Modeling of Crystallization Velocity Dependence on Undercooling and Crystallographic Orientation for FZ Silicon Crystal Growth

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Abstract

This article presents the results of modeling the facet development on the crystallization interface in the FZ silicon growth. The microscopic crystal growth model from [1] and a simplified algebraic heat transfer model were used in the FZ growth model. The silicon crystal growth in (1,1,1) direction was modeled, and the influence of different model parameters on the quasi-stationary form of the crystallization interface was examined.

Introduction

The development of facets on the crystallization interface can significantly affect the silicon crystal growth in the FZ process by modifying the temperature and melt flow distributions. The correct modeling of facet development requires a microscopic crystal growth model that relates the local crystal growth rate with local crystallization interface temperature and the interface orientation towards a facet plane (misdirection angle).

The aim of the authors is develop an axisymmetric FZ process model that would incorporate the microscopic growth model from [1] together with a model for heat transfer in the melt and solid that would allow modeling the facet development in the FZ process. To facilitate the development of such a model, the microscopic growth model was coupled with a simplified algebraic heat transfer model to analyze the influence of various model parameters on the calculated crystallization interface form and to optimize values of these parameters.

1. Microscopic Model of Crystal Growth

1.1 Interface Flatness or Roughness

The microscopic model of crystal growth applied in this article is taken from [1]. Here follows a short description of this model.

In general the crystal growth rate is determined by microscopic flatness or roughness of a crystallization interface. The roughness of a crystal surface at equilibrium for a square-lattice crystal is determined by a simplified Jackson criterion α:

$$\alpha = \frac{4\phi}{k_B T_0},$$
(1.1)

where ϕ is generalized bond energy, k_B is Boltzmann's constant, and T_0 is the melting point. Interfaces with $\alpha > 2$ are flat; interfaces with $\alpha < 2$ are rough. According to Jackson, [2], for silicon, only faces like (1,1,1) can be flat ($\alpha = 2.7$); α for all other faces is less than 2.

1.2 Crystal Growth Rate Model for Different Growth Regimes

The crystal growth rate in the normal direction to the interface is usually expressed as:
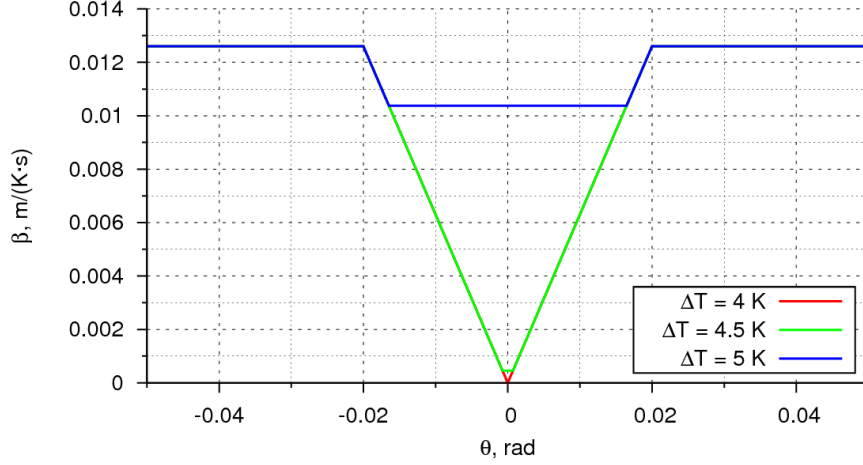
$$V_n = \beta \Delta T , \tag{1.2}$$

Fig. 1. Dependence of the kinetic coefficient on the misdirection angle for different undercoolings

where β is the kinetic coefficient of the crystal growth, and ΔT is the crystallization interface undercooling. Depending on the crystal growth regime, β can itself be a function of undercooling and the angle θ between the crystallization interface and a facet plane (misdirection angle). In this article, three growth regimes are considered: the rough growth, the layered growth from edges, and 2D nucleation.

The rough growth is characterized by a constant kinetic coefficient β_{rough} =0.0126 m/(s·K). In the layered growth on a flat surface, the crystal grows from edges, filling a layer after a layer. Such growth is characterized by the kinetic coefficient β_{SN} =β_{st}|sin θ|, where β_{st}=0.63 m/(s·K). The growth by 2D nucleation mechanism also occurs on a flat surface: 2D atom clusters form spontaneously on the surface, and then grow laterally. Such growth is modeled by the kinetic coefficient β_{2D} =B $exp(-A/\Delta T)$ cos θ, where B=1.5·10^{10} m/(s·K), A=140 K.

