

Modelling of Thermal Field and Point Defect Dynamics During Silicon Single Crystal Growth Using CZ Technique

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Abstract

Mathematical modelling is employed to numerically analyse the dynamics of the Czochralski (CZ) silicon single crystal growth. The model is axisymmetric, its thermal part describes heat transfer by conduction and thermal radiation, and allows to predict the time-dependent shape of the crystal-melt interface. Besides the thermal field, the point defect dynamics is modelled using the finite element method. The considered process consists of cone growth and cylindrical phases, including a short period of a reduced crystal pull rate, and a power jump to avoid large diameter changes. The influence of the thermal stresses on the point defects is also investigated.

Introduction

The Czochralski method is widely used to produce silicon single crystals for the semiconductor industry. Two PID controllers are commonly used to adjust the crystal pull rate and the heater power. The crystal quality depends on the microdefect distribution, which is determined by the self-interstitials and vacancies, as well as the dopants. The whole CZ process is highly non-stationary (transient), which means that it cannot be precisely described using a steady-state model. The dynamical nature of the CZ process is especially actual for the point defect calculations, due to the dependence on the thermal history of the crystal.

In the present paper, the existing model [1] is extended with the possibility to calculate the point defect distribution and thermal stresses in the crystal. Transient calculations of cone and cylindrical growth are carried out, including a pull rate drop. The novelty of the present work is that the power jump is explicitly considered in the simulations to avoid large diameter changes.

1. Mathematical model

1.1. Temperature and phase boundaries

An axisymmetric geometry is considered, see Fig. 1. The non-stationary temperature field and the changing shape of the phase boundaries are calculated with the program CZ-Trans as described in [1]. Heat transfer by conduction and thermal radiation is considered; the influence of the convective heat transfer is modelled indirectly via increased thermal conductivity of the melt. The heater is described as a surface with a homogeneous temperature distribution which changes in time.

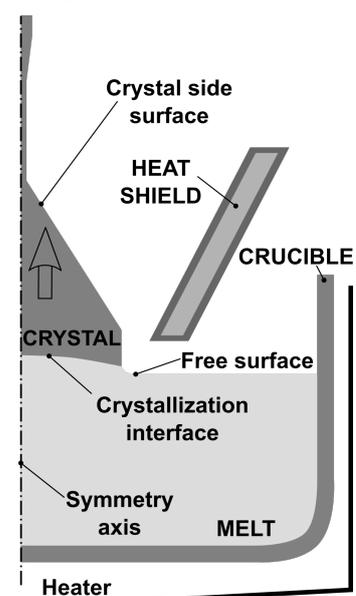


Fig. 1. Scheme of the considered CZ system

1.2. Point defects

Two types of the point defects in the crystal are considered: self-interstitials, denoted by the index “ I ”, and vacancies, denoted by the index “ V ”. The corresponding concentrations C_I and C_V [cm^{-3}] are coupled by the recombination term – the last term in the advection-diffusion-reaction equation (1.1). The subscript “ I,V ” is a shorthand, meaning that (1.1) represents two equations – the first one for I and the second one – for V . The thermodiffusion term is omitted since the corresponding physical parameters are not precisely known and its estimated influence is much weaker than the effect of the equilibrium concentrations [2].

$$\frac{\partial C_{I,V}}{\partial t} + \bar{u} \nabla C_{I,V} = \nabla (D_{I,V} \nabla C_{I,V}) + k_{rec} (C_I^{eq} C_V^{eq} - C_I C_V). \quad (1.1)$$

In the equation (1.1), t is the time, \bar{u} is the velocity (crystal pull rate V_{cryst}), C^{eq} is the equilibrium concentration, D is the diffusion coefficient [m^2/s], and k^{rec} is the reaction constant for recombination [cm^3/s]. On the symmetry axis (see also Fig. 1), the zero flux boundary condition (BC) is set: $\partial C_{I,V}/\partial n = 0$. At the crystallization interface and the crystal side surface, the equilibrium concentration is applied: $C_{I,V} = C_{I,V}^{eq}$.

Once the concentrations C_I and C_V are calculated, the parameter $\Delta = C_I - C_V$ can be used to analyse the excess of the self-interstitials/vacancies in different regions of the crystal. Zero isoline of Δ is the position of the I-V boundary.

