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TEMPERATURE FIELDS IN THIN WIDE-PROFILE PLATES OBTAINED FROM A MELT BY THE STEPANOV TECHNIQUE UNDER NONSYMMETRIC CONDITIONS OF GROWTH

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A mathematical model is suggested allowing one to determine the temperature fields in thin wide-profile plates when growing them from a melt by the Stepanov technique depending on the asymmetry in the position of a growing crystal relative to the nearby screens, as well as on the difference between the surface temperatures of the left and right screens. The model contains the heat conduction equation and a system of integral equations that connects the densities of radiant and temperature fluxes.

Keywords: *Stepanov's technique, temperature fields, radiation heat transfer.*

Introduction. Large-scale crystal sapphire plates have found wide practical applications, for example, as peepholes in the chemical industry, in space-related investigations, and as screens of a great number of multi-purpose reading machines. Moreover, the requirements on their quality have increased constantly. Defects such as, for example, dislocations that appear in crystallization from a melt result from the action of thermoelastic stresses in a nonuniformly heated crystal. Fairly many works are devoted to investigations of temperature stresses in plates, e.g., [1, 2]. The heat transfer conditions used in the calculations in these works are different; therefore it is important to compare their results depending on the mathematical model selected. In our work heat is transferred by radiation described by the "balance" method [3] for a "crystal–screen–shaper" system. In growing large-scale sapphire crystals there exists a serious problem of arranging the thermal unit, since with increase in the dimensions of the thermal zone and in the length of the crystal being grown thermal conditions in the crystallization zone deteriorate substantially and large thermoelastic stresses appear [2]. In real conditions of crystal growth there is necessarily a certain asymmetry in the position of a growing crystal relative to the heaters and the system of screening, and it leads to an appreciable change in temperature over the plate thickness. The present paper is devoted to the study of the influence of the arrangement of screening on the temperature fields of a growing crystal.

Statement of the Problem. We consider the growth of a thin wide-profile crystal plate from a melt by the Stepanov technique. The simplified scheme of growth, coordinate system, and the symbols used are given in Fig. 1. The superscript i will be affixed to the quantities relating to the right side (i = 1) of the thermal unit relative to the crystal plate and and to the left one (i = 2). The determination of the temperature field $T(x, y, z)$ of such a plate is reduced to the solution of the heat conduction equation:

$$k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)-V_0\rho c\frac{\partial T}{\partial y}=0\,. \tag{1}$$

The conditions of heat exchange between the crystal plate and the surrounding medium are determined as follows: on the side surfaces of the plate at $z = -h/2$ and $z = h/2$ the heat flux densities $q_1^{(i)}$ are assigned:

$$-k\left.\frac{\partial T}{\partial z}\right|_{z=h/2}=q_1^{(1)}\,,\quad k\left.\frac{\partial T}{\partial z}\right|_{z=-h/2}=q_1^{(2)}\,. \tag{2}$$

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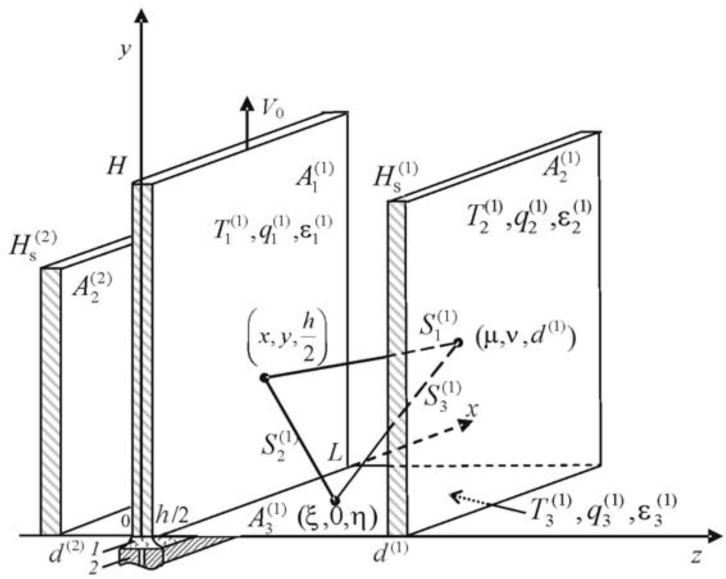

Fig. 1. Simplified scheme of the growth of a crystal tape under asymmetric conditions: 1) meniscus of the melt; 2) shaper.

