Evaluation of Numerical Modeling on Constitutional Supercooling during Heavily Boron Doped Silicon Single Crystal Growth using Cz Method

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The heavy doping of impurities such as boron (B) and phosphorus (P) during the growth of silicon (Si) single crystals using the Cz method has been known to degrade the quality of the grown crystals. This degradation is associated with morphological instabilities, such as cellular growth, caused by constitutional supercooling (CS) at the growth interface [1,2]. Therefore, it is essential to prevent CS during growth in order to produce high-quality, heavily doped Si single crystals.

In this study, we conducted a three-dimensional unsteady numerical simulation which considered the transport and segregation of dopant (B) in the melt to predict the formation of CS during the growth of Si single crystals using the Cz method. The simulation resulted in the determination of the actual and equilibrium temperature gradient in the melt near the growth interface, where the latter was calculated by the local gradient of B concentration. The difference between the gradient of actual and equilibrium temperature is defined as the constitutional supercooling gradient (CSG). Negative values of CSG may indicate the occurrence of CS at the growth interface.

We evaluated the validity of our numerical model by comparing the calculated CSG distributions with experimental results. It was found that the time and rotational averaged CSG distribution over the growth interface obtained by numerical simulation agreed with the region of cellular growth observed in the experiment.

References

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