Global analysis of heat transfer in Si CZ furnace with specular and diffuse surfaces

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Abstract

For the single crystal growth of silicon, a global analysis of heat transfer in a CZ furnace was carried out using the finite element method, where the radiative heat transfer between the surfaces that possess both specular and/or diffuse reflectance components was taken into account, and then the effect of the specular reflection of the crystal and/or melt on the CZ crystal growth was numerically investigated.

1. Introduction

In the Czochralski (CZ) method for the growth of semiconductor single crystals utilized in electronic devices, it is important to understand the heat transfer mechanism in the furnace for controlling the temperature fields, because the crystal quality is closely related to its thermal history in the furnace. One useful way to predict and understand the phenomena in the CZ furnace is numerical simulation, and extensive studies have recently been carried out, especially on the global analysis of heat transfer in the CZ crystal growth system of Si and GaAs single crystals. Most previous studies were concerned with the numerical simulations of the CZ crystal growth processes assuming that all exposed surfaces in the furnace are diffuse and gray in the radiative heat exchange. If the crystal and melt surfaces of silicon are considered to be specular, however, the previous mathematical model can not be used to precisely predict the radiative heat transfer in the CZ furnace.

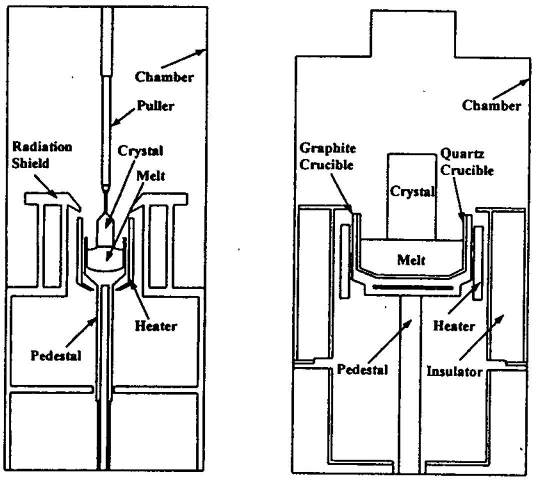
Recently, Maruyama et al.[1,2] have developed the mathematical model of radiative heat transfer between surfaces that possess both specular and/or diffuse reflectance components. In the present work, the global model of heat transfer in the CZ furnace was developed by introducing the radiative heat transfer model, in which one can predict the temperature field in the furnace with arbitrary specular and diffuse surfaces as well as the crystal shape. The effect of the specular reflection of the crystal and/or melt surfaces on the CZ crystal growth process of silicon was then numerically investigated.

2. Theoretical Model

In the global heat transfer model, the temperature distributions in the CZ furnace, the melt/crystal and melt/gas interface shapes and also the crystal pulling speed to keep the crystal diameter constant can be simultaneously computed if the furnace geometry, the temperature at the chamber wall and the heater power are given as input data. In the present work, the global model for the CZ crystal growth of oxide in our previous works [3,4] by use of the finite element method was improved to perform the analysis of the silicon CZ furnace, combining the radiative heat transfer model by Maruyama et al.[1,2].

3. Results and Discussion

In the present work, the global analyses of heat transfer were carried out for the two different CZ furnaces as indicated in Fig.1a and b, where (a) and (b) were utilized in previous studies [5,6] to grow silicon single crystals with 3.5 cm and 15.24 cm diameters, respectively. The following three cases were numerically investigated: Case 1) both the crystal and melt surfaces are diffuse; Case 2) the crystal surface is specular and the melt is diffuse; Case 3) the crystal and melt surfaces are specular. The exposed surfaces in the CZ furnace except for the crystal and melt are assumed to be diffuse.



(a) (b)

Fig.1 Schematic diagram of the CZ furnace.

Fig. 2 shows the relationship between the crystal length and Peclet number, *Pe*, in the CZ furnace shown in Fig.1a, where *Pe* is the dimensionless crystal pulling speed to keep the crystal diameter constant for a given heater power. In the figure, the result of the temperature field in the CZ furnace in Case 2 is also shown. The temperature distributions in Cases 1 and 3 were almost the same as that in Case 2. From the figures, *Pe* decreases as the crystal length increases, in other words, as the crystal growth proceeds. While, for a given crystal length, the magnitude of *Pe* in the case of the specular crystal surface, i.e., Case 2, is larger than that in Case 1 where all exposed surfaces in the CZ furnace are diffuse. This is due to the more reflected fraction of radiation energy in Case 2, which leaves the relatively hot exposed surfaces such as the crucible wall and reaches the crystal surface, to the region with the lower temperature such as the chamber wall, and consequently, the net heat loss from the furnace becomes larger than that in Case 1. The differencies in *Pe* for Cases 1-3 becomes large as the crystal length increases.