We approximate the change in the temperature $T(x, y, z)$ over the plate thickness by a series in powers of z:

$$T(x, y, z) = \sum T^{(i)}(x, y)\, z^i . \tag{3}$$

We substitute this equation into Eq. (1), then multiply by z^k (k = 0, 1, ...), and integrate over z, using boundary conditions (2). Then for the coefficients of expansion of $T^{(i)}(x, y)$ from Eq. (3), restricting ourselves to two terms, we obtain a system of equations:

$$\Delta T^{(0)} = -\frac{V_0 c\rho}{k}\frac{\partial T^{(0)}}{\partial y} = \frac{1}{kh}(q_1^{(1)} + q_1^{(2)}) , \tag{4}$$

$$\Delta T^{(1)} = -\frac{V_0 c\rho}{k}\frac{\partial T^{(1)}}{\partial y} - \frac{12}{h^2} T^{(1)} = \frac{6}{kh^2}(q_1^{(1)} - q_1^{(2)}) , \tag{5}$$

so that for the linear approximation of $T_1(x, y, z)$ over z to the temperature $T(x, y, z)$ we have the expression

$$T_1(x, y, z) = T^{(0)}(x, y) + zT^{(1)}(x, y) .$$

The boundary conditions for $T^{(0)}(x, y)$ and $T^{(1)}(x, y)$ are

$$T^{(0)}(x, y) = T_m \ \text{for}\ \ y = 0 ,\ \ 0 \le x \le L ;\ \ \frac{\partial T^{(0)}}{\partial x} = 0 \ \text{for}\ \ x = 0 ,\ \ x = L ,\ \ 0 \le y \le H ; \tag{6}$$

$$\begin{gathered} T^{(0)}(x, y) = T_0 ,\ \ y = H ,\ \ 0 \le x \le L ;\ \ T^{(1)}(x, y) = 0 \ \text{for}\ \ y = 0 ,\ \ 0 \le x \le L ; \\ \frac{\partial T^{(1)}}{\partial x} = 0 \ \text{for}\ \ x = 0 ,\ \ x = L ,\ \ 0 \le y \le H ;\ \ T^{(1)}(x, y) = 0 ,\ \ y = H ,\ \ 0 \le x \le L . \end{gathered} \tag{7}$$

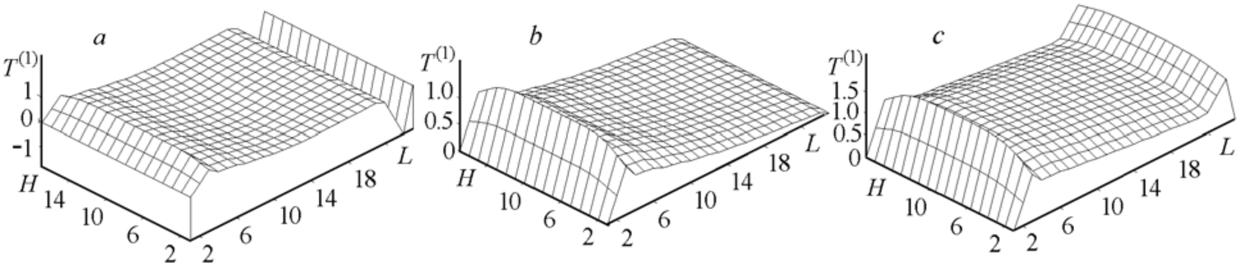

Fig. 2. Gradient of the temperature $T^{(1)}(x, y)$ over the plate thickness as a function of the screen height H_s relative to a growing crystal: a) $H > H_s$; b) $H = H_s$; c) $H < H_s$.

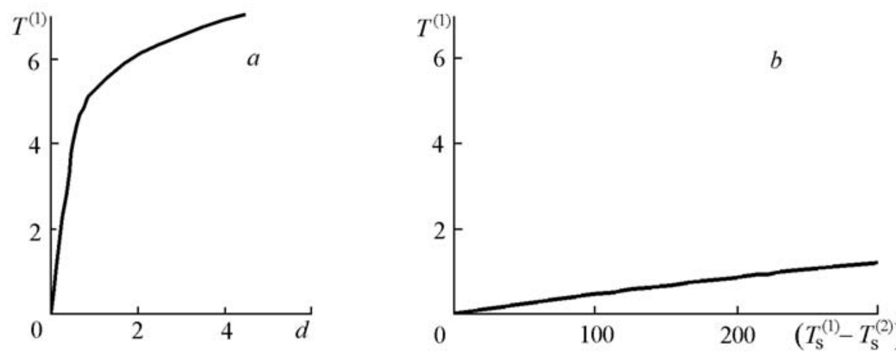

Fig. 3. Dependences of the gradient of $T^{(1)}(x, y)$ on the differences in: a) distances $(d^{(1)} - d^{(2)})$; b) temperatures of the screens $(T_s^{(1)} - T_s^{(2)})$.

