Effect of uniform crystal rotation on convective and radiation-convective heat transfer in the Czochralski method

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Abstract. The conjugate heat transfer in different regimes of heat transfer in the system "crystal – environment – walls of the growth vessel", geometrically similar to the simplified scheme of the upper part of the thermal node in the Czochralski method, is studied numerically by the finite element method. The system of equations of thermo-gravitational and mixed convection in variables of vortex, stream function and temperature is solved. In addition, the uniform rotation of crystals is taken into account. Calculations are carried out at convective and radiation-convective heat transfer with fixed crystal length. Calculations of radiation fluxes are carried out on the basis of the zonal method under the following assumptions: the calculated area is limited by a closed system of surfaces; all surfaces of the system are grey, diffuse-emitting and diffuse-reflecting; the surfaces are divided into zones within which the radiation properties and temperature can be considered constant; the medium filling the growth chamber is diathermic. The calculations were performed with the Prandtl number equal to 0.68 (argon) and the Grashof number of 16000, typical of the real process. The effect of uniform crystal rotation from 1 to 25 rpm on radiation-convective heat transfer is studied. It is shown that under the action of rotation the spatial form of convective flows loses stability. Secondary vortices appear. As a result, the cooling efficiency of the crystal increases significantly.

1. Introduction

The structural perfection of single crystals obtained by pulling from melts by the Czochralski method depends on the shape of crystallization front and the growth rate. In the process of crystal growth, it is necessary to ensure the absence of sharp changes in its diameter, the maximum symmetry of the temperature field and the minimum temperature gradients near the crystallization front [1]. From the results of studies of convective heat transfer in the melt, it follows that for melts with any value of the Prandtl number, there are relations of dimensionless dynamic parameters: Grashof Gr, Marangoni Ma and Reynolds Re numbers, characterizing the intensity and relative role of free and forced convection, in which the crystallization front is flat [2]. The findings are confirmed experimentally using a low-melting substance. Paper [2] presents the results of studies without taking into account heat transfer from the crystal to the environment. But in the real high-temperature technological process heat exchange has a complex conjugate nature and the temperature fields are self-consistent throughout the growth chamber. Control of thermal conditions of the crystal growth is quite a complex task, since the nonlinearity of the problems of convective and conjugate heat transfer between the crystal, the melt and the environment leads to the need to solve them with a large number of geometries of computational regions as the crystal grows.
In the framework of global modeling, the problems should be solved in a complete conjugate formulation, which requires almost impossible precise setting of boundary conditions corresponding to the real process, and large computational and time resources. Therefore, to understand the General laws of the dependence of the temperature fields in crystals on the heat transfer intensity from their generators and corresponding thermal stresses, it is possible to solve the problems in the framework of partial modeling. The results of such studies are necessary to estimate the spatial dependence of the electrophysical characteristics of the crystal on the growth conditions and thermal history of the crystal. Heat transfer from the crystal to the environment of the growth chamber affects the temperature fields in the crystal and in the regime of conjugate heat exchange corrects the curvature of the front and determines the volume distribution of its own point defects [1, 3] and other imperfections. Without claiming to be a complete description of these 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. The coupled radiation-convective heat transfer at a constant crystal rotation speed is investigated numerically by the finite element method [4]. The effect of the crystal rotation speed on the temperature field in the crystal is studied.

2. Model
Taking into account the properties of the axisymmetry of thermal units used in the growing of single crystals by the Czochralski method, the calculations are carried out in the two-dimensional 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, seed crystal, rod, walls of the growth chamber and a screen separating the melt surface from the gas medium in the growth chamber. A dimensionless system of Navier-Stokes equations, energy and continuity in the Boussinesq approximation, recorded in the variables of vortex, current function, azimuthal velocity and temperature, is used to simulate mixed convection:

\[
\frac{1}{\Pr} \left( \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right) + u \frac{\partial T}{\partial r} + v \frac{\partial T}{\partial z} = 0
\]

