Effect of a uniformly rotating crystal length on radiation-convective heat transfer in the Chokhralsky method

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Abstract. Radiation-convective heat transfer from silicon crystals to the environment was investigated with the Chokhralsky method. The systems of equations of thermogravitation and mixed convection in the term vortex, stream function and temperature were solved numerically by the finite element method. The influence of crystal rotation on the spatial forms of convective flows of the surrounding gas and on non-stationary temperature fields in the gas and in the crystals was studied. Calculations were made for crystals of different lengths. The calculations were performed with the Prandtl number equal to 0.68 (argon) and the Grashof number 16000, typical for a real technological process.

1. Introduction

In a real high-temperature technological process of pulling a crystal from the free surface of the melt by the Chokhralsky method, heat exchange has a complex conjugate character and the temperature fields are self-consistent throughout the growth chamber [1]. Controlling the crystal growth conditions is quite a difficult task, since the non-stationary and non-linear problems of coupled radiation-convective heat exchange between the crystal, the melt and the environment are caused by monotonous changes in the geometry and boundary conditions as the crystal grows. As a rule, even in the framework of global modeling, problems are solved with a discrete set of geometries of the calculated regions as the crystal grows. Solving problems in a global conjugate formulation, which requires almost impossible precise setting of boundary conditions corresponding to a real process, requires large computational and time resources. Therefore, in order to understand the general regularities of the dependence of temperature fields in crystals on the intensity of heat transfer from their generatrix and the corresponding thermal stresses, it is advisable to solve problems in the framework of partial modeling [2-4]. The results of such studies are necessary for understanding the characteristics of the thermal history of the crystal. In [4], the effect of uniform rotation of a crystal with a fixed length H/RS = 4 in the rotation speed range from 1 to 25 rpm on radiation-convective heat exchange was investigated. In [5] it was shown that for melts with any value of the Prandtl number, there are relations of dimensionless dynamic parameters: Grashof Number Gr, Marangoni Ma and Reynolds Re, which characterize the intensity and relative role of natural and forced convection of the melt, at which the crystallization front is flat. The conclusions were confirmed experimentally using fusible substances. Therefore, in [4] and in this work, the flat form of the crystallization front is set. Without claiming to be a complete description of all processes, partial modeling allows us to determine the main trends in the behavior of the systems under consideration when changing individual control parameters or their groups. As a follow-up to [4], the coupled radiation-convective heat exchange is studied numerically by the finite element method [6] at the
specified crystal rotation speeds. The influence of the crystal rotation speed on the temperature field in crystals of different lengths, i.e. on the sequence of growth stages, is studied.

2. Model
Taking into account the properties of the axisymmetry of thermal unit used in single crystals grown by the Chokhralsky method, the calculations were performed in a two-dimensional computational domain in cylindrical coordinates. The geometry of the computational domain corresponds to a simplified scheme of the upper part of the growth chamber, consisting of a single crystal, a seed crystal, a rod, the walls of the growth chamber and a screen separating the surface of the melt from the gas medium (argon) in the growth chamber. To simulate mixed convection, a dimensionless system of Navier-Stokes equations and equations of energy and continuity in the Boussinesq approximation is used in terms of vortex, stream function, azimuthal velocity and temperature:

\[
\begin{align*}
\frac{1}{Pr} \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}\right) + \frac{\partial T}{\partial r} + \frac{\partial T}{\partial z} &= 0 \\
\left(\frac{\partial^2 \omega}{\partial r^2} + \frac{1}{r} \frac{\partial \omega}{\partial r} + \frac{\partial^2 \omega}{\partial z^2}\right) + \frac{\partial \omega}{\partial r} + \frac{\partial \omega}{\partial z} + \frac{\partial \omega}{r^2} - u - \frac{1}{r} \frac{\partial W^2}{\partial r} &= -Gr \frac{\partial T}{\partial r} \\
\left(\frac{\partial^2 W}{\partial r^2} + \frac{1}{r} \frac{\partial W}{\partial r} + \frac{\partial^2 W}{\partial z^2}\right) + \frac{\partial W}{\partial r} + \frac{\partial W}{\partial z} + \frac{\partial W}{r^2} - u &= 0 \\
\left(\frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2}\right) - \frac{2}{r^2} \frac{\partial \psi}{\partial r} &= r \cdot \omega \\
u &= \frac{1}{r} \frac{\partial \psi}{\partial z} \\
v &= -\frac{1}{r} \frac{\partial \psi}{\partial r}
\end{align*}
\]

