

Unsteady 3D and analytical analysis of segregation process in FZ Si single crystal growth

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Abstract

3D unsteady calculations of velocity, temperature and dopant concentration fields in molten zone in Floating Zone (FZ) Si single crystal growth process are carried out. The recorded fluctuations of physical fields near the crystallization interface are used to estimate the possible fluctuations of crystal growth velocity. An analytical analysis is carried out to estimate the amplitude of concentration oscillations due to changing local crystal growth rate.

1. Introduction

Silicon single crystals are widely used in production of semiconductor devices. The growing modelling capacities and the high costs of experimental studies of various crystal growth setups have enlarged the role of numerical simulations. As the vast majority of the silicon single crystals are grown with Czochralski method also the modelling of this process has been described in literature more frequently. The Floating zone (FZ) process contributes to only ca. 5% of grown silicon single crystals, however the importance of this process can not be overestimated as the purity of the product is of much higher degree. The FZ products are used in power devices.

Besides the purity of the grown crystal the other important quality parameter is the homogeneity of dopant distribution in the grown crystal. The added dopants are most frequently sprayed on the free surface of the molten zone and later via the crystallization process incorporated in the crystal. The distribution of the dopants depends on convective transport due to the melt hydrodynamics and the segregation process at crystallization interface. The melt motion influences also the temperature gradient near crystallization

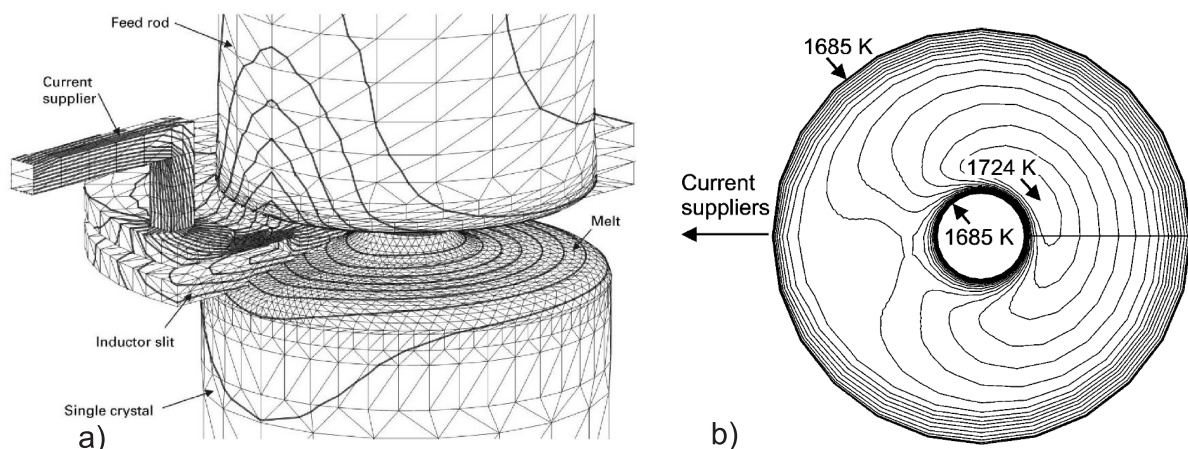


Fig. 1. a) 3D BEM mesh for 3D HF EM calculations, current lines on the surface of silicon parts and inductor; b) calculated temperature distribution on the free surface of the melt.

interface and change the local growth velocity which also influences the dopant segregation process.

It is believed that these changes of crystal growth velocity play a minor role in changing the segregation process in comparison to the influence of convective dopant transport by melt motion and only few references can be found analysing this process. J. P. Garandet [1] have performed analytical estimations and T. Jung. et. al. in [2] carried out 2D numerical analysis and comparison with analytics. However they set external oscillations of temperature and then observed the crystallization process in Bridgman setup. In this paper 3D numerical simulations for melt in FZ process are performed and the observed oscillations of various process parameters near the crystallization interface are used as input data for analytical analysis of the possible influence of thermal oscillations on local crystallization velocity and segregation process.