\[
\frac{\partial^2 \omega}{\partial r^2} + \frac{1}{r} \frac{\partial \omega}{\partial r} + \frac{\partial^2 \omega}{\partial z^2} + u \frac{\partial \omega}{\partial r} + v \frac{\partial \omega}{\partial z} \right) + \frac{\partial W}{\partial z} = 0
\]

\[
\frac{\partial^2 W}{\partial r^2} + \frac{1}{r} \frac{\partial W}{\partial r} + \frac{\partial^2 W}{\partial z^2} + u \frac{\partial W}{\partial r} + v \frac{\partial W}{\partial z} \right) + \frac{\partial W}{\partial z} = 0
\]

\[
\frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2} \right) + \frac{2}{r} \frac{\partial \psi}{\partial r} = r \cdot \omega
\]

\[
u = \frac{1}{\Pr} \frac{\partial \psi}{\partial z}, \quad \frac{\partial \psi}{\partial r}
\]

where T, \( \omega \), \( W \), \( \psi \), u, v is the temperature, vortex, azimuthal velocity, stream function, radial and axial components of velocity, respectively.

In the dimensionless equations \( Gr = (\beta \cdot g \cdot v^2) \cdot \Delta T \cdot R_s^3 \) is the Grashof number. Here \( \beta \) is the coefficient of gas volume expansion, g is the acceleration of gravity, v is the kinematic viscosity of argon, \( \Delta T \) is the temperature difference between the crystallization front and the walls of the growth chamber, \( R_s \) is the radius of the crystal. The Prandtl number of argon \( Pr = \nu / \alpha = 0.68 \), where \( \alpha = \lambda_G / \rho \cdot C_p \) is the coefficient of thermal diffusivity, \( \lambda_G \) is the coefficient of thermal conductivity, \( \rho \) is the density, \( C_p \) is the heat capacity at constant pressure. When the equations are reduced to a dimensionless form, radius of the crystal \( R_s \) is used as a geometric scale. The temperature scale is taken as temperature difference \( \Delta T \). The velocity scale is \( v/R \). Scale radiation fluxes are \( R_s^2 / \lambda_G \cdot \Delta T \). The time scale is \( v/R^2 \).
The calculation of radiation fluxes is carried out on the basis of the zonal method [5] under the following assumptions: the calculated area is limited by a closed system of surfaces; all surfaces of the system are grey, diffuse-emitting and diffuse-reflecting; the surfaces are divided into zones within which the radiation properties and temperature can be considered constant; the medium filling of the growth chamber is diathermic.

The problem was solved under the following boundary conditions. The maximum temperature in the system (1683 K) is set at the crystallization front: \( T_{r_1} = 1 \). On the screen separating the melt surface from the growth chamber, the conditions of thermal insulation, non-flow and adhesion are set: \( \frac{\partial T}{\partial n}_{r_2} = 0, \quad \psi|_{r_2} = 0, \quad a\|_{r_2} = \frac{\partial V}{\partial x}_{r_2} \). The minimum temperature in the system is maintained on the walls of the growth chamber, the condition of non-flow and adhesion is set: \( T_{r_3} = 0, \quad \psi|_{r_3} = 0, \quad a\|_{r_3} = \frac{\partial V}{\partial r}_{r_3} \). On the crystal generators, the conditions of non-flow, adhesion are set, the rotation speed and the ideal contact condition are set taking into account the radiation fluxes: \( \psi|_{r_4} = 0, \quad a\|_{r_4} = \frac{\partial V}{\partial x}_{r_4}, \quad W|_{r_4} = w, \quad T|_{r_4^+} = T|_{r_4^-}, \quad -\lambda_s \frac{\partial T}{\partial n}_{r_4^+} = -\lambda_s \frac{\partial T}{\partial n}_{r_4^-} + Q \).