where \( T, \omega, W, \psi, u, v \) are the temperature, vortex, azimuthal velocity, stream function, radial and axial velocity components, respectively, and \( Gr = (\beta g/\nu^2) \cdot \Delta T \cdot R_s^3 \) is the Grashof number. Here \( \beta \) is the volume expansion coefficient of the gas, \( g \) is the acceleration of gravity, \( \nu \) is the kinematic viscosity of argon, \( \Delta T = 1330 \text{K} \) is the temperature difference between the crystallization front and the walls of the growth chamber, and \( R_s \) is the radius of the crystal. The argon Prandtl number \( Pr = v/a = 0.68 \), where \( a = \lambda_C/\rho C_P \) is the thermal diffusivity, \( \lambda_C \) is the thermal conductivity coefficient, \( \rho \) is the density, and \( C_P \) is the heat capacity at constant pressure. When reducing the equations to a dimensionless form, the \( R_s \) is the radius of the crystal used as a geometric scale. The temperature scale is assumed to be the temperature difference \( \Delta T \). The speed scale is \( v/R_s \). The radiation flux scale is \( R_s^2/\lambda_C \cdot \Delta T \). The time scale is \( R_s^2/v \).

Calculation of radiation fluxes is based on the zonal method \([6]\) under the following assumptions: the computational domain is limited by a closed system of surfaces; all surfaces are gray, diffusely emitting and diffusely reflecting; the surface is divided into zones, within which the radiative properties and temperature can be considered constant; and the medium filling the growth chamber is determined. The problem is solved under the following boundary conditions. At the crystallization front, the maximum temperature in the system is set (1683 K): \( T_{\Gamma_1} = 1 \). On the screen separating the surface of the melt from the growth chamber, the conditions of thermal insulation, non-flow and adhesion are set: \( \frac{\partial T}{\partial n}_{\Gamma_2} = 0, \quad \psi_{\Gamma_2} = 0, \quad \omega_{\Gamma_2} = \left. \frac{\partial V}{\partial z} \right|_{\Gamma_2} \). The minimum temperature in the system is maintained on the walls of the growth chamber, the condition of non-flow and adhesion is set: \( T_{\Gamma_3} = 0, \quad \psi_{\Gamma_3} = 0, \quad \omega_{\Gamma_3} = -\left. \frac{\partial V}{\partial r} \right|_{\Gamma_3} \).
The conditions of non-flow, adhesion, rotation speed and ideal contact condition are set for the crystal generatrix, taking into account the radiation flows:

\[ \psi|_{t_4} = 0, \quad \phi|_{t_4} = \frac{\partial V_r}{\partial t} \left|_{t_4} \right. - \frac{\partial V_z}{\partial t} \left|_{t_4} \right. , \quad W|_{t_4} = w, \]

\[ T|_{t_4} = T|_{t_4} , \quad -\lambda_S \frac{\partial T}{\partial n}_{t_4} = -\lambda_G \frac{\partial T}{\partial n}_{t_4} + Q. \]

Numerical simulation is carried out by finite element method on irregular grid with 101x501 nodes of the triangular finite element with given linear functions. The calculations are carried out with the thermal conductivity of the crystal \( \lambda_S = 26 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1} \), characteristic of monocrystalline silicon. The radius of the crystal \( R_S = 0.05 \text{ m} \), the thermal conductivity of argon \( \lambda_G = 5.83 \times 10^3 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1} \), the thermal diffusivity of the gas \( \alpha = 3.74 \times 10^{-4} \text{ m}^2 \cdot \text{s}^{-1} \), the volumetric expansion coefficient \( \beta = 6.4 \times 10^4 \text{ K}^{-1} \), and the kinematic viscosity of the gas \( \nu = 2.54 \times 10^{-4} \text{ m}^2 \cdot \text{s}^{-1} \). The properties of argon are taken at a temperature of 1600 K [6]. The degree of blackness of all surfaces of the system is 0.5. Rotation speeds in the range from 1 to 25 rpm are considered.

