shaded area in Fig. 2a) includes the crystal, melt, crucible and heater. Diameter of the crystal was set to 32 mm in this calculation. The other regions in the furnace are included in the 2D domain. A local view of the computational grid system is shown in Fig. 2b. In a series of computations with various magnetic field intensities and crystal pulling rates, the crystal is rotated at 2 rpm. In these cases, the melt–crystal interface shapes are almost rotationally axisymmetric [7].

Figure 3 shows the influence of crystal-pulling rate (0.3 and 1.5 mm/min) on the melt–crystal interface shape and temperature distribution (Fig. 3a and b) in the crystal and melt [8]. Diameter of the crystal was set to 32 mm in this calculation. Figure 3c shows the calculated interface shapes with the two different crystal-pulling rates. The intensity of the magnetic field is set to 0.2 T in both cases. The temperature distribution in the melt is less homogeneous and the interface is more convex to the melt when a lower pulling rate is applied to the crystal. This phenomenon is related to the heat balance between the solid and the liquid through their interface where the heat of solidification is generated. The similar results were obtained by experiment [9].

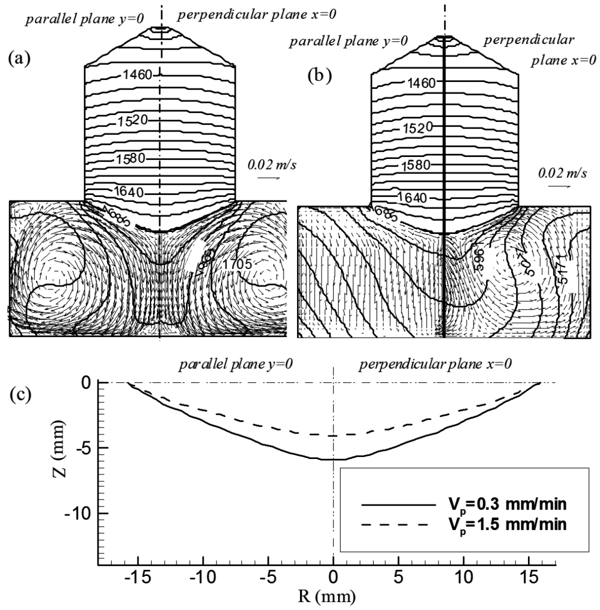

Fig. 3. Melt flow, thermal field and melt–crystal interface profiles in symmetric planes $x = 0$ (right half-plane) and $y = 0$ (left half-plane) for different crystal-pulling rates of (a) 0.3 and (b) 1.5 mm/min. Isotherms plotted every 15 and 5 K in the crystal and melt, respectively. Comparison of melt–crystal interface shapes with different crystal-pulling rates (c).

3. Control of point defect

Voronkov [8, 10] reported that the ratio between the local crystal growth rate (V_g) and the temperature gradient in the crystal near the interface (G) are a key parameter in the formation of voids and interstitial clusters. The basis of the theory is the reaction between vacancies and interstitials. Vacancies are transferred mainly by advection, while interstitials are transferred by diffusion in a crystal during cooling. Therefore, the temperature gradient in a crystal, which affects the diffusion process, and the crystal growth velocity, which affects advection, are important parameters for controlling point defects in a crystal.

Figure 4 shows the axial temperature gradients in both the crystal and the melt at the melt–crystal interface as a function of crystal pulling rate [11, 12]. Diameter of the crystal was set to 32 mm in this calculation. Solid lines show results with and without the transverse magnetic field, while dashed lines show the results without convection in the melt, approximately corresponding to the case for an infinite magnetic field intensity. The arrows in Fig. 4 show the contribution from convection in the melt. The values of axial temperature gradients in the melt and crystal were obtained by averaging the central area of the interface. These values are not identical even when the crystal-pulling rate is zero because of the difference in thermal conductivity between the crystal and the melt. These results show that the axial temperature gradients in the melt and crystal near the interface increase

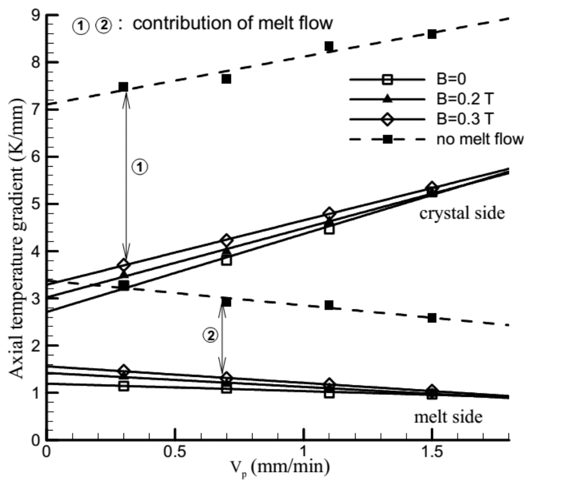

Fig. 4. Axial temperature gradients in crystal (upper part) and melt (lower part) near the interface as a function of crystal pulling rate at different applied magnetic field intensities.

with increase in magnetic field intensity. The temperature gradient near the interface in the crystal increases, while that in the melt decreases with increase in crystal-pulling rate. Meanwhile, the difference is reduced for the case with magnetic field intensity of finite value including zero and the case without melt convection. Since this difference occurs because of the melt convection, this result indicates that the contribution of melt flow is reduced with increase in crystal-pulling rate.