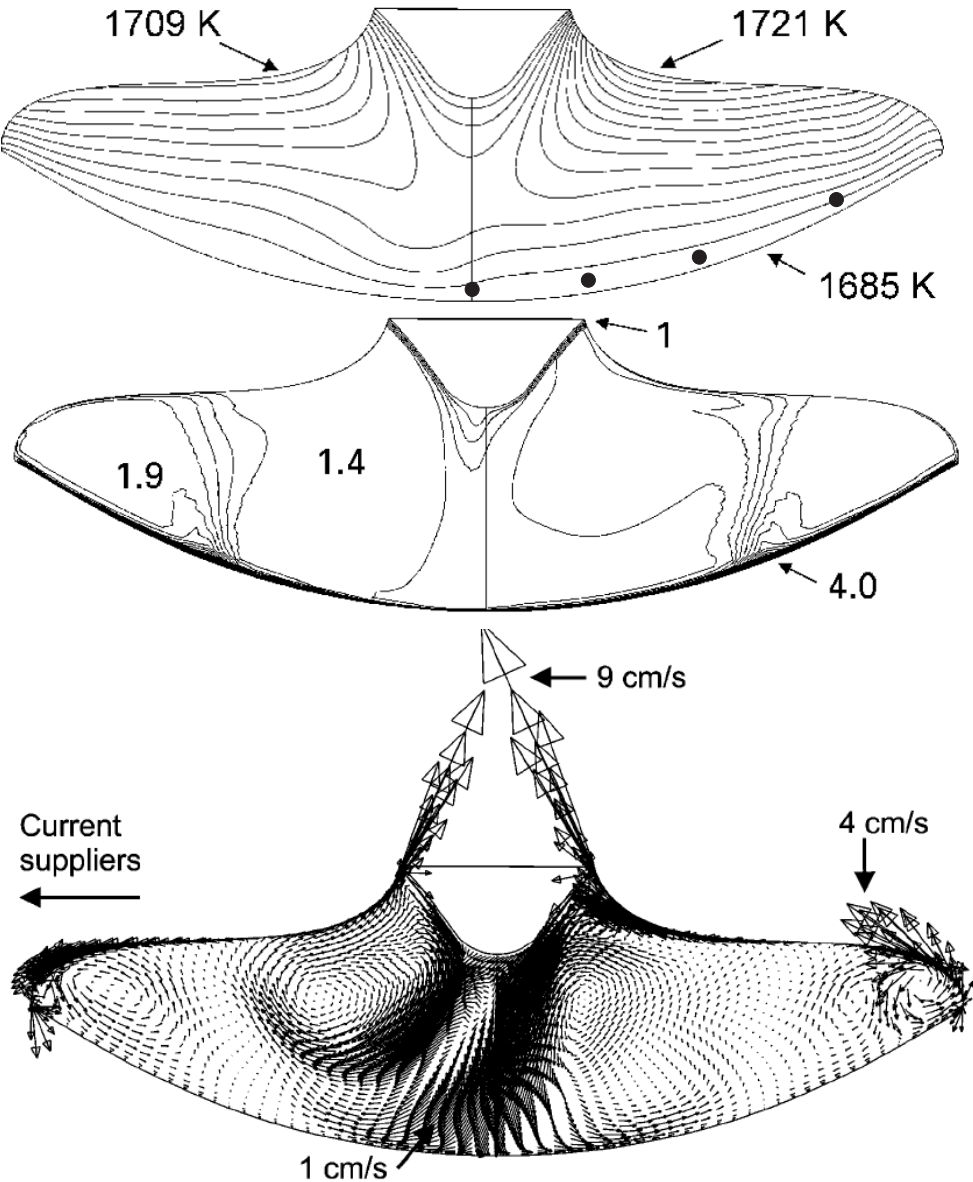


Fig. 2. Temperature (top), dopant concentration (middle) and projected velocity vectors (bottom) in vertical cross-section in the plane of main slit. The probe points are highlighted on temperature distribution.

2. 3D model and calculations of unsteady velocity, temperature and concentration fields

Calculations of unsteady velocity, temperature and dopant concentration fields in molten zone in FZ system from Institute for Crystal Growth (Berlin) for 100 mm silicon single crystal growth are carried out. For the studies the mathematical model [3] and the self developed calculation package FZSIFOAM based on open source code library OpenFOAM were used. The crystal rotation rate was set to 5 rpm.

The calculation of molten zone phase boundaries with specialized 2D program FZone [4], the generation of 3D mesh and the 3D calculation of boundary conditions for molten zone, see Fig. 1a, are described in [4] and [5]. In 3D HD calculations structured mesh with 180000 elements and time step 1.5 ms were used. 4 probe points for monitoring of the calculated physical fields were designated, see Fig. 2 top. These probe points were put at four different radii – 0, 10, 20 and 35 mm. In each position the probes were placed 1.5 mm above crystallization interface.