The relationship between the surface temperatures $T_j^{(i)}(r_j^{(i)})$ and radiation densities $q_k^{(i)}$ are assigned by the following system of integral equations:

$$\frac{q_k^{(i)}(r_k^{(i)})}{\varepsilon_k^{(i)}} - \sum_{j=1}^{3} \frac{1-\varepsilon_j^{(i)}}{\varepsilon_j^{(i)}} \int_{A_j^{(i)}} K_{kj}^{(i)} q_j^{(i)}(r_j^{(i)})\, dA_j^{(i)} = \sigma T_k^{(i)4}(r_k^{(i)}) - \sigma \sum_{j=1}^{3} \int_{A_j^{(i)}} K_{kj}^{(i)} T_j^{(i)4}(r_j^{(i)})\, dA_j^{(i)}\,, \tag{8}$$

$$k = 1, 2, 3\,; \quad i = 1, 2\,,$$

where

$$K_{12}^{(i)}(r_1^{(i)}, r_2^{(i)}) = K_{21}^{(i)}(r_1^{(i)}, r_2^{(i)}) = \frac{1}{\pi}\frac{(d^{(i)} - h/2)^2}{S_1^{(i)4}}\,; \quad K_{13}^{(i)}(r_1^{(i)}, r_3^{(i)}) = K_{31}^{(i)}(r_1^{(i)}, r_3^{(i)}) = \frac{1}{\pi}\frac{(\eta - h/2)\, y}{S_2^{(i)2}}\,;$$

$$K_{23}^{(i)}(r_2^{(i)}, r_3^{(i)}) = K_{32}^{(i)}(r_2^{(i)}, r_3^{(i)}) = \frac{1}{\pi}\frac{\nu(d^{(i)} - \eta)}{S_3^{(i)4}}\,; \quad K_{11}(r_1^{(i)}) = K_{22}(r_2^{(i)}) = K_{33}(r_2^{(i)}) = 0\,;$$

$$S_1^{(i)} = \sqrt{(x-\mu)^2 + (y-\nu)^2 + (d^{(i)} - h/2)^2}\,; \quad S_2^{(i)} = \sqrt{(x-\xi)^2 + y^2 + (\eta - h/2)^2}\,;$$

$$S_3^{(i)} = \sqrt{(\xi-\mu)^2 + \nu^2 + (d^{(i)} - \eta)^2}\,;$$

$$T_1^{(1)}(x, y) = T_0(x, y) + \frac{h}{2} T_1(x, y)\,, \quad T_1^{(2)}(x, y) = T_0(x, y) - \frac{h}{2} T_1(x, y)\,.$$

The temperatures $T_2^{(i)}(\mu, \nu)$ and $T_3^{(i)}(\xi, \eta)$ are the known functions, viz.: $T_3^{(i)}(\xi, \eta)$ (i = 1, 2) is considered equal to the temperature of the melt T_m contained in the shaper, whereas $T_2^{(i)}(\mu, \nu)$ (i = 1, 2) changes linearly over the screen height ν from T_0 (ν = 0) to a certain known temperature of the upper edge of the screen $T_s^{(i)}$ ($\nu = H_s^{(i)}$):

$$T_2^{(i)}(\mu, \nu) = T_m + \frac{\nu}{H_s^{(i)}} (T_s^{(i)}(\mu) - T_m) .$$

The boundary-value problems (4)–(7) will be solved by the method of finite elements, i.e., by the direct method of mathematical physics consisting in the minimization of such a functional for which the Euler–Lagrange equation yields an initial differential equation for it. For example, for Eq. (4) with boundary-value conditions (6) such a functional has the form

$$L(T^{(0)}, T^{6(0)*}) = \iint_{A_1} \left[(\nabla T^{(0)} \nabla T^{(0)*}) + \frac{\xi}{2} T_1^* (\mathbf{V} \cdot \nabla T^{(0)}) - \frac{\xi}{2} T^{(0)} (\mathbf{V} \cdot \nabla T^{(0)*}) \right] dxdy , \tag{9}$$

where $T^{(0)*}$ is the quantity conjugate of the temperature $T^{(0)}$ and $\xi = \frac{\rho c}{k}$, $\mathbf{V} = (V_0, 0)$.

We reduce the system of integral equations (8) to a discrete form replacing all the integrals entering into it by the integral sums corresponding to them. According to the method of finite elements, the minimization of functional (9) allows one to obtain a system of linear algebraic equations which, together with the system of equations corresponding to Eqs. (8), yields a general system of equations whose solution allows one to obtain the distribution of temperature over the entire volume of the plate and to follow its change depending on the magnitude of the asymmetry in the disposition of screens relative to a growing crystal in the conditions of different ambient temperatures.

