The influence of crucible and crystal rotation on the hydrodynamics of a melt with a Prandtl number 16 and on heat transfer in the Czochralski method

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Abstract. The effect of crucible rotation on the evolution of the melt flow structure at a Prandtl number 16 on the temperature and velocity fields and on convective heat transfer in the Czochralski method is simulated numerically in the mixed convection regimes at a given crystal rotation rate. The ranges of similarity parameters corresponding to stationary and unsteady melt flows and heat transfer regimes, as well as regimes with the most uniform radial distributions of local heat fluxes are determined. In the initial regime Reynolds, Grashof and Marangoni numbers are set to ReK = 95, Gr = 4870 and Ma = 5835.

1. Introduction
Despite the widespread use of the Czochralski method, the thermophysical processes during crystal growth have not been fully studied, and crystal growth is still an art and depends on the experience of the technologist [1-7]. The need for a deeper and more complete study of thermophysical processes in the growth of crystals is objectively due to continuously emerging new crystalline materials and strict requirements for their quality. An oxide crystal of bismuth ortho-germanate (BGO, Prandtl number Pr = 16) has practical importance and wide range of applications [3]. The BGO melt has individual thermophysical properties that affect the processes of convective heat transfer at the melt-solid transition stage [2-7]. Melts of garnets have similar properties, for example, the gallium gadolinium garnet.

In the Czochralski method, there is a radial temperature gradient on the free surface of melts; therefore, in addition to the buoyancy forces the thermocapillary effect acts and a heated melt flows along the free surface on the edge of the crystallization front (FC), melting the periphery of the FC. In addition, the radial inhomogeneity of the local heat flux at the FC increases [5, 7]. Thus, in all variations of the method, a fundamentally unavoidable and poorly controlled thermal gravitational-capillary convection occurs [5, 7]. In the classical Czochralski method with a fixed crucible, the selection of the crystal rotation speed is used to control hydrodynamics and convective heat transfer [1-7]. In particular, it is necessary to displace the thermocapillary flow of the superheated melt from the edge of the crystallization front [5, 7]. An additional method for controlling the hydrodynamics of melts and convective heat transfer is crucible rotation [2, 4, 6]. Uniform rotation of the crystal and crucible in one direction leads to a decrease in the intensity of the free convective flow and approaches the thermal conductivity regime with increasing rotation speed [2]. The results of investigations [2, 4] show that by choosing the crucible rotation speed it is possible to suppress the development of instabilities and to laminarize the initial unsteady mixed convection regime. There are few parametric studies in the regimes of crystal and crucible rotation. Therefore, studies of the effect of crucible rotation are carried out as a...
continuation of the investigations of [3, 5], in which the initial regime was thermogravitational convection in melts with Prandtl numbers 0.01 ≤ Pr ≤ 0.07. In this work, the presence of the thermocapillary effect is taken into account and the initial regime is the unsteady mixed convection in the melt with Pr = 16.

To determine the optimal conditions for crystal growth, it is necessary to know the limits of transitions to unsteady flow regimes, i.e. critical values of the Grashof number Gr, Marangoni number Ma, and Reynolds number ReK in the regimes of free and mixed convection [3-5]. It is necessary to determine the limits of the transitions under the combined influence of buoyancy forces, thermocapillary effect and centrifugal forces, including the rotation of the crucible. In the regions of laminar-turbulent transition and in turbulent regimes, temperature fluctuations at the FC lead to the appearance of crystal imperfections, for example, a streaky inhomogeneity.

2. Problem definition

The system of equations of the mixed convection in the Boussinesq approximation in terms of vortex, stream function, temperature, and azimuthal velocity is solved:

\[
\frac{\partial \omega}{\partial t} + U \frac{\partial \omega}{\partial r} + V \frac{\partial \omega}{\partial z} + \frac{U \omega}{r} \frac{\partial \omega}{\partial r} + \frac{1}{r} \frac{\partial W^2}{\partial r} = \frac{1}{Re} \left( \frac{\Delta \omega - \omega}{r^2} \right) - \frac{Gr}{Re^2} \frac{\partial \theta}{\partial r};
\]

\[
\Delta \psi - \frac{2}{r} \frac{\partial \psi}{\partial r} = r \omega; \quad \frac{\partial \theta}{\partial t} + U \frac{\partial \theta}{\partial r} + V \frac{\partial \theta}{\partial z} = \frac{1}{Pr \cdot Re} \Delta \theta;
\]

\[
\frac{\partial W}{\partial t} + U \frac{\partial W}{\partial r} + V \frac{\partial W}{\partial z} + \frac{U W}{r} = \frac{1}{Re} \left( \frac{\Delta \omega - W}{r^2} \right);
\]

