Optimization of temperature distribution transition in Directional Solidification method without restriction of growth furnace structure

Hiroyuki Tanaka[1*], Kentaro Kutsukake[2], Takuto Kojima[3], Xin Liu[1], Noritaka Usami[1].
*lead presenter: t.hero.material.1753@gmail.com
1 Graduate School of Engineering, Nagoya University
2 Center of Advanced Intelligence Project, RIKEN
3 Graduate School of Informatics, Nagoya University

In the crystal growth of Si by directional solidification (DS) method, it has been reported that the temperature distribution around the crystal has a significant effect on the crystal quality and the growth furnace structure affects the temperature field during the process. However, there has been no investigation of crystal growth with flexible changes in the temperature field independent of the growth furnace structure. In this study, we created an original calculation model that can perform crystal growth simulations focusing on the crystal surroundings without assuming a specific growth furnace and performed transient calculations for various temperature distribution transitions. Using the obtained calculation results, a machine learning model was constructed, and a mathematical optimization method was used to search for the temperature distribution transition around the crucible for high-quality Si ingot.
Crystal growth analysis software CGSim (STR) was used for the two-dimensional transient thermo-fluid simulation and the dislocation propagation calculation based on the Alexander-Haasen model. The geometry of the model to represent Si in a quartz crucible in an Ar atmosphere is shown in Fig. 1. The time series temperatures were given as the boundary conditions on the perimeter of the simulation area for the transient calculations of the cooling process from the melt. Firstly, the boundary condition temperatures were randomly generated for selected 13 nodes using a quartic function with constraints where the initial and final temperatures were fixed, and the continuity and temperature range of the profiles were considered. Then, the temperatures at all boundary nodes were obtained by cubic spline interpolation. From the results of 200 converged simulations, a deep neural network (DNN) was constructed to predict the solid-liquid interface shape transition during crystal growth and the dislocation density distribution of the ingot from the temperature distribution transition around the crucible. Then, the genetic algorithm (GA) equipped with the predictor searched for the optimal recipe according to multi-objective combination of the lower dislocation density and shorter crystallization time. Fig. 2 shows the optimum temperature distribution transition of the crucible side wall. Fig. 3 shows a comparison of the dislocation density distribution of Si ingot simulated by our experimental recipe and the optimum temperature distribution transition. The dislocation density was decreased in the upper Si ingot by the optimal recipe.

Acknowledgment: This work was partially supported by JST/CREST, Grant No. JPMJCR17J1 (2017-2023).

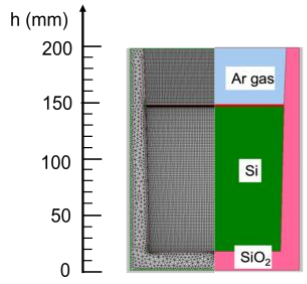

Fig. 1. Calculation model

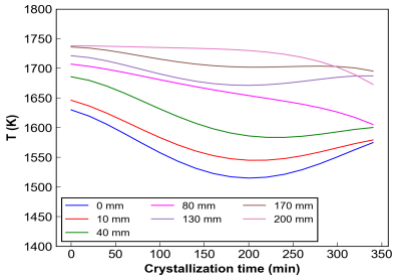

Fig. 2. Optimum temperature. distribution transition

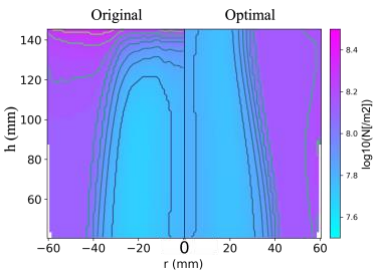

Fig. 3. Dislocation density distribution