The physical parameters strongly depend on the absolute temperature, T . The general expressions for the diffusion coefficient and the equilibrium concentration are given by equation (1.2), where $k = 8.617 \cdot 10^{-5}$ eV/K is the Boltzmann constant, and the parameters D^0 , E^m , C^0 , H^f and S^f are taken from [3].

$$D(T) = D^0 \exp\left[-\frac{E^m}{kT}\right], \quad C^{eq}(T) = C^0 \exp\left[-\frac{H^f - S^f T}{kT}\right]. \quad (1.2)$$

At the melting point of silicon, $T_0 = 1685$ K, the values are $C_I^{eq} = 6.9 \cdot 10^{14} \text{ cm}^{-3}$, $C_V^{eq} = 8.5 \cdot 10^{14} \text{ cm}^{-3}$, and $\Delta = -1.6 \cdot 10^{14} \text{ cm}^{-3}$, which means that at the crystallization interface more vacancies are formed than interstitials. Further from the interface the crystal can be interstitial-rich since at high temperatures $D_I > D_V$.

The recombination coefficient is given by the equation (1.3), where $a_r = 1$ nm is the capture radius for recombination, and the energy barrier $E = 1.5$ eV [4], [5].

$$k_{rec}(T) = 4\pi a_r (D_I + D_V) \exp\left[-\frac{E}{kT}\right]. \quad (1.3)$$

1.3. Thermal stresses

The thermal stresses in the crystal are calculated in an axisymmetric manner as described in [6]. The physical parameters are: Poisson’s ratio 0.25, Young’s modulus $1.56 \cdot 10^{11}$ Pa, coefficient of thermal expansion of crystal $3.2 \cdot 10^{-6} \text{ K}^{-1}$.

The influence of the thermal stresses on the formation enthalpy of point defects is considered using the parameters for the isotropic case from [7], given by $\Delta H_I^f = -0.068 \sigma_{ave}$, $\Delta H_V^f = +0.153 \sigma_{ave}$, where enthalpy is expressed in eV, and stress – in GPa. The mean thermal stress $\sigma_{ave} = (\sigma_{rr} + \sigma_{zz} + \sigma_{\phi\phi})/3$.

2. Results and discussion

Cone and cylindrical growth (crystal diameter 200 mm) stages are considered in the same way as it was previously done in [8]. Additionally, a crystal pull rate drop is applied following the experiment by Abe, see [9], [10] and references therein: during the cylindrical phase V_{cryst} is changed from 1 mm/min to 0.2 mm/min for 30 minutes. The hot zone geometry (and hence, the heater power) is different from the one used in [9].

As noted in [9], heater power jump should be applied in advance to counteract the large crystal diameter changes due to V_{cryst} jump. This turned out to be difficult to achieve in our calculations, contrary to models where the diameter is fixed [9], [10], therefore several power curves have been tried. The considered velocity and power curves are plotted in Fig. 2, where V0 and P0 denote the reference case with no jumps. V1 corresponds to the experiment by Abe [9], while V2 is a test case to investigate the long-term pull rate change. In the case P1 the power jump of +5 kW is applied 40 min before the pull rate jump; for P2 the jump +3 kW is 25 min before and ends when V_{cryst} jump ends; for P3 the power jump +4 kW is 25 min before and ends 5 min after V_{cryst} jump begins. It should be noted that in the calculations [10] no power change is mentioned, and the crystal radius seems to stay perfectly constant.

Most of the considered cases exhibit a rather strong crystal radius oscillations, see Fig. 3, left. The smallest radius deviations are for the cases (V1, P2) and (V1, P3).

According to Voronkov [11], the dominating point defect specie is determined by the ratio $\Gamma = v/G$, where v is the crystal growth rate and G – the temperature gradient. Above the critical value $\Gamma_{crit} \approx 1.4 \cdot 10^{-3} \text{ cm}^2/\text{min}/\text{K}$ the crystal will be vacancy-rich, and below – interstitial-rich. The calculation results shown in Fig. 3, right (thick grey line – Γ_{crit}), indicate that the pull rate jump indeed can introduce interstitials in the originally vacancy-rich crystal.

The response of the growth rate at the triple point on the crystal pull rate and power jumps is shown in Fig. 4. An exponential time dependence is observed. During the jump the growth rate does not catch up with the pull rate, the case with a prolonged jump (V2) shows that 50 min are needed for it to happen. The influence of the power jump is rather weak.