### 3. Results and discussion

The rotation of crystals is used not only to control the melt hydrodynamics and, as a result, to manage the shape of the crystallization front, but also to exclude the influence of imperfections of the thermal unit. The rotation of the crystal affects the processes of heat transfer to the environment in the growth chamber. Calculations are performed for \( Pr = 0.68 \) and \( Gr = 160000 \), and relative crystal lengths \( H/R_S = 2, 4, 6, 8 \). Calculations are performed for fixed crystals and at rotation speeds \( \omega_K = 10 \) and \( 25 \) rpm. Figures 1-5 show the fields of stream function isolines and isotherms in the regime of radiation-convective heat exchange at crystal lengths \( H/R_S = 2, 6, 8 \). For the relative length of the crystal \( H/R_S = 4 \), detailed information is provided in [2, 4]. The Results [2, 4] serve as a base for the comparative analysis of the data obtained at \( H/R_S = 2, 6, 8 \).

**Figure 1.** Fields of stream function isolines (left) and isotherms (right) at the moment \( t = 200 \) at the height of the crystal 2 (a, b) and 6 (c, d) and rotation speeds \( \omega_K \): a, c – 0 rpm; b, g – 25 rpm.

Figures 1a, 1b and 2a show the fields of stream function isolines and isotherms in the regime of radiation-convective heat exchange without rotation of crystals. In these cases, the convection has a
thermogravitational nature. Here, the convection is caused by the action of buoyancy forces. But the heat exchange in these regimes is radiation-convective.

In the absence of rotation of the crystal $H/R_S = 2$, as with $H/R_S = 4$, a stationary temperature field is formed and a three-vortex convective flow of a complex shape is established with the separation of the boundary layer on the rod forming at the level $z = 4.5$ (figure 1a). The gas is heated at the incandescent base of the crystal and under the influence of buoyancy force rises up the crystal generatrix. Then the gas flows cool down on the walls of the growth chamber and again fall down on the base of the crystal. On the cold walls of the vessel of the growth chamber, descending streams of cold gas are formed, reach the thermal insulation screen, unfold and flow to the red-hot base of the crystal. Thus, convective heat exchange leads to local cooling and a sharp increase in radial and axial gradients near the crystallization front. As a consequence, the radial distributions of axial local heat fluxes are also uneven.

Accordingly, the distribution of radial and axial temperature gradients in the crystal is inhomogeneous. As a result of radiative fluxes from the crystal surface its temperature decreases. The flow of heated gas ascending along the generatrix warms the upper part of the crystal.

**Figure 2.** Fields of stream function isolines (left) and isotherms (right) at time $t = 200$ at the crystal height of 8 and rotation speeds: a - 0; b - 25 rpm.

**Figure 3.** Fields of stream function isolines (left) and isotherms (right) at the height of the crystal 2 and the rotation speed of 10 rpm at times: a - t = 110; b – 140; c – 170; d – 200.
As a result, the axial temperature gradients in the crystal are reduced. Figures 1b, 1d and 2b show the fields of isolines of the stream function and isotherms in the regime of radiation-convective heat exchange at the speed of rotation of crystals of 25 rpm at the same time.

![Figure 4](image_url1)

**Figure 4.** Fields of stream function isolines (left) and isotherms (right) at the height of the crystal 6 and the rotation speed of 10 rpm at times: a – t = 110; b – 140; c – 170; d – 200.

At the same time, at a rotation speed $\omega_K = 10$ rpm, the fields of isolines of the stream function and isotherms in the regime of radiation-convective heat exchange during the rotation of crystals are shown in figures 3d – 5d. When centrifugal forces and buoyancy forces are simultaneously applied, the flows become unsteady and oscillatory.

![Figure 5](image_url2)

**Figure 5.** Fields of stream function isolines (left) and isotherms (right) at the height of the crystal 8 and the rotation speed of 10 rpm at times: a - t = 110; b – 140; c – 170; d – 200.
Figures 3-5 show the time evolution spatial flow forms and temperature fields at a fixed speed of rotation of crystals of different lengths. In the regime of gravity-centrifugal convection and radiation heat transfer at a rotation speed of 10 rpm, the axial temperature gradients increase (figures 3-5) relative to the case without rotation.

When the speed of the crystal rotation increases to $\omega_K = 25$ rpm, the axial temperature gradients in the lower part of the crystal decrease in comparison with the cases of $\omega_K = 10$ rpm and $\omega_K = 0$. As the length of the crystal increases, the axial temperature gradients in the lower part of the crystal increase. This can be seen from the temperature distributions and temperature gradients in figures 6-9. The regularities of heat transfer and temperature fields are related to changes in the spatial shape of the gas flow. A convective vortex with a clockwise direction of movement (to the right of the symmetry axis) is formed between the crystal-forming and cold walls of the housing at $\omega_K = 0$. This same vortex occupies part of the space above the crystal. A similar vortex is formed between the rod generatrix and the vessel walls, which partially blocks the penetration of the gas heated at the base of the crystal into the upper region of the growth chamber.

