Journal of Theoretical
and Applied Mechanics
Soifia, 1992, Year XXIII, No 2

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Mathematical Modelling of Heat Transfer in Silicon Czhochralski Growth

1. Introduction

In the Czhochralski (CZ) growth of silicon it is important to know the temperature distribution in the puller both for process control and defect engineering. The productivity of silicon crystals is directly related to the temperature distribution near the crystal-melt interface; and crystal quality parameters (like the precipitation of oxygen and the growth of stacking faults during device process) are significantly affected by the thermal history of crystals during growth. In particular, a reliable understanding of relation between the thermal history and the quality parameters is a major target of current research in silicon growers.

Since the direct measurement of the temperature distribution in a growing crystal is very difficult, the empirical approach is time-consuming and often unsuitable. This paper describes a mathematical model for analyzing the thermal history of crystals during the growth.

2. Global modelling of heat transfer in a CZ puller

Since the temperatures in a puller are strongly coupled by radiative heat exchange, thermal modelling of a whole puller is needed to predict accurately the temperature distribution. In spite of the complexity in such a modelling, several global models have been recently developed, and computer simulation of heat transfer becomes possible on the basis of reasonable boundary conditions and actual input parameters [1 - 5]. An example of the model geometry is shown in Fig.1. The whole puller is analyzed by the global model. Like other global models, our early model is based on three critical assumptions: 1) axially symmetrical temperature distribution, 2) conduction dominant heat transfer in the melt, and 3) diffuse grey radiation.

By using the model, two types of pullers are analyzed. One is a laboratory scale puller with a 6 inch crucible and a 2 inch crystal, and the other is an industry scale puller with a 16 inch crucible and a 6 inch crystal. Fig.2 shows the calculated thermal history of a 2 inch crystal in a laboratory scale puller. The dashed line in Fig.3 shows the same data, as in Fig.2. This result shows that the temperature distribution in a growing crystal is mainly determined by the distance from the free surface, but less sensitive to the grown crystal length and to also to the growth rate. This result implies also that the thermal history or cooling rate of the crystal depends almost on the pull rate only. The model results were verified by the experiments on a laboratory puller. Measured temperatures in a test crystal are also plotted in Fig.3. Calculation predicts well the measured results. Temperatures in the heat shield and heater power were also measured and compared with the calculated results, and both results were in good agreement.

For an industry scale puller, the temperature distribution in a crystal is also determined mainly by the distance from the melt, but the calculated heater power appreciably overestimates the measured value by 20 %.

3. Modelling of heat transfer in the melt

The validity of the conduction dominated heat transfer in the melt is studied by comparing three different computer models: conduction dominated model, 2D laminar convection model, and 2D k-epsilon model of turbulence [6]. The results show that the conduction dominated model is valid for a small scale melt only, but heat transfer is convection dominated for an industrial size melt.

Although 2D laminar models are widely used for analyzing melt convection [1,2,4], recent studies reveal that the melt convection is most likely turbulent [7]. The possibility of a k-epsilon model of turbulence is studied for modelling the heat transfer in the melt [8].

Surface temperatures at the centre of the Si CZ melt was measured by using a two-colour optical pyrometer in an industry scale puller, and the effects of crucible rotation on the temperature were examined. An example of temperature record is shown in Fig.4. The mean temperature decreased with the increase of the crucible rotation rate, while the heater temperature was kept constant through the measurements. Relationship between the melt temperature and crucible rotation rate are shown in Fig.5a for two runs. As shown in Fig.4, the measured temperature always fluctuated around the mean value. Fig.5b shows the peak-to-peak values of temperature fluctuation in connection with the crucible rotation rates.

The mean temperatures and temperature fluctuation in the melt were analyzed on the basis of k-epsilon model of turbulence. The boundary conditions of temperature were extracted from the results of conduction dominant global model for run A. The results are shown in Fig.6. It is remarkable that both tendency and order of calculated values agree fairly good with the experimental results. The k-epsilon model of turbulence seems to reproduce the nature of heat transfer in a silicon CZ melt.

4. Summary

The temperature distribution in a growing crystal is almost independent of the pull rate and crystal length. It is mainly determined by the distance from the melt surface. This implies that the thermal history (cooling rate) of a crystal depends almost on the pull rate only. These model results are verified for a laboratory scale puller by the experimental work, and important for understanding the relation between the thermal history and the quality parameters of the silicon crystal.

For analyzing an industrial scale puller, modelling of convective heat transfer in the melt is necessary for a more quantitative prediction. The capability of the k-epsilon model of turbulence is shown. Integration of the global model with the turbulence model is now in progress.

