The influence of conjugate natural convective heat transfer on the temperature field in a monocrystalline sapphire tape in the Stepanov method

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Abstract. Natural convective heat transfer in the system "monocrystalline tape – environment – walls of the growth vessel", geometrically similar to the simplified scheme of the upper part of the heat node in the Stepanov method, is studied numerically by the finite element method in the conjugate formulation. The calculations were performed with a Prandtl number equal to 0.68 (argon), in the range of Grashof numbers 1000 ≤ Gr ≤ 25000 and with a discrete set of tape lengths in the range from 1 to 5.

1. Introduction
The Stepanov method is one of the methods for growing single crystals from melts with a free surface [1, 2]. The key feature of the Stepanov method is the use of a shaper and the ability to pull single crystals from the melt with a wide range of cross-sectional profiles of the crystal from flat tape, rods and cylindrical pipes to more complex shapes. When the crystal grows, the melt enters the crystallization front through the capillary channels of the shaper. As a result, a thin layer of melt is formed between the single crystal and the shaper, which determines the shape of the crystal cross-section, from which the crystal is growing [1, 2]. The main difficulties in the practical implementation of obtaining high-quality single crystals by this method are associated with the control of processes in the meniscus zone. In this case, the meniscus zone is a column of melt between the shaper and the crystallization front (CF). The shape of the area occupied by the melt under the crystallization front is significantly affected by the conjugate radiation-convective heat transfer between the shaper, the melt, the CF and the environment. By adjusting the relative role of the buoyancy forces and the thermocapillary effect on the convective heat transfer under the CF, it is possible to pull a crystal with a flat CF. An important but poorly studied factor is heat transfer from the crystal to the environment and dependence of the temperature fields in the crystal on its shape and size as it grows.

The uniformity of the distribution of optical and electrical properties and, in general, the structural perfection of the grown single crystal depend on the thermal history of the crystal [1, 2]. In the process of crystal growth, it is necessary to ensure minimum temperature gradients and thermal stresses in the crystal. The complexity of the analysis of crystal growth processes and the difficulties in developing a well-controlled automated and optimal technology for growing single crystals are largely due to a complex of unsolved problems of non-stationary conjugate heat transfer. As the crystal grows, its length changes and the configuration of the region where complex conjugate heat transfer occurs changes. As a result, the patterns of conjugate heat transfer between a single crystal and the environment of the growth chamber change. Within the framework of global modelling, it is necessary
to solve the non-stationary problem of complex conjugate heat transfer in the entire thermal node of the growth node, considering changes in the geometry of the computational domain [3]. This will require a lot of computing and time resources. To understand the general regularities of the dependence of the temperature fields in a single crystal on conjugate heat transfer necessary for the design of growth nodes and optimization of technological processes for the growth of single crystals, it is advisable to use the partial modelling approach [4–7]. Partial modelling allows us to determine at a qualitative level the main trends in the behavior of the systems under consideration when individual control parameters or a group of them change.

Conjugate heat transfer in the natural convective heat transfer regime in the "single – crystal tape – environment – walls of the growth vessel" system, geometrically similar to the upper part of the heat node in the Stepanov method, was studied numerically by the finite element method [8]. The results of calculations for a discrete set of Grashof numbers and lengths of a single-crystal tape are presented. The influence of the tape length and the Grashof number (temperature drop) on the temperature fields and temperature gradients in the crystal is studied.

2. Model

For the geometry used for growing single-crystal tapes, numerical simulation is carried out in a two-dimensional formulation in Cartesian coordinates. When simulating thermogravitational convection, a dimensionless system of Navier-Stokes, equations of energy and continuity in the Boussinesq approximation is used, written in the terms of vortex, stream function and temperature:

\[
\frac{\partial T}{\partial t} + V_x \frac{\partial T}{\partial y} + V_y \frac{\partial T}{\partial x} = \frac{1}{Pr} \left( \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial x^2} \right)
\]

\[
\frac{\partial \omega}{\partial t} + V_y \frac{\partial \omega}{\partial y} + V_x \frac{\partial \omega}{\partial x} = \left( \frac{\partial^2 \omega}{\partial y^2} + \frac{\partial^2 \omega}{\partial x^2} \right) + Gr \frac{\partial T}{\partial y}
\]

\[
\frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial x^2} = -\omega \quad V_x = \frac{\partial \psi}{\partial y} \quad V_y = -\frac{\partial \psi}{\partial x}
\]