Dimensionless form of the equations uses the following parameters: the length scale is the radius of the crystal – Rk; the temperature scale is the temperature difference between the edge of the crystal and the walls of the crucible - ΔT; and the speed scale is the linear speed of the edge of the crystal – ωkRk.

There is a group of dimensionless numbers in the system: the Grashof number (Gr), which approximates the ratio of the buoyancy to viscous force acting on a fluid; the Marangoni number (Ma) represents the role of thermocapillary effect; and the Prandtl number (Pr) represents thermophysical properties of the melt.

\[
Gr = \frac{g \beta T}{\nu^2} \Delta T \cdot R^3, \quad Ma = \left( -\frac{\partial \sigma}{\partial T} \right) \frac{R_k}{\alpha \mu} \cdot \Delta T, \quad Pr = \frac{v}{\alpha}, \quad Re_k = \frac{\Omega K \cdot R_k^2}{v}, \quad Re_T = \frac{\Omega T \cdot R^2}{v}.
\]

σ is the surface tension coefficient, μ, ν are the dynamic and kinematic viscosity coefficients, and α is the thermal diffusivity.

The system of equations is solved with the following boundary conditions. The bottom of the crucible (rigid and adiabatic):

\[
\psi = 0, \quad \frac{\partial \psi}{\partial z} = 0, \quad W = (\Omega_T / \Omega_K)^* r, \quad \frac{\partial \theta}{\partial z} = 1, \quad z = 0, \quad 0 \leq r \leq R_T / R_k;
\]

the lateral surface of the crucible:

\[
\psi = 0, \quad \frac{\partial \psi}{\partial r} = 0, \quad W = (\Omega_T / \Omega_K)^* r / R_k, \quad \theta = 1, \quad 0 \leq z \leq H / R_k, \quad r = R_T / R_k;
\]

free melt surface (adiabatic):

\[
\psi = 0, \quad \omega = -\frac{Ma}{Pr \cdot Re} \frac{\partial \theta}{\partial r}, \quad \frac{\partial W}{\partial z} = 0, \quad \frac{\partial \theta}{\partial z} = 0, \quad z = H / R_k, \quad 1 \leq r \leq R_T / R_k;
\]
crystallization front:
\[
\psi = 0, \quad \frac{\partial \psi}{\partial z} = 0, \quad W=r, \quad \theta = 0, \quad z=H/R, \quad 0 \leq r \leq 1;
\]
the axis of symmetry:
\[
\psi = 0, \quad \omega = 0, \quad W=0, \quad \frac{\partial \theta}{\partial r} = 0, \quad 0 \leq z \leq H/R, \quad r=0;
\]
The calculations were carried in the regimes of uniform rotation of the crucible in the direction of the crystal rotation at the given parameters \( Pr = 16, \) \( Gr = 5835, \) \( Ma = 4870, \) \( Re = 95, \) \( H/R_T = 0.7, \) \( R_f/R_K = 2.76. \)

3. Result and Discussion
Investigations are aimed at clarifying the effect of uniform crucible rotation on the mixed convection regimes in the Czochralski method. Here the results of investigations of crucible rotation in the direction of crystal rotation in the range of angular velocities \( 0 \leq \Omega \leq 50.5 \) rpm are presented. These regimes can be technologically optimal, because the initial regimes of mixed convection during crystal rotation interact with uncontrolled thermal gravitational-capillary convection and can be unsteady. At the same time, the uniform rotation of the system in some cases leads to a decrease in the intensity of the free convective flow and stabilization [8 - 10]. As a result, it is possible to increase the stability threshold not only for a free convective flow, but also for a flow in the mixed convection regime.