All the three growth mechanisms are incorporated into one expression:

$$\beta(\Delta T, \theta) = \min(\beta_{rough}, \max(\beta_{2D}(\Delta T, \theta), \beta_{SM}(\theta))) . \tag{1.3}$$

Fig. 1 shows dependence of the kinetic coefficient on the misdirection angle for different undercooling values.

2. Numerical Algorithm for Interface Motion Based on the Microscopic Model

In 2D axisymmetric approximation, a crystallization interface is represented by a set of straight segments in the meridional plane. The numerical modeling of the crystallization interface requires parallel solution of the temperature distribution in the melt and solid, which provides the interface temperature distribution. Assuming that the interface temperature distribution is given, one can calculate the new crystallization interface in two steps. In the

first step, the vertical displacements for ends of each linear segment are calculated. For example, segment n in Fig. 2 has two ends, points i and $i+1$, which locally can be designated as 1 and 2. To calculate their vertical displacements, at first their distances ΔR_1^n and ΔR_2^n to the facet plane are calculated. For the end with highest distance, end 2 in the example, it is assumed that it grows in the direction normal to the facet plane, so that the vertical displacement for it is calculated as:

$$\Delta H_2^n = \frac{\beta(0, \Delta T_2^n) \Delta T_2^n}{\vec{n}_f \cdot \vec{e}_y} \Delta t_i,$$
(2.1)

where Δt_i is the crystal growth time step. For the end that is closest to the facet plane (end 1), the vertical displacement is calculated as:

$$\Delta H_1^n = \frac{\beta(\theta, \Delta T^n) \Delta T^n}{\vec{n} \cdot \vec{e}_y} \Delta t_i,$$
(2.2)

where ΔT^n is average undercooling of the segment: $\Delta T^n = (\Delta T_1^n + \Delta T_2^n)/2$.

In the second step, the final value of the vertical displacement for each interface point is calculated as a maximum of the segment displacements on its either side, for example:

$$\Delta H_{i+1} = \max(\Delta H_2^n, \Delta H_1^{n+1}).$$
(2.3)

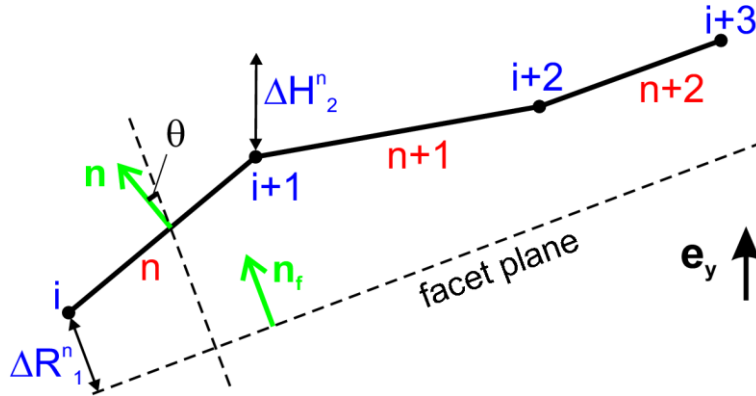
Fig. 2. Calculation of a new crystallization interface form

3. A Simplified Model for the Heat Flow Calculation on the Crystallization Interface

The heat flow densities in the melt and solid on the crystallization interface are modeled with a simplified algebraic model. It is assumed that the melt is above the solid crystal and that the forms of $T_+=1705$ K and $T_-=1665$ K isotherms are given as predefined functions of radius x and height y. Then the vertical projections of the heat flow densities in the melt and solid, q_m and q_s, on a crystallization interface point with interface temperature T_f can be calculated as:

$$q_m = \lambda_m \frac{T_+ - T_f}{\Delta z_+},$$
(3.1)

$$q_s = \lambda_s \frac{T_f - T_-}{\Delta z_-},\qquad(3.2)$$

where Δz_+ and Δz_- are the distances between the interface point and T_+ and T_- isotherms, see Fig. 3.