References

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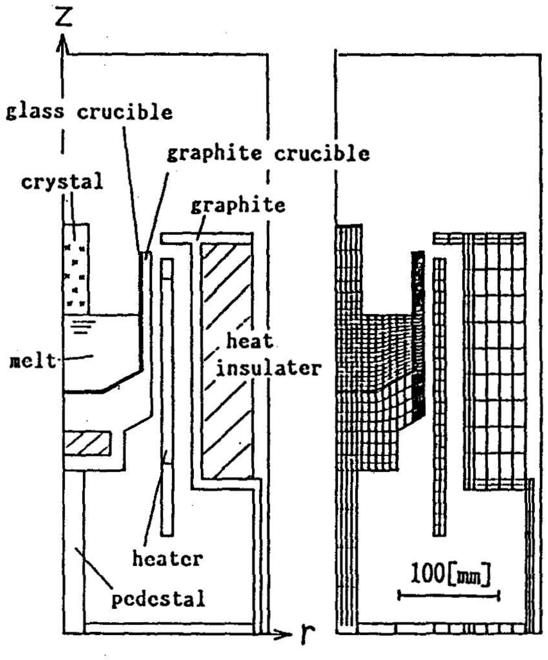

(a) geometry (b) grid

Fig.1 Model geometry of a CZ puller.

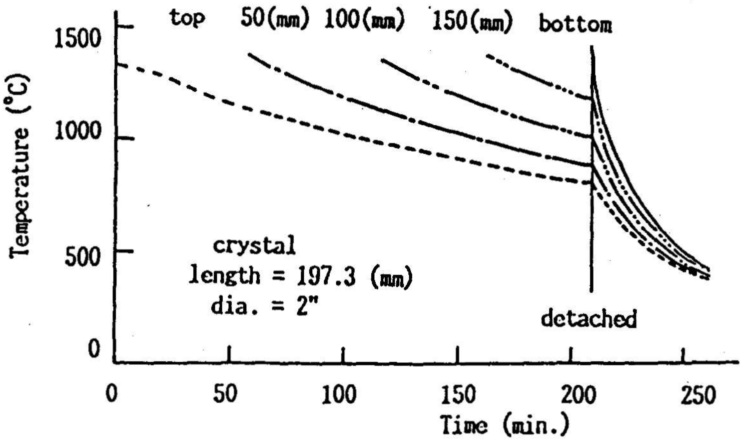

Fig.2 Thermal history of a growing crystal (calculated).

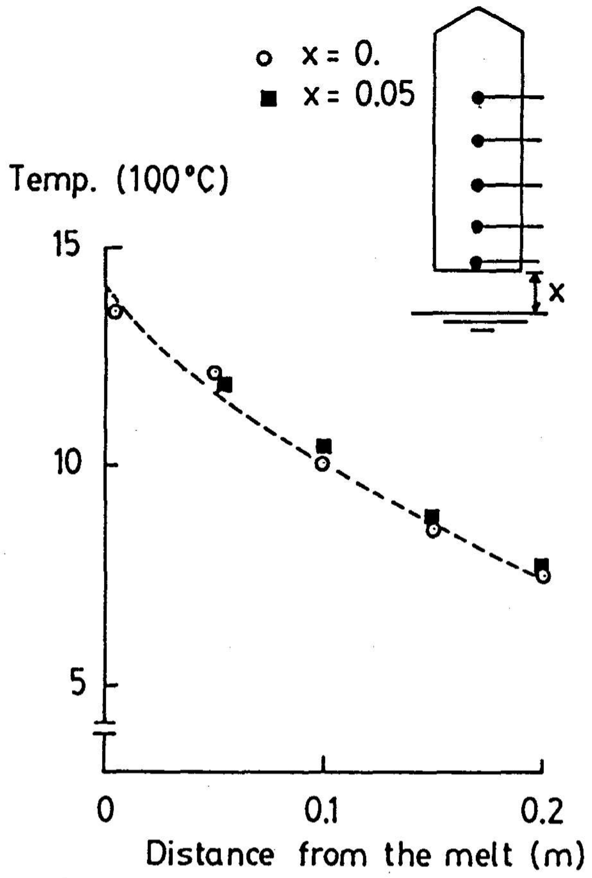

Fig.3 Calculated and measured temperature distribution in a crystal. — — — calc., o ■ measured