The mixed convection regime is selected as the initial regime at \( Gr = 4870 \) and \( Ma = 5835 \) and \( Re_K = 95 \) (Figures 1, 2). It was shown in [5] that at the Grashof and Marangoni numbers, as well as at Reynolds numbers \( 0 \leq Re_K \leq 81 \) and \( 104 \leq Re_K \leq 250, \) the flow has a stationary axisymmetric character. In the range of \( 82 \leq Re_K \leq 103, \) the flow loses its stability and axisymmetric oscillations occur (Figure 1). The Reynolds number \( Re_K = 95 \) (at \( \Omega_K = 6.4 \) rpm) is approximately in the middle of this range. Fluctuations are complex. As a result, the radial distributions of local heat fluxes depend on time (Figure 2a) and the instantaneous values of the dimensionless heat transfer coefficient (Nusselt number Nu on crystallization front (Figure 2b).

Figure 1 shows the flow structure (stream function (a) and isotherms (b)) in the initial mixed convection regime at \( Re_K = 95 \) with a stationary crucible at times corresponding to the extreme values of the Nusselt number Nu. Figure 2b shows the Nusselt numbers, which are determined by integrating the instantaneous radial distributions of local heat fluxes at the crystallization front (Figure 2a):
\[
Nu = \frac{\left\{ \int_0^{2\pi} \left( \frac{\partial \theta}{\partial z} \right)_{z=H/R} r dr d\varphi \right\}}{Q_k},
\]
where \( Q_k \) is the integral heat flux on the crystallization front in the thermal conductivity mode. Figures 1 and 2a show only the right-hand sides of the axisymmetric fields of the stream function and isotherms and the distributions of local heat fluxes. Stream function (a) and isotherms (b) at the time \( t = 204 \) s are practically identical to the fields at the time \( t = 30.5 \) s. At the qualitative level, the fields of stream functions and isotherms coincide at the times \( t = 113 \) s and \( t = 251 \) s; \( t = 125.5 \) s and \( t = 345 \) s. The fluctuations of the integral heat fluxes and the dimensionless heat transfer coefficient have a quasiperiodic character. Fluctuations of temperature under the crystallization front and local heat fluxes on the crystallization front are the cause of various imperfections of monocrystals. Fluctuations of local characteristics are a consequence of various hydrodynamic instabilities. The crucible rotates in order to laminarize the initial unsteady mixed convection regime. In addition to eliminating temperature pulsations, it is necessary to control the radial distributions of local heat fluxes, which influence the local shape of the crystallization front.

To determine the optimal conditions for crystal growth, the crucible rotation speed is selected to search for the most uniform radial distribution of the local heat flux on the crystallization front. To reduce the intensity of the free convection flow, at a fixed crystal rotation speed of \( 6.4 \) rpm (\( Re_K = 95 \)), the crucible rotation speed is gradually increased in the same direction in the range of \( 0 \leq \Omega \leq 50 \) rpm.
(Figures 3, 4). Figure 3b shows the fields of isolines of the stream function (a) and isotherms (b) in the regime of uniform rotation of the crystal and crucible at the same speed at $R_e_K = 95$ ($\Omega_K = 6.4$ rpm) and $R_e_T = 723$, $\Omega_T = 6.4$ rpm, i.e. in stationary mode. At $Pr = 0.05$ [2], in the regimes of uniform rotation of the crystal and crucible with the same rate, heat transfer occurs practically in the regime of thermal conductivity or low-intensity thermogravitational convection. The data in Figure 3b correspond to a complex stationary mixed convection regime with a significant influence of the thermocapillary effect.

At crucible rotation speeds of $0 \leq \Omega_T \leq 2.56$ rpm or at $0 \leq R_e_T \leq 289$, the flow is unsteady. With increasing the crucible rotation speed to $\Omega_T = 3.84$ rpm ($R_e_T = 434$, $Nu = 19.8$) and more, the flow stabilizes and becomes stationary (Figure 3). With increasing the crucible rotation speed, the position of the boundary, where flows merge, moves under the edge of the crystallization front. Figure 5 shows that the most uniform distribution of the local heat flux on the crystallization front is observed at $R_e_T = 434$. This regime, therefore, corresponds to the crystal growth with an almost flat shape of crystallization front. But the energetically optimal regime is $R_e_T = 1060$ with the minimum value of $Nu = 15.72$. According to the data presented in Figures 3, 4, it can be seen that at $R_e_T \geq 434$ the flow is stationary, but has a complex spatial shape. The directions of flows in a complex vortex structure can be understood from the profiles of the axial and radial velocity components shown in Figures 6, 7. Together with the data presented in Figure 3, these profiles explain the patterns in changes in the radial distributions of local heat fluxes. This is due not only to the flow of hot melt onto the edge of the crystallization front (Figure 3a, b), but also to changes in the flow direction along the normal to the crystallization front (Figure 3c, d). The influence of the thermocapillary effect on the formation of the flow shape can be seen from a comparison of Figures 3 and 7b. A radial temperature gradient along the free surface of the melt initiates a thermocapillary flow from the hot crucible wall to the cold edge of the crystallization front. With increasing the crucible rotation speed above the critical one and changing direction of the flow under the crystallization front, the thermocapillary effect remains and intensifies the flow from the crystallization front to the rotating bottom of the crucible. The radial distributions of local heat fluxes on the crystallization front, presented in Figure 5, show that at high crucible rotation speeds, the regimes are not technological. In these regimes, the shapes of crystallization front will be convex into the melt.