Numerical simulation is carried out by finite element method on irregular grid of 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 \( R_s \) is 0.05 m, the thermal conductivity of argon \( \lambda_G = 5.83 \times 10^{-2} \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1} \), the thermal diffusivity of the gas \( a = 3.74 \times 10^{-4} \text{ m}^2 \cdot \text{s}^{-1} \), the volumetric expansion coefficient \( \beta = 6.4 \times 10^{-4} \text{ K}^{-1} \), 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

Numerical simulation is carried out with \( Pr = 0.68, \quad Gr = 16000, \quad \text{crystal length } H/R_s = 4 \) in the range of rotation speeds from 1 to 25 rpm.

Figure 1 shows the isolines of the current function and distribution of the temperature field in the entire region during radiation-convective heat exchange at different speeds of crystal rotation. In the absence of rotation of the crystal, a stationary temperature field is formed and a three-vortex convective flow of complex shape is established with the separation of the boundary layer from the forming rod at the level of \( z = 5.5 \). It is noticeable that the temperature field in the crystal is inhomogeneous. Accordingly, distribution of radial and axial temperature gradients in different parts of the crystal is inhomogeneous. As a consequence, the radial distributions of axial local heat fluxes are also uneven. This is due to the fact that on the cold walls of the vessel the descending streams of cold gas are formed, which reach the thermal insulation screen, unfold and flow onto the hot base of the crystal. Then the gas is heated and under the action of buoyancy rises up the crystal. Then the gas flows cool down on the walls of the growth chamber and again fall down to the base of the crystal. Thus, natural convective heat transfer leads to effective cooling and increase in radial and axial gradients near the crystallization front. Depending on the geometry of the computational domain, convective gas flows can reduce temperature gradients in colder areas of the crystal by heating the heated gas with ascending flows. Accounting for radiation fluxes significantly affects the temperature distribution on the surface and inside the crystal. Cooling efficiency increases in the entire volume of the crystal. The temperature on the forming crystals decreases. Accordingly, the temperature difference between the cold walls of the growth chamber and the crystal surface decreases. Axial temperature gradients increase significantly. Radial temperature gradients increase dramatically [7, 8].
Figure 1. Isolines of the stream function (left) and isotherm (right) at the moments of dimensionless time \( t = 104 \) at a speed of rotation: a – 0 rpm, b – 1 rpm, c – 10 rpm, d – 25 rpm.

Figure 2. Isolines of the current function (left) and the isotherm (right) at the crystal rotation speed 10 rpm at the moments of dimensionless time: a – \( t = 0 \), b – 30, C – 60, D – 90.
Under the influence of crystal rotation, the system loses its stability; secondary vortices are formed in the upper part of the growth chamber and fall down on the rod (figure 2). Then the secondary vortices reach the convective cell formed above the crystal, which prevents the penetration of hot gas masses rising from the crystal into the upper part of the growth chamber, and destabilizes it. As a result, hot gas is released into the upper part of the chamber, during which a secondary vortex is formed, rising along the cold walls of the vessel. The vortex, cooled down on the walls of the body, reaches the upper wall of the body, changes its direction and flows along the rod. Thus, the cooling efficiency of the upper part of the crystal and rod is significantly increased (figures 3-4). More effective cooling of the rod leads to an increase in the conductive heat sink from the crystal.

Figure 3. Temperature profiles at different levels in height $z$ at a crystal rotation speed of 10 rpm at moments of time: 1 – 0; 2 – 30; 3 – 60; 4 – 90.

Figure 4. Profiles of the vertical velocity component at different levels in height $z$ at a crystal rotation speed of 10 rpm at moments of time: 1 – 0; 2 – 30; 3 – 60; 4 – 90.

Thus, the cooling efficiency of the crystal grows noticeably, which can be seen by the concentration of isotherms at the base of the crystal, and temperature fluctuations occur inside the crystal (figure 5). Also, on the slope of the isotherms in figure 5, it is noticeable that despite the more effective cooling of the crystal during rotation, the radial temperature gradients decrease. It is evident that with the growth of the crystal rotation speed from 1 rpm to 10 rpm, the temperature field inside the crystal changes slightly. With a further increase in the speed of rotation, the cooling efficiency of the crystal decreases slightly.
Figure 5. Temperature fields in the crystal at the moment of dimensionless time $t = 104$ at a speed of rotation: a – 0 rpm, b – 1 rpm, c – 10 rpm, d – 25 rpm. The stroke indicates 4 additional isotherms with values: 0.975, 0.925, 0.875, 0.825. Fat isolated isotherm with a value of 0.8.

