3D Finite Volume Scheme for Czochralski Crystal Growth

Jing Lu, Zibing Zhang, Qisheng Chen [*]

Institute of Mechanics, Chinese Academy of Sciences, 15 Beisihuanxi Road, Beijing, 100080, China
e-mail: qschen@imech.ac.cn

Abstract

Czochralski (Cz) technique, which is used for growing single crystals, has dominated the production of single crystals for electronic applications. The Cz growth process involves multiple phases, moving interface and three-dimensional behavior. Much has been done to study these phenomena by means of numerical methods as well as experimental observations. A three-dimensional curvilinear finite volume based algorithm has been developed to model the Cz process. A body-fitted transformation based approach is adopted in conjunction with a multizone adaptive grid generation (MAGG) technique to accurately handle the three-dimensional problems of phase-change in irregular geometries with free and moving surfaces. The multizone adaptive model is used to perform a three-dimensional simulation of the Cz growth of silicon single crystals.

Since the phase change interface are irregular in shape and they move in response to the solution, accurate treatment of these interfaces is important from numerical accuracy point of view. The multizone adaptive grid generation (MAGG) is the appropriate scheme for thi s purpose. Another challenge encountered is the moving and periodic boundary conditions, which is essential to the numerical solution of the governing equations. Special treatments are implemented to impose the periodic boundary condition in a particular direction and to determine the internal boundary position and shape varying with the combination of ambient physicochemical transport process and interfacial dynamics. As indicated above that the applications and processes characterized by multi-phase, moving interfaces and irregular shape render the associated physical phenomena three-dimensional and unsteady. Therefore a generalized 3D model rather than a 2D simulation, in which the governing equations are solved in a general non-orthogonal coordinate system, is constructed to describe and capture the features of the growth process.

All this has been implemented and validated by using it to model the low pressure Cz growth of silicon. Accuracy of this scheme is demonstrated by agreement of simulation data with available experimental data. Using the quasi-steady state approximation, it is shown that the flow and temperature fields in the melt under certain operating conditions become asymmetric and unsteady even in the absence of extrinsic sources of asymmetry. Asymmetry in the flow and temperature fields, caused by high shear initiated phenomena, affects the interface shape in the azimuthal direction thus results in the thermal stress distribution in the vicinity, which has serious implications from crystal quality point of view.

REFERENCES

[1]   V. Prasad, H. Zhang, A. P. Anselmo. *Transport phenomena in Czochralski crystal growth*, in J. P. Harnett, Thomas F. Irvine Jr. eds. *Advances in heat transfer*, vol. 30, (1997).
[2]   H. Zhang, V. Prasad, M. K. Moallemi, *A numerical algorithm using multizone adaptive grid generation for multiphase transport process with moving and free boundaries*, Num. Heat Transfer, Part B, 29, (1996), 339-421.