The boundary condition for the heat flow balance on the crystallization interface requires that the following relation between the heat flow densities and the pulling velocity v_p hold:

$$q_m + v_p \rho q_0 = q_s,\qquad(3.3)$$

$$q_m + v_p \rho q_0 = q_s$$

Fig. 3. An algebraic model for heat transfer on the crystallization interface
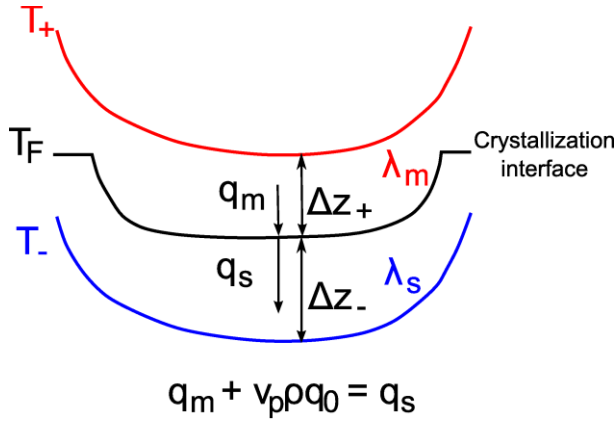
where ρ is the crystal silicon density, and q_0 is latent heat of fusion. Thus if the crystallization interface form is given, (3.1), (3.2), and (3.3) can be used to calculate such interface temperature value T_f that ensures this boundary condition.

4. Final Model for Quasi-stationary Crystallization Interface Form

The quasi-stationary crystallization interface form is calculated iteratively with a given temperature recalculation time step, which is equal or larger than the crystal growth time step. Every iteration consists of two steps: temperature and crystallization interface recalculation steps. The calculation begins with an initial crystallization interface form. As a first step, the interface temperature distribution is calculated from (3.1), (3.2), and (3.3). After that the crystallization interface form is recalculated according to (2.1), (2.2), and (2.3) with fixed interface temperature. Since the crystal growth time step could be smaller than the temperature time step, several crystal interface recalculations can be made during the iteration. This iterative procedure is repeated until the crystallization interface stops changing.

5. Calculation Examples

To investigate the influence of the model parameters on the form of the calculated crystallization interface, the following silicon material properties were used: solid state density ρ=2329 kg/m^3, latent fusion heat 1.8·10^6 J/kg, λ_s=22 W/(m·K), λ_m=67 W/(m·K). The crystal pulling rate was set normally to 1 mm/min.

The crystal radius was set to 0.05 m. A parabolic form of the T_+ and T_- isotherms is chosen, which is described by formula:

$$T_i = T_0 - A_T x^2 + B_T y,\qquad(5.1)$$

where A_T=8000 K/m^2, and B_T=1000 K/m.

The calculations were carried out with 100, 200, and 400 point grids. The calculation results are shown for 400 point grid, unless specified differently. Both the crystal growth and temperature recalculation time steps were set to 0.001-0.0001 s, depending on the grid size.

The crystal growth in (1,1,1) direction was modeled, so that facet plane (1,1,1) was a constant height surface. Therefore the triple point (TRP) was at the maximum distance from the facet plane, and facets developed at the TRP line, see Fig. 4, left.
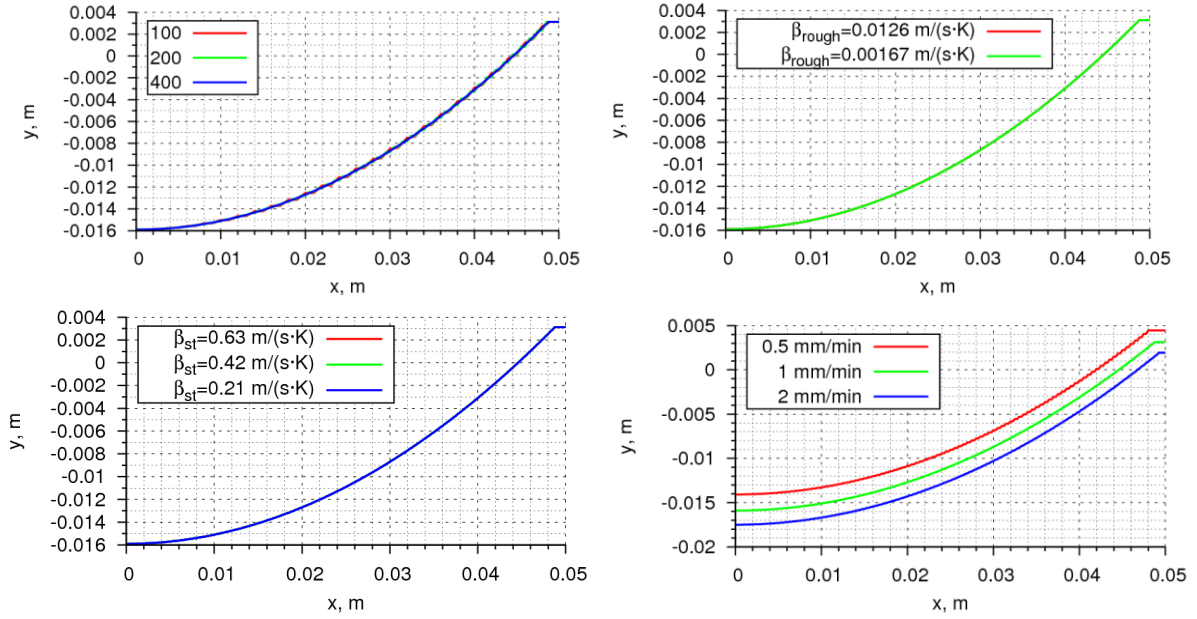

