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3D Crystallization Interface Correction in Simulation of Czochralski Crystal Growth with Asymmetric Magnetic Fields

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Introduction

An important topic in numerical simulation of Czochralski is crystallization interface correction. In 2D axisymmetric model or 3D model with almost axisymmetric flow, crystallization interface can be adjusted to same temperature or same crystallization rate by direct nodal motion without extra data treatment.

While with non-axisymmetric flow, some issue will happen. Fig. 1a) shows a non-axisymmetric temperature distraction on flat interface (before correction) when transverse magnetic field is applied. If the interface is adjusted to the averaged temperature of triple points(TPs), then local grid distortion will occur near TPs whose temperature are below the mean temperature. A solution to this issue will be described below.

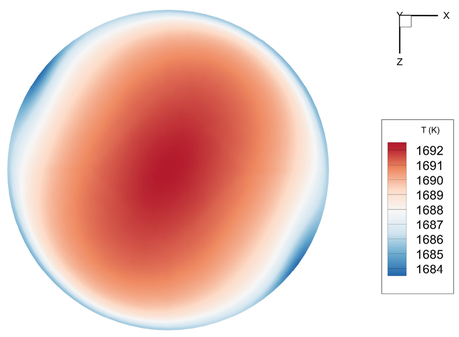

Fig. 1a) Temperature distribution on flat crystallization interface (before correction).

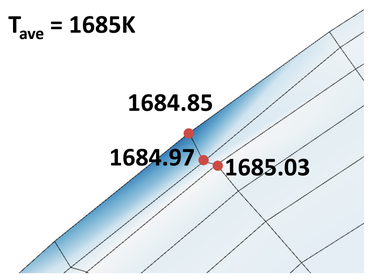

Fig. 1b) Local grid distortion at crystallization at interface after directly correction to same temperature.

Modeling approach

The crystallization interface is corrected by two methods according conservation of heat flux (Equation 1). One is temperature-based; another is crystallization-rate-based.

The main point is T_f and V_n are polynomial fitted to an axisymmetric distributed $T_f(r)$ and $V_n(r)$. The nodal displacement is also axisymmetric. Finally, an axisymmetric interface can be obtained.

$$\left(k\frac{\partial T}{\partial n}\right)_c - \left(k\frac{\partial T}{\partial n}\right)_m = \rho_c \Delta H V_n \qquad (1)$$

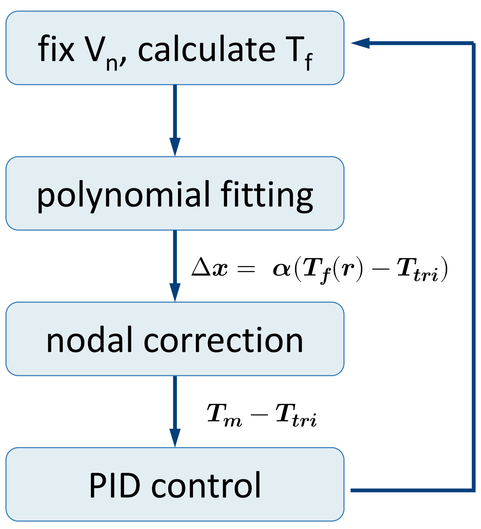

Fig. 2a) Flow diagram of temperature-based interface correction

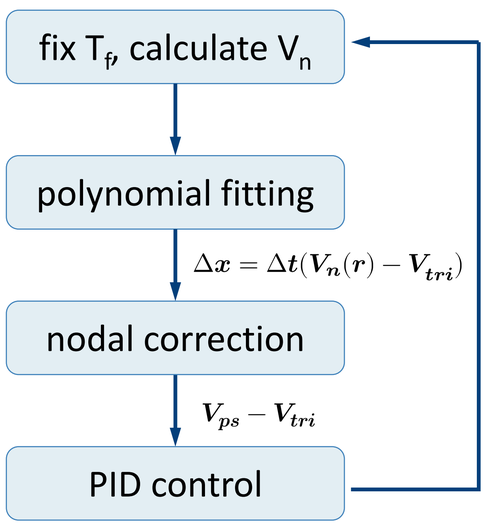

Fig. 2b) Flow diagram of crystallization-rate-based interface correction

Result & Discussion

Fig. 3 shows the scatter distribution of face center temperature on flat interface. The polynomial fitting function $T_f(r)$ is assumed as circumferential averaged temperature. Then T_{tri} is calculated by $T(d/2)$, where d is the diameter of the crystal.