Due to the significantly larger size of the convective vortex near the single crystal and the higher intensity of convective flows in the bottom region, the radial gradients at the base of the crystal grow noticeably stronger than in the centrifugal radiation-convective mode. Also, the overall cooling efficiency of the single crystal, which is more evenly warmed up in height, decreases more significantly.

In regime with the combined action of buoyancy forces, centrifugal forces, and radiation heat transfer at a crystal rotation speed of 10 rpm, the following feature is observed. From the gas heated on the forming crystal, pop-up vortexes, which move to the cold wall of the housing, are periodically formed. In the boundary layer, small-scale vortexes are formed on the rod, flowing down. As a result of the
periodic release of heated gas from the lower part of the region, the temperature field in the crystal becomes quasi-periodic.

![Figure 9. Time dependence of the radial gradient at 10 rpm and the ratio of the height to the radius of the crystal: 1 – H/R_S = 2, (1, 1.7504); 2 – 6, (1, 5.7504); 3 – 8, (1, 7.7504).](image)

![Figure 10. Time dependence of the Nusselt number at 10 rpm and the ratio of the height to the radius of the crystal: 1 – H/R_S = 2; 2 – 6; 3 – 8.](image)

Significant differences in the spatial form of convective flows and the distribution of the temperature field throughout the region in the gravitational-centrifugal radiation-convective regime compared to the thermogravitation radiation-convective regime are primarily associated with a violation of the stability of the spatial form of convective flows. The gas heated at the base of the crystal can periodically penetrate into the upper part of the growth chamber, and portions of cold gas penetrate into the lower part of the growth chamber (figures 3 – 5). When the spatial form of convective flows becomes fluctuating, the temperature field inside the crystal, seed crystal, and rod begins to oscillate (figures 7b and 8b). A heat wave propagates in the crystal (figure 9). The fluctuating nature of heat transfer (figure 10) generates temperature fluctuations in the crystal, with the maximum amplitude in the upper part of the crystal. The Nusselt number (figure 10) is calculated as the ratio of the integral heat flux from the crystal surface in the radiation-convective mode to the heat flux in the conductive regime.

At the rotation speed of a single crystal from 1 to 10 rpm, the spatial shape of convective flows and the temperature distribution in the single crystal do not differ significantly [2, 4]. This is due to the relatively small amount of centrifugal acceleration compared to the acceleration of gravity. When the speed of rotation of the crystal increases to 25 rpm, under the influence of centrifugal forces, the intensity of oscillations decreases, that is, the effect of laminarization of the gas flow is observed. A vortex begins to increase above the crystal, partially blocking the penetration of the gas heated at the base into the upper part of the growth chamber. As the height of the crystal increases, this effect increases. As a result, the amplitude of local heat flux fluctuations decreases.

**Conclusions**

The conjugate heat transfer in the regime of radiation-convective heat transfer from a silicon crystal to the ambient gas medium has been studied numerically by the finite element method. Calculations have been made for crystals of a discrete set of relative length 2 ≤ H/R_S ≤ 8 with heat transfer from stationary and uniformly rotating crystals at speeds of 10 and 25 rpm. The geometry of the calculated area is similar to the simplified scheme of the upper part of the heat unit in the Chokhralsky method. We solved the system of equations of thermo-gravitational and mixed convection in terms of vortex, stream function and the temperature. Calculations of radiation flows are based on the zonal method. The calculations have been performed with the Prandtl number equal to 0.68 (argon) and the Grashof number 16000, which is typical for a real technological process. The rotation of the crystal is shown to increase the cooling efficiency of the crystal. This is due to the loss of stability of the spatial form of convective
flows and the emergence of a system of non-stationary secondary vortexes, under the influence of which there is a more efficient cooling of the rod and crystal due to conductive heat exchange, and emissions of heated gas masses into the cold upper part of the growth chamber. Increasing the rotation speed to 25 rpm has a stabilizing effect on the spatial shape of convective flows and reduces the cooling efficiency of the crystal. The results obtained are useful in developing optimal technological modes for obtaining single crystals by directed crystallization methods and in designing and creating modern equipment for growth.

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