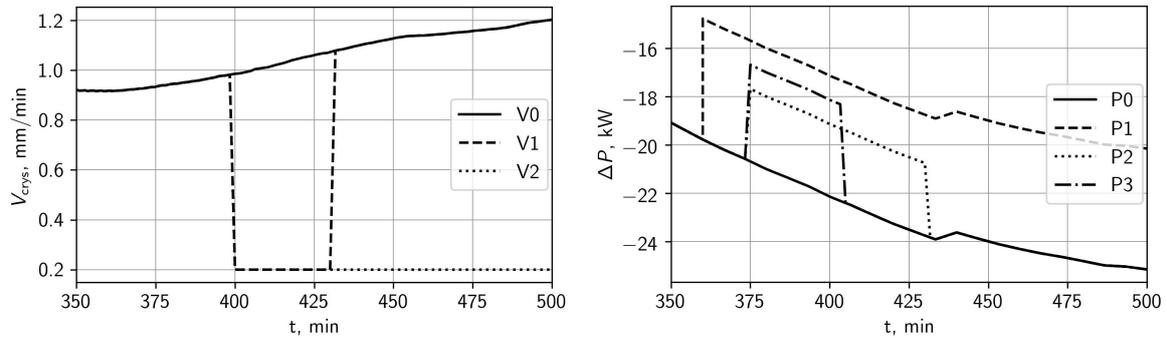


Fig. 2. Time-dependence of the crystal pull rate (left) and heater power change (right).

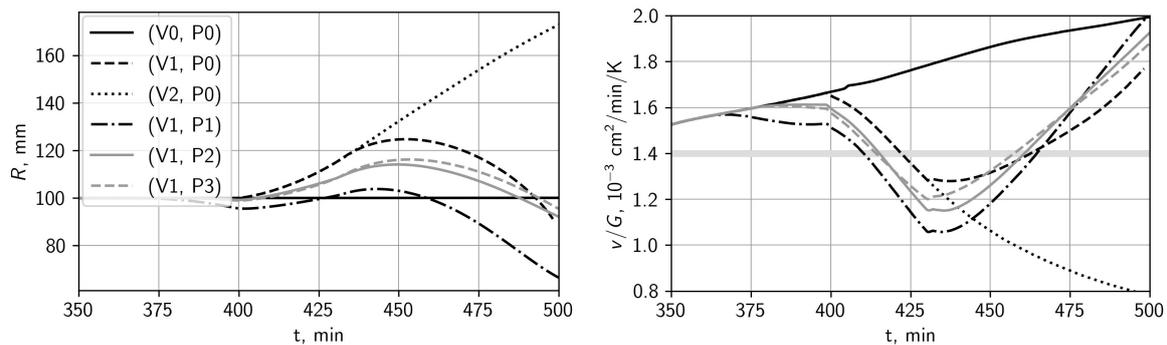


Fig. 3. Time-dependence of the crystal radius (left) and v/G ratio at centre (right)

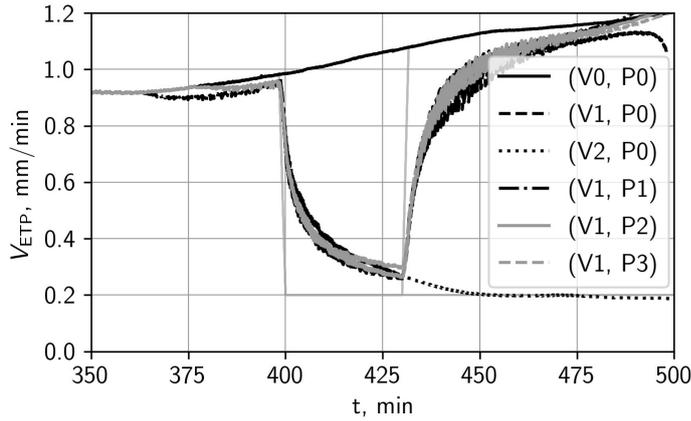


Fig. 4. Time-dependence of the growth rate at the ETP

A fine mesh in the crystal has to be used for the thermal stress and point defect calculations. An example of the used quasi-structured grid and the calculated temperature field is shown in Fig. 5.

Fig. 6 shows the calculated thermal stresses in the crystal. Near the crystallization interface the mean stress $\sigma_{ave} < 0$ close to the centre, and $\sigma_{ave} > 0$ close to the crystal rim. According to subsection 1.3 and [7], more vacancies will be formed at the centre, and more interstitials – at the rim.