After interface correction, the scatter distribution of face center temperature is shown in Fig. 4. It shows the circumstantial averaged temperature is at melting point (1685K).

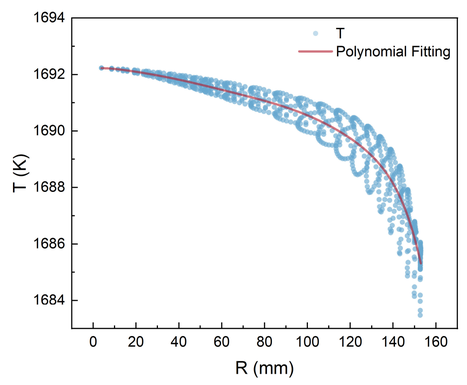

Fig. 3 Scatter distribution of face center temperature on flat interface after T_{tri} are modified to melting point. The read line shows the polynomial fitted value.

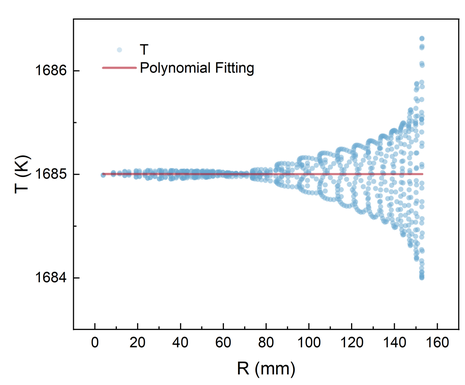

Fig. 4 Scatter distribution of face center temperature on corrected interface after T_{tri} are modified to melting point. The read line shows the polynomial fitted value.

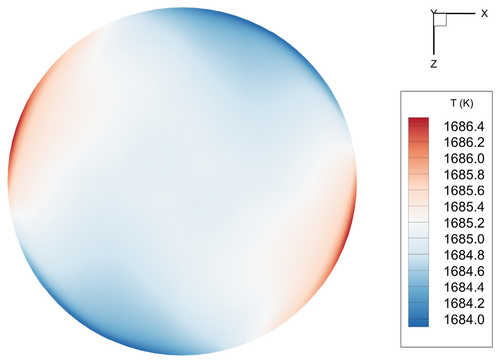

Fig. 5a) temperature distribution of interface after correction

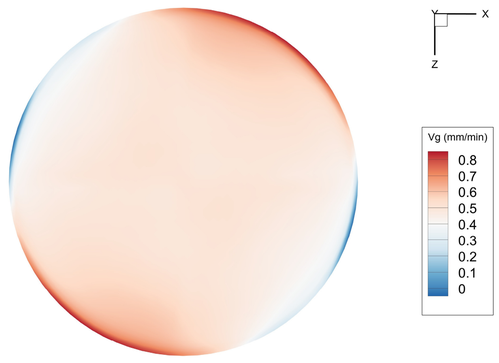

Fig. 5b) crystallization rate distribution of interface after correction

Fig. 5 shows the temperature and crystallization distribution after interface correction. The cold areas at Fig. 5a) correspond to the high crystallization rate area at Fig. 5b), which presents a good consistency. The non-axisymmetric features are well captured.

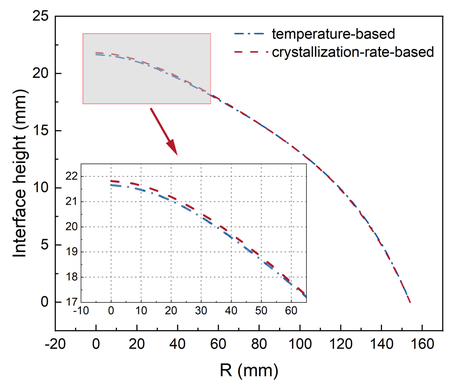

Fig. 6 Interface shape of two different correction methods

Fig. 6 shows the nodal position of the interface corrected by two methods. The interfaces corrected by the two methods are almost coincident, and the maximum deviation is about 0.2 mm.

Conclusion

Considering the crystal rotation, the crystallization interface is almost axisymmetric in actual situation. Here, polynomial fitting is considered as a method of circumferential averaging due to the convenience of data processing. The interface is corrected based on the polynomial fitted data. Finally, an axisymmetric interface can be obtained by two correction methods, and the results showed great consistency.