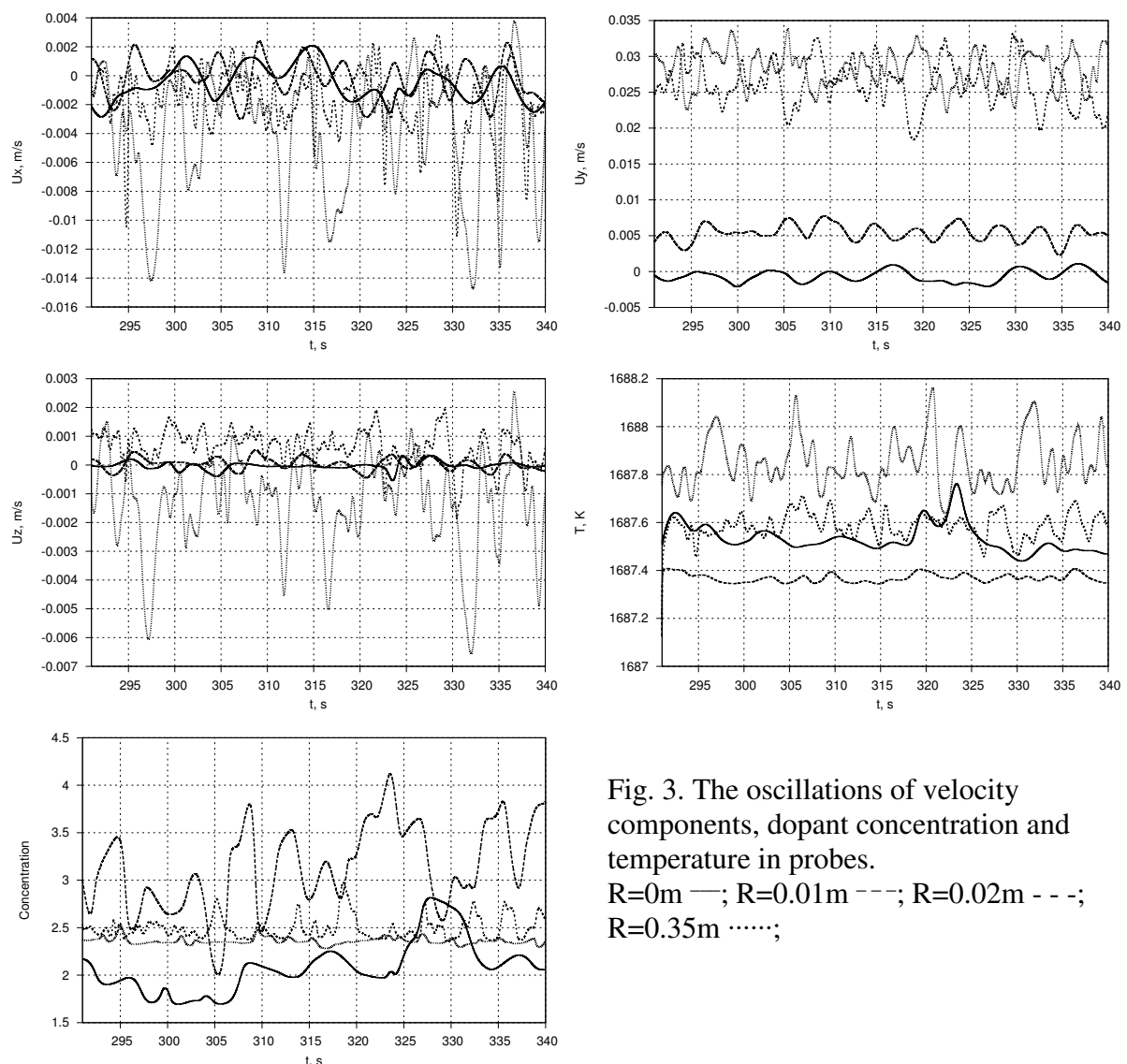


Fig. 3. The oscillations of velocity components, dopant concentration and temperature in probes.
 $R=0\text{m}$ —; $R=0.01\text{m}$ ---; $R=0.02\text{m}$ - - -; $R=0.35\text{m}$ ····;

The calculated temperature field on the free surface for the case with crystal rotation 5 rpm are shown in Fig. 1b. The corresponding calculated averaged in time over 50 s temperature, dopant concentration and velocity fields in vertical cross-section are shown in Fig. 2.