The calculated point defect distributions in the crystal at the same time instant are shown in Fig. 7; “stress infl.” means that the influence of the thermal stresses on the point defects has been considered, and “ $\partial C/\partial n = 0$ ” – that the no-flux BC has been set at the crystal side surface. The thermal stresses increase C_V at the centre, as expected, but the overall influence is weak. The no-flux BC only slightly changes the concentrations near the crystallization interface, and considerably – further away from it. The cases with velocity curve V1 and various power curves have the same qualitative behaviour: before the radius increase a local C_I minima and C_V maxima develops near the crystal side surface, and when the radius starts to decrease, an additional C_I maxima develops.

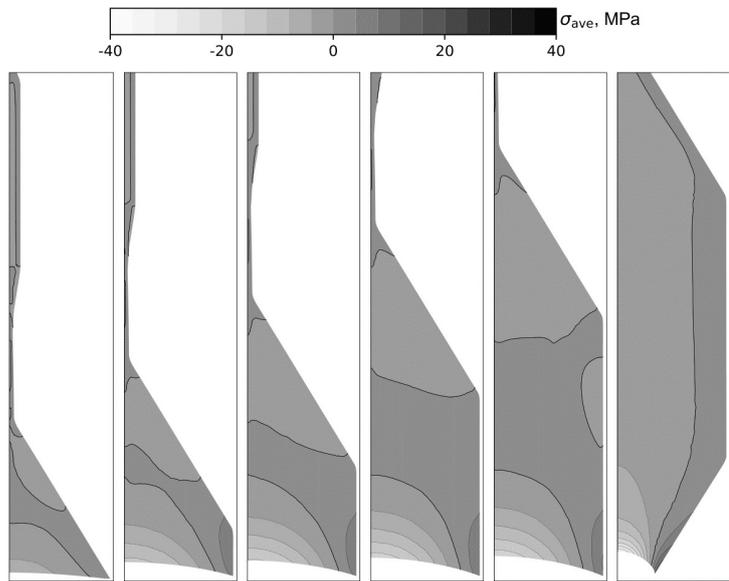


Fig. 6. Mean thermal stress σ_{ave} in the crystal for the case (V0, P0) at $t = 5, 6, 7, 8, 9, 10$ h (from left to right)

The crystallization interface shape plotted in Fig. 8 visualizes the slow growth rate at the triple point and indicates that the decrease in the growth rate for the points near the centre is not as strong (in fact, it only drops to ~ 0.6 mm/min). According to the Δ field, in the basic case the crystal is vacancy-rich, except for a small region in the cone. The thermal stresses make it slightly more vacancy-rich, while the no-flux BC make the outer region of the cylindrical part and the cone interstitial-rich. As observed before for the concentrations, Δ

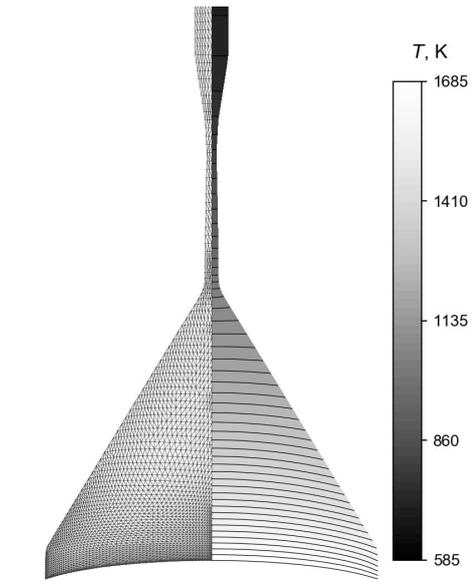


Fig. 5. The finite element mesh and temperature field in the crystal. Spacing between isotherms 20 K

field for the velocity curve V1 and different power curves is qualitatively the same: an interstitial-rich region develops at the crystal surface due to the crystal pull rate drop.

The I-V boundary does not reach the symmetry axis, which agrees with [9], [10]. However, it is known from these sources that when applying the same V_{cryst} jump for crystals with smaller radius, the I-V boundary reaches the centre. Since we modelled only one crystal (diameter 200 mm), it was decided to apply the pull rate drop indefinitely, case (V2, P0). The results are shown in Fig. 9: the crystal radius change is very large, and about 1.5 h after the jump the I-V boundary spreads to the symmetry axis.