Conclusions
Numerical simulation of the effect of crucible rotation on the flow structure at fixed Prandtl number $Pr=16$, Grashof, Marangoni and Reynolds numbers, on the temperature and velocity fields, on local and integral heat transfer was carried out in the mixed convection regimes using the Czochralski method. When the crucible rotated in the direction of crystal rotation, the limits of the transition to a steady flow of the melt were determined. The regimes with the most uniform radial distributions of heat fluxes at the crystallization front were determined to be the main criterion for the optimal conditions for crystal growth with minimal thermal stresses.
**Picture 1.** Dependence of the flow structure in mixed convection regime with a fixed crucible:
a) \( t = 134 \text{s} \), b) \( 204 \text{s} \), c) \( 251 \text{s} \), d) \( 345 \text{s} \).
Picture 2. The corresponding radial distributions of local heat fluxes at the crystallization front as a function of time (a) instantaneous and average values of Nusselt number vs time: 1 – t = 30.5 s, 2 – 113 s, 3 – 125.5 s, 4 – 134 s, 5 – 204 s, 6 – 251 s, 7 – 345 s.
Dependence of the flow structure (stream function and isotherm) in the regime of uniform unidirectional rotation of the crystal and crucible: a) $\text{Re}_T = 434$, $\text{Nu} = 19.8$; b) $723$, $\text{Nu} = 18.3$; c) $1157$, $16.42$; d) $5707$, $27.17$

**Picture 3.** Dependence of the flow structure (stream function and isotherm) in the regime of uniform unidirectional rotation of the crystal and crucible: a) $\text{Re}_T = 434$, $\text{Nu} = 19.8$; b) $723$, $\text{Nu} = 18.3$; c) $1157$, $16.42$; d) $5707$, $27.17$
Dependence of the flow structure (stream function and isotherm) in the regime of uniform unidirectional rotation of the crystal and crucible: $\text{Re}_T = 1060$, $\Omega_T = 9.38 \text{ rmp}; \text{Nu} = 15.72$

**Picture 4.** Dependence of the flow structure (stream function and isotherm) in the regime of uniform unidirectional rotation of the crystal and crucible: $\text{Re}_T = 1060$, $\Omega_T = 9.38 \text{ rmp}; \text{Nu} = 15.72$

**Figure 5.** Radial distributions of local heat fluxes at the crystallization front: 1 – $\text{Re}_T = 0$, $z = 3H/4$; 1 – $\text{Re}_T = 434$, $2 – 723$, $3 – 761$, $4 – 867$, $2 – \text{Re}_T = 434$, $3 – 723$, $4 – 761$, $5 – 867$, $5 – 1157$, $6 – 3044$, $7 – 5707$

**Figure 6.** Profiles of the axial velocity component at $z = (3H/4)$:
1 – $\text{Re}_T = 434$, $2 – 723$, $3 – 761$, $4 – 867$, $5 – 1157$, $6 – 3044$, $7 – 5707$

**Figure 7.** Profiles of the horizontal velocity component at $r = 0.95$ (a) and $r = 1.4$ (b):
1 – $\text{Re}_T = 434$, $2 – \text{Re}_T = 723$, $3 – \text{Re}_T = 761$, $4 – \text{Re}_T = 867$, $5 – \text{Re}_T = 1157$, $6 – \text{Re}_T = 3044$
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