Fig. 4. Top left: crystallization interface obtained with basic parameter values. Calculation results with 100, 200, and 400 point grids. Top right: Dependence of the calculated crystallization interface form on the parameter β_{rough}. Bottom left: dependence of the calculated crystallization interface form on the parameter β_{st}. Bottom right: dependence of the calculated crystallization interface form on the pulling velocity v_p

Fig. 4 and 5 show the dependence of the calculated crystallization interface on different model parameters. Fig. 6 shows the form of the crystallization interface for the isotherms with a maximum at the symmetry axis, described by equation:

$$T_i = T_0 + 1000y + 8000x^2 - 6 \cdot 10^6 x^4 . \tag{5.2}$$

Conclusions

A program for calculation of steady-state crystallization interface form for silicon growth in (1,1,1) direction was written using [1] as a source. A series of calculations have been carried out with this model coupled with a simplified algebraic model for heat transfer at the crystallization interface, in which the influence of the various model parameters was examined.

The calculations have shown that facets develop near the TRP line for a parabolic temperature profile. If there is a local maximum at the symmetry axis in the temperature profile, then a facet can also develop at the symmetry axis. The crystallization interface form depends very little on the rough and layered growth parameters β_{rough} and β_{st}. The size of the facets increases with the decrease of the temperature profile steepness near the TRP and decrease of the pulling velocity.
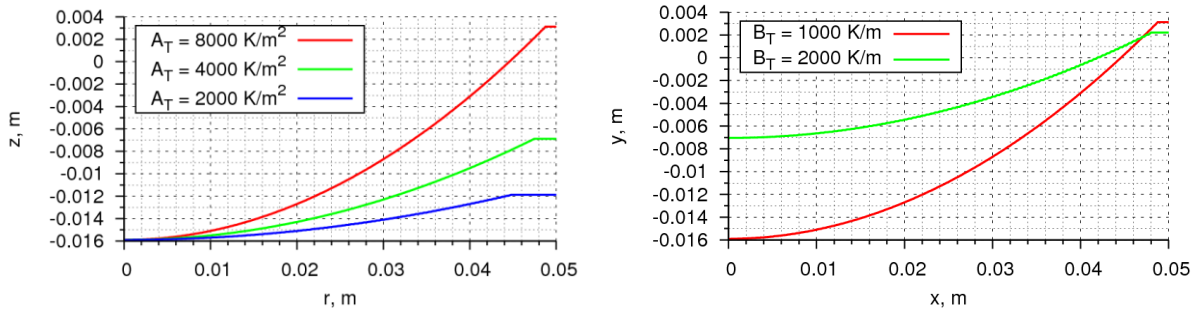
Fig. 5. Left: dependence of the calculated crystallization interface form on the temperature profile steepness near the TRP. Right: dependence of the calculated crystallization interface form on the temperature vertical gradient
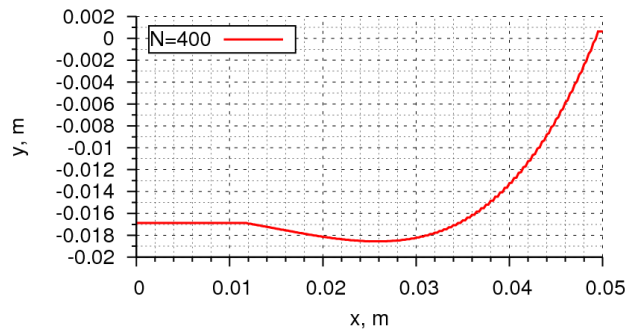

Fig. 6. The crystallization interface for a temperature profile with a maximum at the symmetry axis

Acknowledgements

References

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[2] Jackson, K.: *Kinetic Processes*. WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2004.

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