Here \(Gr = g \cdot \beta \cdot L^2 (T_{\text{max}} - T_{\text{min}}) \cdot v^{-2}\) is the Grashof number, where \(g\) is the acceleration of gravity, \(\beta\) is the volume expansion coefficient of gas, \(v\) is the kinematic viscosity of argon, \(\Delta T\) is the temperature difference between the crystallization front and the walls of the growth vessel. \(L\) is the distance from the center of the growth chamber to the cold walls of the vessel. The Prandtl number \(Pr = v/\alpha_f\), where \(\alpha_f\) is the coefficient of thermal diffusivity of liquid. \(T\) is the dimensionless temperature, \(\omega\) is the dimensionless vortex, \(\psi\) is the dimensionless stream function, \(V_x\) and \(V_y\) are the vertical and horizontal components of the velocity vector, \(x\) and \(y\) are the horizontal and vertical spatial coordinates, respectively.

When reducing the equations to a dimensionless form, the \(L\) is distance from the center of the growth chamber to the cold walls of the vessel is used as a geometric scale. The temperature difference \(\Delta T\) is taken as the temperature scale. The velocity scale is selected as \(v/L\).

The problem was solved under the following boundary conditions. At the crystallization front, the maximum temperature in the system is set: \(T_{|I_1} = 1\). On the screen separating the melt surface from the growth chamber, the conditions of thermal insulation, non-leakage and adhesion are set: \(\frac{\partial T}{\partial n}_{|I_2} = 0\), \(\psi_{|I_2} = 0\), \(\omega_{|I_2} = \frac{\partial V}{\partial z}_{|I_2}\). The minimum temperature in the system is maintained on the walls of the growth vessel, the condition of non-leakage and adhesion is set: \(T_{|I_3} = 0\), \(\psi_{|I_3} = 0\), \(\omega_{|I_3} = -\frac{\partial V}{\partial r}_{|I_3}\). On
the generators of a single-crystal tape, the conditions of non-flow, adhesion and the condition of ideal thermal contact are set: \( \psi_{|z} = 0, \ \frac{\partial \psi}{\partial t}_{|z}, -\lambda_s \frac{\partial T}{\partial n}_{|z} = -\lambda_r \frac{\partial T}{\partial n}_{|z} \), where \( \lambda_s \) and \( \lambda_r \) are the thermal conductivity of a solid and a gas, respectively.

\[ 4 \begin{align*}
\psi_{|z} &= 0, \\
\frac{\partial \psi}{\partial t}_{|z} &= -\lambda_s \frac{\partial T}{\partial n}_{|z}, \\
-\lambda_r \frac{\partial T}{\partial n}_{|z} &= 0.
\end{align*} \]

\[ 4 \begin{align*}
\frac{\partial^2 \psi}{\partial z^2} &= -\frac{\partial V}{\partial z}, \\
\frac{\partial^2 \psi}{\partial r^2} &= -\frac{\partial V}{\partial r}, \\
\frac{\partial T}{\partial n} &= 0.
\end{align*} \]

Figure 1. The fragment of the grid in the area near the crystallization front -0.3 < x < 0.3, 0 < y < 0.3