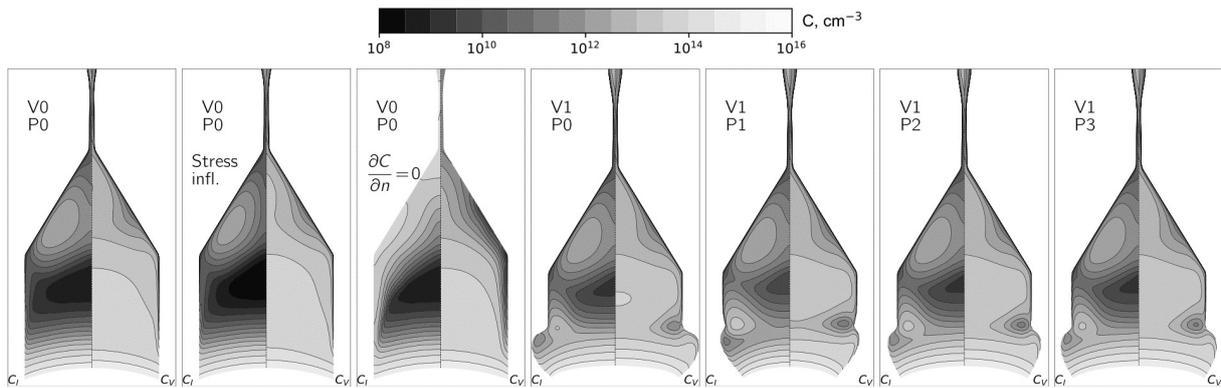


Fig. 7. Point defect concentrations in the crystal

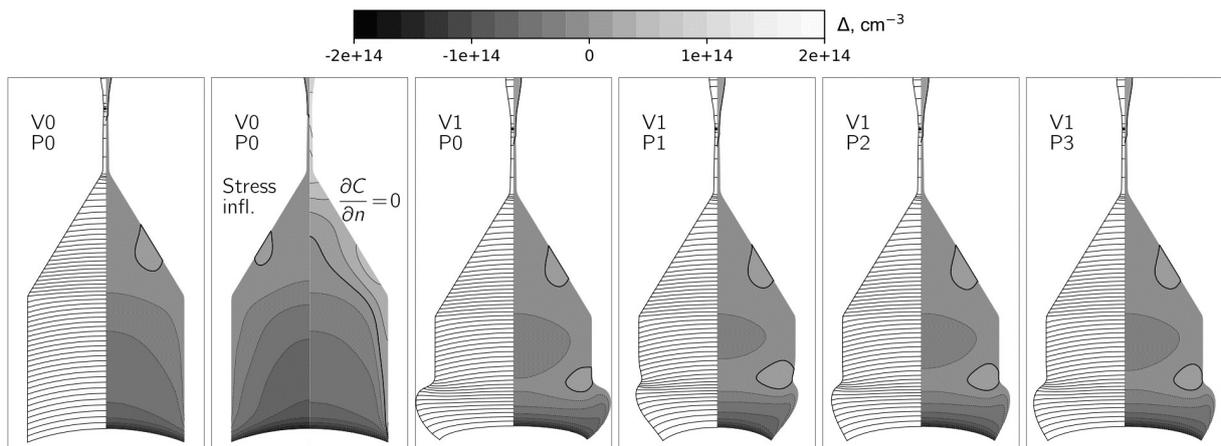


Fig. 8. Crystallization interface shape plotted each 200 s (left) and Δ field in the crystal (right). Thick solid line – zero Δ isoline