These phenomena can be explained as follows. When we apply a magnetic field of large intensity, natural convection in the melt is suppressed, resulting in an inhomogeneous temperature distribution in the melt. Therefore, the temperature gradient in the melt increases with increase in magnetic field intensity. Meanwhile, because of the heat balance between the liquid and solid at the interface, the temperature gradient in the crystal near the interface also increases. However, melt convection still remains even if we apply a magnetic field with relatively large intensity to the melt. As a result, even when a relatively large magnetic field of 0.3 T is applied to the system, the temperature gradients near the interface in both the crystal and the melt are far from those without melt convection, as shown in Fig. 4.

However, since a larger crystal growth rate always results in lower heater power, the temperature on the side wall of the melt decreases because of the lower heater power. The temperature difference is reduced and becomes more homogeneous in the melt. This leads to weaker melt convection because of a decrease in the thermal buoyant force induced by the temperature gradient in the melt. Therefore, with an increase in crystal-pulling rate, both the axial temperature gradient in the melt near the interface and the contribution from melt convection decrease. However, since the heat release of solidification at the interface is proportional to the crystal growth rate

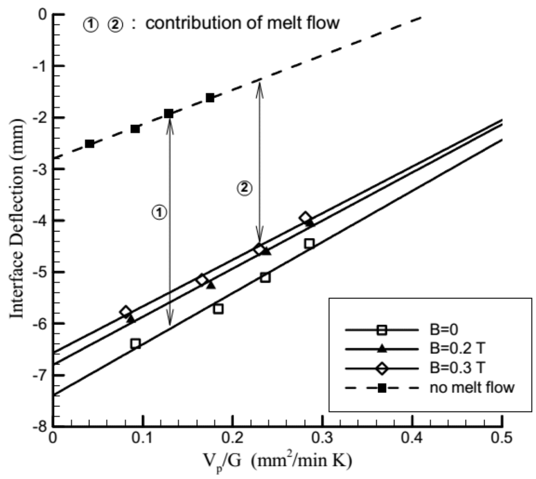

Fig. 5. Interface deflection as a function of crystal pulling rate at different applied magnetic field intensities.

and is transported away from the interface through the crystal, a larger axial temperature gradient field is generated in the crystal near the interface when the crystal--pulling rate is increased.

Figure 5 shows the interface deflection toward the melt as a function of the ratio between the crystal pulling rate ($V_{\rm p}$) and the temperature gradient in the crystal near the interface (G) [12]. Diameter of the crystal was set to 32 mm in this calculation. The values of interface deflection and the parameter $V_{\rm p}/G$ were obtained by averaging the central area of the interface. The arrows in Fig. 5 show the contribution of convection in the melt. The interface moves upward to the crystal side with increase in either the magnetic field intensity or $V_{\rm p}/G$. This tendency is consistent with that of the axial temperature gradient in the crystal near an interface shown in Fig. 4. This is because the interface shape is determined mainly by the temperature distribution in the crystal close to the interface and the melt convection in a crucible. When a magnetic field of large intensity is applied to the system or a larger pulling rate is applied to the crystal, the melt convection is suppressed and the axial temperature gradient in the crystal near the interface increases. The melt–crystal interface then moves upward to the crystal side to accommodate the increased axial temperature gradient in the crystal near the interface and the contribution from the melt convection in the crucible decreases.

4. Summary

We have reported results of defect formation, heat and mass transfer during the silicon single crystal growth by the Czochralski method. A reflector can be used to separate heating and cooling areas in the furnace and increase crystal growth velocity. Transverse magnetic fields used in a large-scale silicon Czochralski furnace allow for control of the melt flow. The TMCZ system can allow for the modification of important parameters affecting the formation of point defects such as vacancies and interstitials. A 3D calculation enabled predictions of the tendency to form vacancy rich or interstitial rich crystals by estimating the value of the ratio between the growth rate and temperature gradient in the crystals.

Acknowledgments

This work was partly supported by a Grant-in-Aid for Scientific Research (B) 24360012 of the Japanese Ministry of Education, Science, Sports and Culture.

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