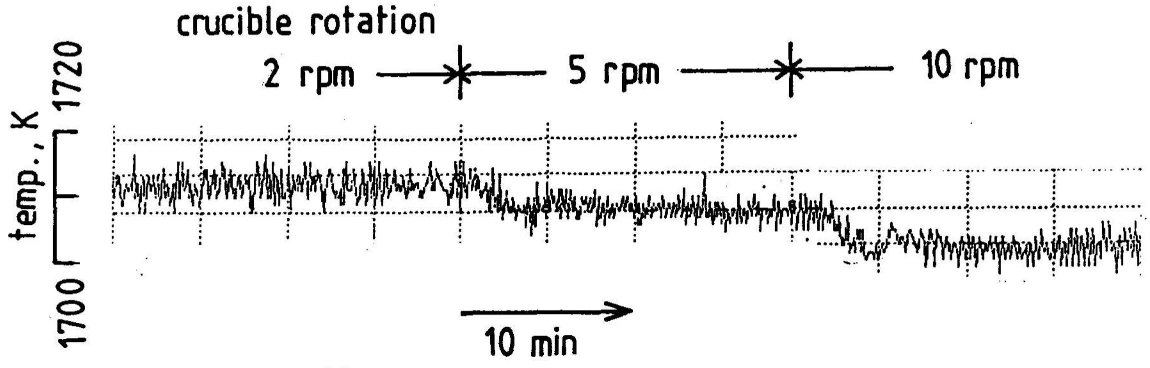

Fig.4 An exmaple of temperature record (run A)

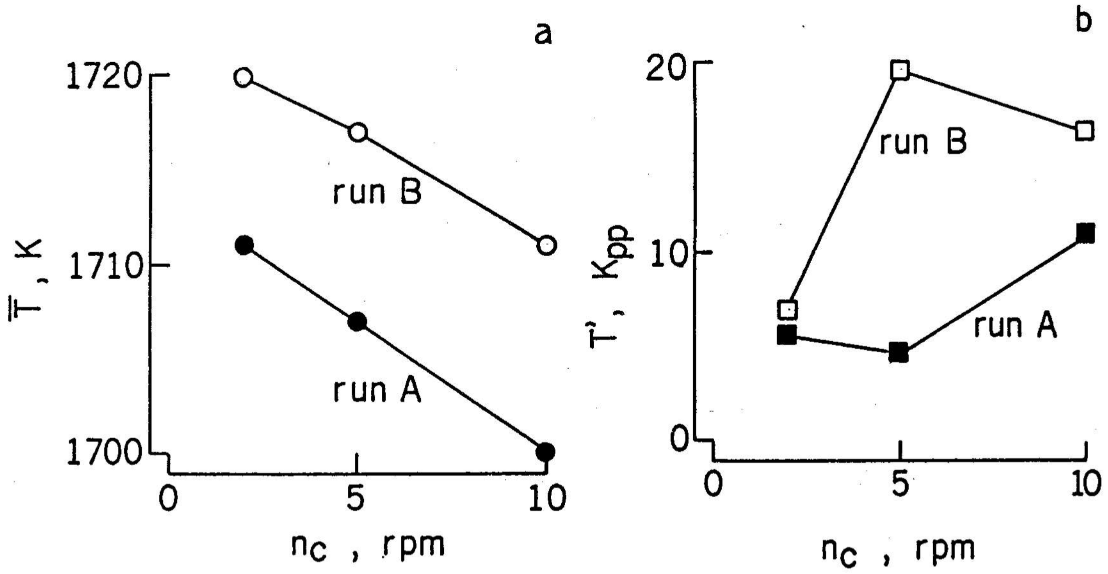

Fig.5 Measured dependence of melt temperature on crucible rotation rate. (a) mean temperature, (b) temperature fluctuation.

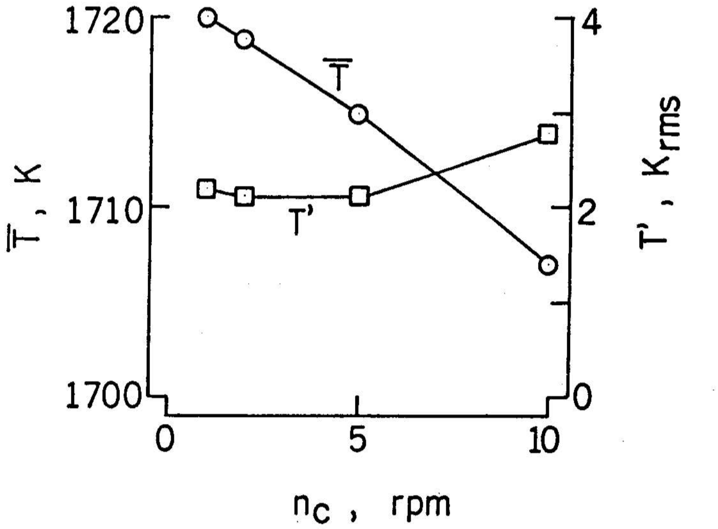

Fig.6 Calculated dependence of melt temperature on crucible rotation rate. $\bar{T}$: mean value, T': fluctuation.