This is due to the fact that the intensity of the flow in the convective cell formed above the crystal increases, which prevents the emission of hot gas masses into the upper part of the growth chamber. This reduces the cooling efficiency of the upper part of the crystal and the rod (figures 6-7).

Figure 6. Temperature profile in cross-section $r = 1.5$ at crystal rotation speed: 1 – 0 rpm; 2 – 1; 3 – 10; 4 – 25.

Figure 7. The profile of the radial component of the velocity in the cross-section $r = 1.5$ when rotation speed of crystal: 1 – 0 rpm; 2 – 1; 3 – 10; 4 – 25.
Figure 8. Temperature profiles at different levels in height z at the speed of rotation of the crystal: 1 – 0 rpm; 2 – 1; 3 – 10; 4 – 25.

Figure 9. Profiles of the vertical velocity component at different levels in height z at the crystal rotation speed: 1 – 0 rpm; 2 – 1; 3 – 10; 4 – 25.
Figures 8-9 show the temperature distribution and the vertical velocity component in the gap between the crystal and the cold walls of the vessel at different levels in height. It is noticeable that the greatest amplitude of the axial components of the velocity of gas flow is achieved in the absence of rotation. Despite this, it is in this regime the crystal cools least effectively. This is due to the fact that when the crystal rotates due to the loss of stability and more efficient cooling of the rod, the conductive heat sink through the seed increases.

![Temperature distribution and vertical velocity component](image)

**Figure 8.** Temperature distribution and vertical velocity component in the gap between the crystal and the cold walls of the vessel at different levels in height.

**Figure 9.** Vertical velocity component in the gap between the crystal and the cold walls of the vessel at different levels in height.

**Figure 10.** Temperature profiles in different sections along the radius at crystal rotation speeds: 1 – 0 rpm; 2 – 1; 3 – 10; 4 – 25.

Figure 10 shows the temperature profiles in different sections along the radius of the crystal. It is well seen that under the influence of rotation the crystal cools much more efficiently. The maximum cooling efficiency of the crystal is achieved in the rotation speed range from 1 to 10 rpm. Then, as the rotation speed increases, the cooling efficiency of the crystal decreases.

**Conclusion**

The conjugate heat transfer in different regimes of heat transfer in the system "crystal – environment – walls of the growth vessel", geometrically similar to the simplified scheme of the upper part of the thermal node in the Czochralski method, is studied numerically by the finite element method. The system of equations of thermo-gravitational and mixed convection in variables of vortex, stream function and temperature is solved. In addition, the uniform rotation of the crystals is taken into account. Calculations are carried out at convective and radiation-convective heat transfer with a fixed crystal length. Calculations of radiation fluxes are carried out on the basis of the zonal method under the following assumptions: the calculated area is limited by a closed system of surfaces; all surfaces of the system are grey, diffuse-emitting and diffuse-reflecting; the surfaces are divided into zones within which the radiation properties and temperature can be considered constant; the medium filling of the growth chamber is diathermic. The calculations were performed with the Prandtl number equal to 0.68 (argon) and the Grashof number 16000, typical of the real process. The effect of uniform crystal rotation from 1 to 25 rpm on radiation-convective heat transfer is studied.

It is shown that the rotation of the crystal increases significantly the cooling efficiency of the crystal. First of all, this is due to the loss of stability of the spatial form of convective flows and emergence of secondary vortices, under the influence of which there is more effective cooling of the rod and, therefore, the crystal due to conductive heat exchange, and emissions of hot 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 form of convective flows and the cooling efficiency of the crystal decreases.

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