Numerical simulation was carried out by the finite element method on an uneven grid of 17557 nodes consisting of triangular finite elements with linear functions. In a solid, the grid thickens 8 times, relative to the grid in the area filled with gas. Figure 1 shows a fragment of the tape above the crystallization front (CF is shown by the red line). The calculations were performed at thermal conductivity of a single-crystal tape \( \lambda_s = 11 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1} \) (sapphire at 1000 K), the thermal conductivity of the gas (argon) \( \lambda_r = 5.83 \cdot 10^{-2} \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1} \), the thermal diffusivity of gas \( \alpha = 3.74 \cdot 10^{-4} \text{ m}^2 \cdot \text{s}^{-1} \), the kinematic viscosity of gas \( \nu = 2.54 \cdot 10^{-4} \text{ m}^2 \cdot \text{s}^{-1} \), and the volume expansion coefficient of gas \( \beta = 6.4 \cdot 10^{-4} \text{ K}^{-1} \). The properties of argon were taken at a temperature of 1600 K [9]. The distance from the center of the growth chamber to the cold walls of the vessel is \( L = 51 \text{ mm} \). The width of the single-crystal tape is \( 2 \cdot L/31 \). The height of the growth chamber is fixed and assumed to be equal to \( 5 \cdot L \).

3. Results and discussion
In the field of such a simplified technological geometry of the growth node of the Stepanov method, calculations of natural convective heat transfer from a single-crystal tape to the cold walls of the vessel in the regime of thermogravitational convection are carried out. The simulation is carried out with a discrete set of Grashof numbers \( Gr = 1000 \) (\( \Delta T = 77.5 \text{ K} \)), 10 000 (\( \Delta T = 775 \text{ K} \)) and 25 000 (\( \Delta T = 1940 \text{ K} \)) and in the range of single-crystal tape lengths \( 1 \leq H/L \leq 5 \).

Figure 2 shows the fields of isotherms and isolines of the stream function at different lengths of a single-crystal tape and Grashof numbers. In the range of the tape length from 1 to 4, a single-vortex circulation flow is established in the gap between the tape and the cold walls of the vessel (figures 2a – 2b). The gas heats up at the base of the tape (the crystallization front), rises along the crystal generatrix, breaks off from the upper edge of the tape and reaches the cold cover of the vessel. Then the gas flow unfolds, reaches the cold walls of the vessel, cools and descends to the heat-insulated screen. After that, the cold gas flow unfolds and runs over the heated base of the monocryalline tape. As a result, the cooling efficiency of the tape increases significantly near the crystallization front, and the longitudinal and transverse temperature gradients in the volume of the tape increase sharply.
Figure 2. The isolines of the stream function (left) and the isotherm (right) for the Grashof number: a, b, c – Gr = 10 000; d – 25 000; e – 1000 and the length of the tape: a – h = 3; b – 4; c, d, e – 5.

As it grows, the length of the tape reaches the height of the area (H/L = 5). The structure of convective flows in the area filled with gas is changing. The region of boundary layer separation appears (figure 2b). At a level equal to y = 3.2, the ascending gas flow breaks off from the generatrix of monocrystalline tape and goes to the cold walls of the vessel. The reason for the separation of the boundary layer is the formation of an oncoming flow of cold gas and the formation of a second vortex in the upper part of the gas layer. The flow of cold gas descends along the forming upper part of the tape, meets the ascending hot flow, turns around, goes to the center of the area filled with gas, and rises to the cold cover of the vessel. As a result, local temperature gradients grow in the region of boundary layer separation and the patterns of heat transfer change.

With an increase in the temperature drop (figure 2d), the intensity of convective flows increases, but the spatial shape does not change qualitatively. The region of separation of the boundary layer is slightly shifted up to the level y = 3.3. With a decrease in the temperature drop (figure 2e), a qualitative change in the spatial structure of convective flows occurs, the region of separation of the boundary layer disappears and the flow becomes single-vortex.

The information obtained is of practical interest. As the height of the growth chamber increases, new areas of separation of the boundary layer will appear, and a multi-vortex convective flow will form.

Figure 3 shows the evolution of the isotherm field inside a single-crystal tape as its length increases. At the initial stage of crystal growth, the temperature field in the tape changes significantly (figure 3a - 3c) but starting from the length H/L = 3, it is seen that the temperature field in the lower part of the tape stabilizes. This is due to the influence of a cold gas flow running on the base of the tape.

Starting from H/L = 2, the intensity and spatial shape of the cold gas flow from the walls of the vessel to the lower part of the tape ceases to change (figure 4a - 4b). The subsequent increase in the length of the tape affects the spatial shape and intensity of convective flows only in the upper part of the calculated domain.