In order to estimate the possible influence of the temperature oscillations on the local crystal growth velocity and segregation process, the results obtained in probes, Fig. 3, are analyzed. As the probes were put in xz plane, the U_x and U_z are respective components of meridional velocity while U_y can be accounted as azimuthal velocity. The characteristic velocities are in the range of few mm/s to few cm/s, and its oscillation amplitude reaches some mm/s. The amplitude of concentration oscillations strongly depends of the probe position and the amplitude can vary from few percent to 50 percent and even more. The oscillation amplitude of temperature gradient at crystallization interface reaches about 25% of characteristic temperature gradient value, and both increase with distance from rotation axis.

3. Analysis of local crystal growth velocity oscillations

To derive the local crystal growth velocity oscillation amplitude from numerically calculated temperature gradient oscillations, the following equations can be written. The averaged in time heat flow density due to crystallization process is $\bar{q}_{cr} = v_p \rho q_0$, where v_p is pulling velocity of crystal, ρ is density of solid silicon and q_0 is latent heat of fusion. The instantaneous value of q_{cr} can vary in time as the instantaneous crystallization velocity v_{cr} depends on temperature gradient fluctuations at crystallization interface. The averaged in time heat flow density from the melt due to thermal gradient \bar{q}_m is $\bar{q}_m = \lambda \delta\bar{T} / \delta n$, where $\delta\bar{T} / \delta n$ is the characteristic thermal gradient in normal to the crystallization interface direction and λ is thermal conductivity of the melt. Obviously, the averaged in time heat flow density from crystallization interface into crystal can be written as a sum $\bar{q}_{inc} = \bar{q}_{cr} + \bar{q}_m$. Still as in laboratory reference system the crystallization interface can be considered as steady and the instant value of $q_{inc} \approx \bar{q}_{inc}$, it follows that the thermal fluctuations in melt are compensated by the changes of local instantaneous crystallization velocity. Therefore we can write that

$$v_{cr} = \frac{\bar{q}_{inc} - q_m}{\rho q_0} = v_p + \frac{\delta\bar{T} / \delta n \cdot \lambda}{\rho q_0} \xi, \quad \xi = \left| 1 - \frac{\delta T / \delta n}{\delta\bar{T} / \delta n} \right|, \quad (1)$$

where overlined parameters are averaged in time, while plain symbols denote the instantaneous values. In the graphs shown in Fig. 3, it can be seen that the highest amplitude of thermal oscillations are at the radius value $R=0.035m$, i.e. $\Delta T = 0.9K \pm 0.2K$. From this we can get that characteristic ξ value is about 0.2 to 0.25. The local crystallization velocity can be written as $v_{cr} = v_p (1 + \beta(t))$, where $\beta = (v_{cr} - v_p) / v_p$. Using the following material properties and process parameters: $v_p = 2.4$ mm/min, $\rho = 2329\text{kg/m}^3$, $q_0 = 1.8 \cdot 10^6$ W/m², $\delta\bar{T} / \delta n = 600$ K/m, $\lambda = 67$ W/mK we obtain that for $\Delta T = 0.9K \pm 0.2K$ follows $|\beta| \leq 0.05$.

4. Analytical estimation of concentration fluctuations due to changes of growth velocity

In 3D calculations used concentration transport equation in the melt is as follows:

$$\frac{\partial C}{\partial t} + U_x \frac{\partial C}{\partial x} + U_y \frac{\partial C}{\partial y} + U_z \frac{\partial C}{\partial z} = D \left[\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right]. \quad (2)$$

3D calculations show that the concentration boundary layer is about 0.5 mm thick. For analytical estimations in this boundary layer, we use an approximation that only melt flow

through the crystallization interface with averaged in time crystallization velocity $\bar{v}_{cr} = v_p$ determines dopant convective transport. Assuming this we can rewrite (2) for concentration boundary layer

$$\frac{\partial C}{\partial t} - v_p \frac{\partial C}{\partial n} = D \frac{\partial^2 C}{\partial n^2}, \quad (3)$$

where n denotes the normal crystallization interface coordinate. We consider the particular solution of (3) as a series in regard to small β