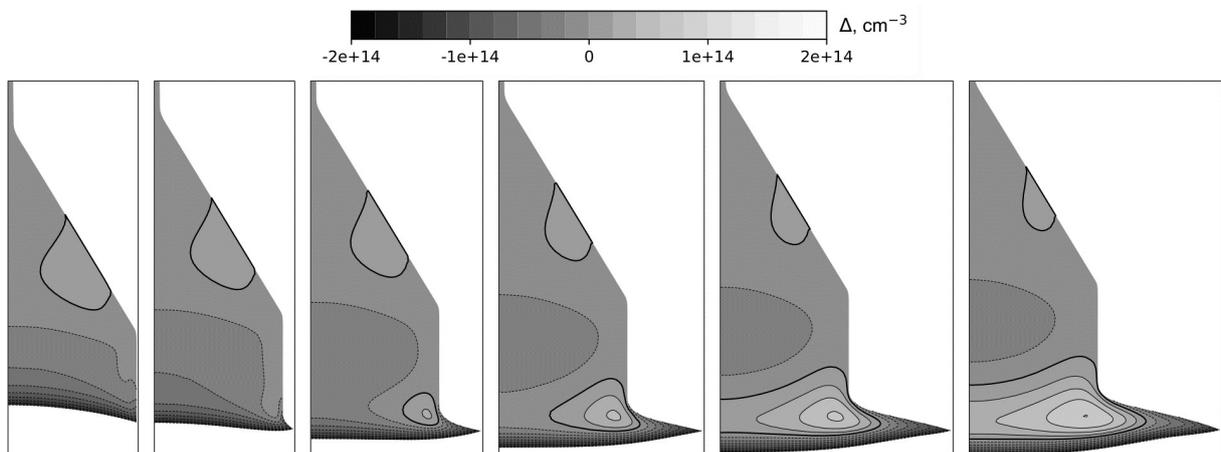


Fig. 9. Δ field in the crystal for the case (V2, P0) at $t = 6.5, 7, 7.5, 8, 8.5, 9$ h (from left to right). Thick solid line – zero Δ isoline

Conclusions

Non-stationary numerical modelling of CZ silicon single crystal growth has been carried out, including calculation of thermal stresses and point defects in the crystal. The influence of the thermal stresses on the point defects is weak.

A qualitative reproduction of the pull rate drop experiment is achieved. Due to the too large change in the crystal radius, a power jump has to be applied as well. Even then a constant crystal radius cannot be maintained – possibility to use a better power curve should be investigated in future. A longer period of a reduced pull rate is needed for the I-V boundary to reach the centre of the considered $D = 200$ mm crystal.

References

- [1] Sabanskis, A., Bergfelds, K., Muiznieks, A., Schröck, T., Krauze, A.: *Crystal shape 2D modeling for transient CZ silicon crystal growth*. Journal of Crystal Growth, Vol. 377, 2013, pp. 9-16.
- [2] Sinno, T., Brown, R.A., von Ammon, W., Dornberger, E.: *Point Defect Dynamics and the Oxidation-Induced Stacking-Fault Ring in Czochralski-Grown Silicon Crystals*. Journal of the Electrochemical Society, Vol. 145, 1998, No. 1, pp. 302-318.
- [3] Sinno, T.: *A bottom-up multiscale view of point-defect aggregation in silicon*. Journal of Crystal Growth, Vol. 303, 2007, No. 1, pp. 5-11.
- [4] Brown, R.A., Maroudas, D., Sinno, T.: *Modelling point defect dynamics in the crystal growth of silicon*. Journal of Crystal Growth, Vol. 137, 1994, No. 1-2, pp. 12-25.
- [5] Prostomolotov, A.I., Verezub, N.A.: *Two-dimensional model of the intrinsic point defects behaviour during CZ silicon crystals growth*. Intl. Conference on Solid State Crystals 2000, 2001, pp. 97-103.
- [6] Muiznieks, A., Raming, G., Mühlbauer, A., Virbulis, J., Hanna, B., Ammon, W.V.: *Stress-induced dislocation generation in large FZ-and CZ-silicon single crystals—numerical model and qualitative considerations*. Journal of Crystal Growth, Vol. 230, 2001, No. 1, pp. 305-313.
- [7] Sueoka, K., Kamiyama, E., Vanhellefont, J., Nakamura, K.: *Stress and doping impact on intrinsic point defect behavior in growing single crystal silicon*. Phys. Status Solidi B, Vol. 251, 2014, No. 11, pp. 2159-2168.
- [8] Sabanskis, A., Bergfelds, K., Virbulis, J.: *Transient 2D modelling of Czochralski crystal growth process*. Proceedings of the international scientific colloquium “Modelling for Electromagnetic Processing”, 2014, pp. 87-92.
- [9] Abe, T., Takahashi, T.: *Intrinsic point defect behavior in silicon crystals during growth from the melt: A model derived from experimental results*. Journal of Crystal Growth, Vol. 334, 2011, No. 1, pp. 16-36.
- [10] Dornberger, E., Von Ammon, W., Virbulis, J., Hanna, B., Sinno, T.: *Modeling of transient point defect dynamics in Czochralski silicon crystals*. Journal of Crystal Growth, Vol. 230, 2001, No. 1, pp. 291-299.
- [11] Voronkov, V.V., Falster, R.: *Vacancy and self-interstitial concentration incorporated into growing silicon crystals*. Journal of Applied Physics, Vol. 86, 1999, No. 11, pp. 5975-5982.

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