Figure 4c shows the evolution of the vertical distribution of longitudinal temperature gradients in a single-crystal tape as its length increases. It is noticeable that the longitudinal temperature gradients are distributed non-linearly.
Figure 3. Isotherms in the tape with the Grashof number: a, b, c, d, e – Gr = 10 000; f – Gr = 25 000 and the length of the tape a – h = 1; b – 2; c – 3; d – 4; e, f – 5.

The maximum value is reached in the lower region of the tape and, starting from the length H/L = 2, it does not change depending on the length of the single-crystal tape. This is due to the steady flow of cold gas flowing onto the base of the tape. At the same time, with the increase in the length of the tape, the longitudinal gradients in the upper part of the tape grow. This is due to the intensification of convective heat transfer from the crystal caused by the growth of the heat removal surface.

When the tape length H/L = 5 is reached, a qualitative change in the shape of the distribution of longitudinal temperature gradients occurs. This is due to the fact that the tape has reached the cold cover of the vessel, as a result of which the role of conductive heat transfer has significantly increased. It can be seen that the distribution of the longitudinal temperature gradients in the lower part of the tape remained unchanged. That is, the strengthening of the role of the conductive heat transfer mechanism had an impact only on the upper part of the tape. The significant influence of the separation region of the boundary layer is also visible. It can be seen that under its influence, local longitudinal temperature gradients increase significantly.

Figure 4d shows the transverse distribution of longitudinal temperature gradients near the crystallization front. It is clearly noticeable that in the range of lengths of a single-crystal tape 1 ≤ H/L ≤ 2, a significant increase in longitudinal temperature gradients occurs. In the range 2 ≤ H/L ≤ 3, the growth of longitudinal temperature gradients slows down significantly and in the range 3 ≤ H/L ≤ 4, they practically do not change. When H/L = 5 is reached and the upper part of the monocrystalline tape comes into contact with the cold cover of the vessel, under the influence of a significant increase in the role of conductive heat transfer, the longitudinal temperature gradients at the base of the monocrystalline tape increase insignificantly.
Figure 4. The profile of the horizontal velocity component in the cross-section \( x = 5 \) (a), the profile of the vertical velocity component at the level \( y = 0.25 \) (b), the vertical distribution of longitudinal temperature gradients in the cross-section \( x = 0 \) (c), the horizontal distribution of longitudinal temperature gradients at the level \( y = 0.25 \) (d) with the Grashof number \( Gr = 10000 \) and the length of the tape: 1 – \( h = 1 \); 2 – 2; 3 – 3; 4 – 4; 5 – 5.

In addition, it is noticeable that the transverse distribution of longitudinal temperature gradients in a thin tape is markedly inhomogeneous. The maximum of the longitudinal gradients is reached on the surface of the tape, and the minimum is located in the center of the tape. The information obtained is important, since the analysis of the dislocation distribution during crystal growth uses the Voronkov theory, which assumes a homogeneous distribution of longitudinal temperature gradients.

4. Conclusion
As the length of the single-crystal tape increases, the fields of temperature, temperature gradients and thermal stresses in the volume of the resulting crystal change significantly in the Stepanov method. The features of convective heat transfer have a significant influence on the temperature fields. The spatial shape of convective flows changes with the increase in the length of the single-crystal tape. Region of separation of the boundary layer may form, which noticeably change the local patterns of heat transfer. At the same time, starting from a certain length, the spatial shape and intensity of convective flows are established in the lower region of the growth chamber, which does not change.
with increasing the length of the tape. A cold gas flow runs over the base of the tape, under the influence of which the cooling efficiency of the area at the crystallization front increases noticeably and longitudinal temperature gradients grow. After that, a temperature field is set in the lower part of the tape, which becomes insensitive to the conductive heat sink through the crystal to the cold cover of the vessel.

It is shown that the transverse distribution of the longitudinal temperature gradient in a single-crystal tape near the crystallization front is expressed inhomogeneously. This is important information when analyzing the causes of the appearance and distribution of dislocations in the crystal.

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