Fig.3 shows the relationship between the crystal length and the crystal pulling speed in the CZ furnace shown in Fig.1b, together with the temperature distribution in the furnace in Case 2. The variation in *Pe* with the crystal length is the same as that in Fig.2, and *Pe* in Case 2 is the largest for the three cases. However, the difference between Cases 1 and 2 becomes larger compared to the CZ system in Fig.2.

Comparing the results in Fig.2 with those in Fig.3, it is noted that the relative magnitude of *Pe* in Case 3 to that in Case 1 is significantly different in these two figures; in Fig.2, *Pe* in Case 3 is larger than that in Case 1, on the other hand, in Fig.3, the opposite trend occurs. This can be explained by the difference in the shape of the melt surface; the melt surface corresponding to Fig.2 is the curved one, while the surface in Fig.3 is almost flat. When the melt free surface is flat and specular, the radiation energy from the hot crucible is purely reflected by the melt surface and reaches the crystal surface, especially, near the tri-phase point, and consequently heats it, thus, *Pe* is decreased. On the other hand, for the curved melt surface, radiative energy reflected by the melt surface partially goes out to the relatively colder region, and thus the net heat loss from the crystal surface near the tri-phase point is relatively large, and *Pe* becomes larger than that in the case of a flat surface.

4. Conclusion

For the CZ crystal growth of silicon, a global analysis of heat transfer was carried out using the finite element method, where the radiative heat transfer between surfaces that possess both diffuse and/or specular reflection components could be taken into account. As a result, it was found that the pulling rate of the crystal with a purely specular surface becomes faster than that with a diffuse surface to maintain the crystal diameter constant for a given heater power. Also, the effect of the radiative characteristic of the melt surface on the crystal growth strongly depends on the surface shape. The effect of the specular reflection should be considered in the precise numerical simulation of heat transfer in the CZ furnace, if the crystal and/or melt surfaces are specular.

Acknowledgements

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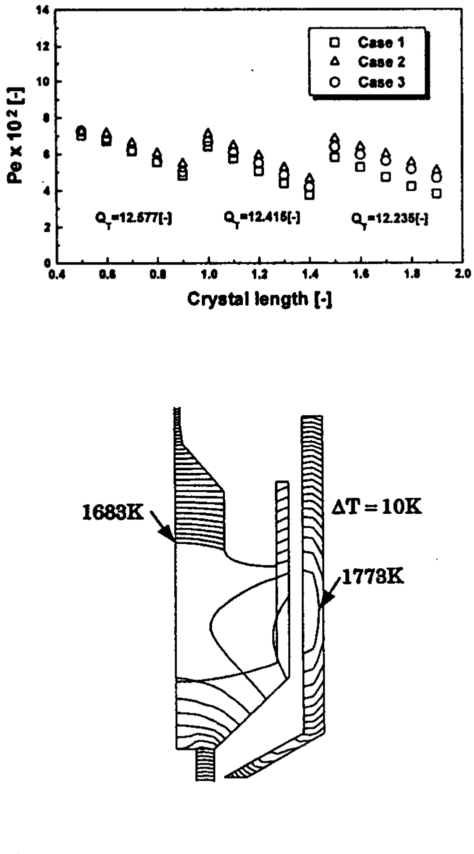

Fig.2 Variation of the crystal pulling speed with the crystal length in the CZ furnace in Fig.1a

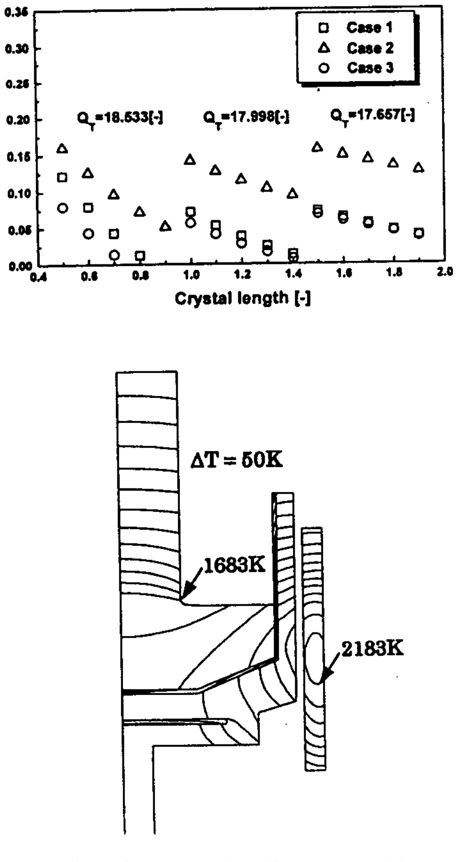

Fig.3 Variation of the crystal pulling speed with the crystal length in the CZ furnace in Fig.1b