$$C = C_0 + \sum_{k=1} \beta^k C_k(t, n), \quad C_k(t, n) = c_k e^{k\omega t - \lambda_k n}, \quad (4)$$

where C_0 denotes the non-oscillating part of the solution and all C_k tend to zero for large n . Simple substitution of (4) in (3) gives expressions for complex $\lambda_k = \lambda_k^r + i\lambda_k^i$:

$$\lambda_k^r(\omega_k) = \frac{\bar{v}_{cr}}{2D} \left[1 + \sqrt{\frac{1}{4} + 4 \frac{\omega_k^2 D^2}{\bar{v}_{cr}^4} + \frac{1}{2}} \right], \quad \lambda_k^i(\omega_k) = \frac{\bar{v}_{cr}}{2D} \sqrt{\frac{1}{4} + 4 \frac{\omega_k^2 D^2}{\bar{v}_{cr}^4} - \frac{1}{2}}, \quad (5)$$

while by definition $\omega_k = k\omega_1$. Segregation condition on crystallization surface ($n = 0$) states

$$D \frac{\partial C}{\partial n} = -\gamma C, \quad \gamma = (1 - k_s) v_{cr}, \quad (6)$$

where k_s is segregation coefficient. For simplicity only one frequency of crystal growth rate oscillations will be considered further. Equations (4-6) give simple, recursive expression for complex c_k values

$$c_k = \frac{\gamma c_{k-1}}{\lambda_k^r - \gamma + i\lambda_k^i}, \quad k = 1, 2, 3, \dots \quad c_0 = 1/k_s. \quad (7)$$

In order to estimate an upper limit of C pulsation component $C' = C - 1/k_s$ amplitude $\max|C'|$, we consider the sum with modulus $|c_k|$

$$\sum_{k=1}^{\infty} \beta^k |c_k| \geq \max|C'(0)|. \quad (8)$$

For small $\beta \ll 1$ all but terms with c_0 and c_1 in (8) can be omitted. Then condition (8) gives simple estimation for the ratio r' between pulsation and mean concentration component at the crystallization interface:

$$r' = \frac{\beta}{c_0} |c_1| = \frac{\beta \gamma}{\sqrt{(\lambda_1^r - \gamma)^2 + (\lambda_1^i)^2}} = \beta R', \quad \text{where } R' = \frac{\gamma}{\sqrt{(\lambda_1^r - \gamma)^2 + (\lambda_1^i)^2}}. \quad (9)$$

Fig. 4. shows normalized pulsation to mean ratio R'_0 versus pulsation period $\tau = \omega_1 / 2\pi$. For characteristic frequency of pulsations of about $\tau = 5s$ (see CFD simulations), (9) yields $R' \approx 0.07$. Corresponding absolute pulsations for typical value $\beta = 0.05$ is far below 1% of mean, therefore neglecting of crystal growth speed pulsations in our CFD models is partially justified.

Conclusions

The performed 3D calculations with the following analytical estimations have shown that characteristic amplitude of concentration fluctuations in the grown crystal due to convection are by one order

and more higher than fluctuations due to changes of local growth velocity, therefore the use of constant crystal growth rate in 3D calculations can be used as good approximation.

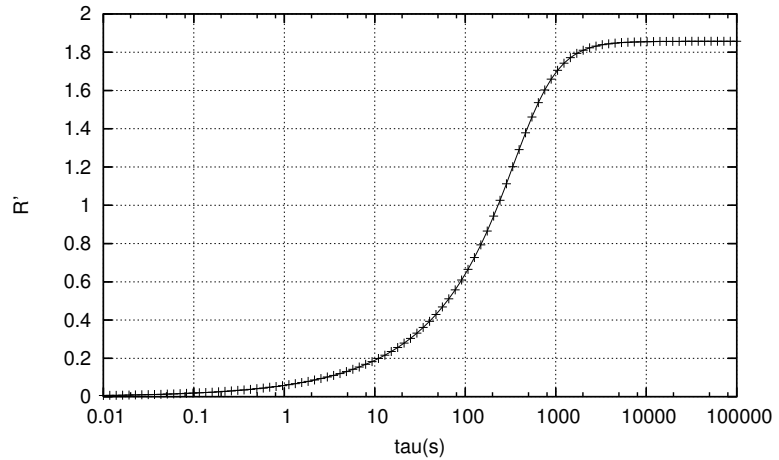


Fig. 4. Values of R' as a function of characteristic period τ .

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