Numerical Results. Figure 1 demonstrates a typical behavior of the temperature gradient $\frac{\partial T_1(x, y, z)}{\partial z} = T^{(1)}(x, y)$ over the plate thickness depending on the screen height H_s relative to the height H of a crystal being grown. Computations were carried out at the following thermal and geometric parameters of the thermal unit: L = 15 cm, H = 25 cm, h = 0.8 cm, T_m = 2050°C, T_0 = 1000°C, $T_s^{(1)}$ = 950°C, $T_s^{(2)}$ = 750°C; the distance between the side surfaces of the crystal and screens was 4 cm and the difference between the surface temperatures of the right, $A_2^{(1)}$, and left, $A_2^{(2)}$, screens was 200°C.

From the figures given it is seen that at all the relationships between the crystal height H and screen height H_s the gradient of the temperature $T^{(1)}(x, y)$ increases sharply from the crystallization front to the upper edge of the crystal plate over its entire width. For the case of equal heights of the screen and plate ($H = H_s$), the maximum of the gradient of 1.5 deg/cm is attained at a distance approximately equal to 2 cm from the crystallization front and afterwards decreases gradually to the upper edge of the plate up to the values equal to 0.3 deg/cm (Fig. 2b). But if the crystal is higher than the screen ($H > H_s$), then $T^{(1)}(x, y)$ decreases sharply from 0.3 deg/cm ($z = H_s$) to −1.7 deg/cm ($z = H - H_s/2$) and then increases to values practically equal to zero on the upper edge of the plate ($z = H$, see Fig. 2a). And, finally, when $H < H_s$, then on the upper edge of the crystal plate the behavior of the gradient of $T^{(1)}(x, y)$ is analogous to the case of $H > H_s$ accurate to the decimal place (Fig. 2c).

Figure 3a presents the dependence of a maximum value of the gradient of the temperature $T^{(1)}(x, y)$ on the difference of distances $d = (d^{(1)} - d^{(2)})$ at a fixed value of $d^{(2)}$ = 2 cm. It is seen from the figure that the gradient of $T_1(x, y)$ increases monotonically from zero in the case of symmetric disposition of screens (d = 0) to values equal to 7 deg/cm at d = 5 cm. Now, we consider the behavior of a maximum gradient of $T^{(1)}(x, y)$ depending on the difference of the temperatures of the left, $T_s^{(1)}$, and right, $T_s^{(2)}$, screens, when the temperature varies within the range 0–300°C at identical distances $d^{(1)}$ and $d^{(2)}$ from the middle plane of the crystal plate to the screens equal to 2 cm and at a fixed temperature of the left screen $T_s^{(2)}$ = 750°C. The dependence presented in Fig. 3b shows that at a temperature difference $T_s^{(1)} - T_s^{(2)}$ equal to 300°C maximum values of the gradient do not exceed 1.2 deg/cm.

Conclusions. The calculations carried out show that the asymmetry in the disposition of screens relative to a crystal being grown exerts a much greater influence on the nonuniform distribution of temperature over the plate thickness than the asymmetry in the temperatures of heaters. Thus, in growing large-scale sapphire tapes attention should be specially paid to the dimensions and disposition of the screens.

NOTATION

$A_1^{(1)}$, $A_1^{(2)}$, crystal surfaces; $A_2^{(1)}$, $A_2^{(2)}$, surfaces of the right and left screens, respectively; $A_3^{(1)}$, $A_3^{(2)}$, shaper surfaces; c, specific heat of a crystal, J/K; $d^{(1)}$, $d^{(2)}$, distances from the middle plane of the crystal to the surfaces of screens $A_1^{(1)}$ and $A_2^{(2)}$, respectively, cm; h, plate thickness, cm; H, crystal height, cm; $H_s^{(1)}$, $H_s^{(2)}$, height of the right and left screens, respectively, cm; k, heat conduction coefficient, J/(K·m·sec); $K_{kj}^{(1)}$, kernels of integral equations; L, crystal width, cm; $q_j^{(1)}$ (i = 1, 2; j = 1, 2, 3), heat flux densities, J/(m^2·sec); $r_j^{(1)}$ (i = 1, 2; j = 1, 2, 3), radius-vectors describing the surfaces $A_j^{(1)}$; $S_j^{(i)}$ (i = 1, 2; j = 1, 2, 3), distances between arbitrary points belonging to the surfaces of the crystal, screen, and shaper, cm; $T(x, y, z)$, crystal temperature, K; $T^{(0)}$, temperature of the middle plane of the crystal, $^{\circ}$C; $T^{(0)*}$, quantity conjugate to the temperature $T^{(0)}$; $T^{(1)}$, temperature gradient over the plate thickness, $^{\circ}$C/cm; T_m, melting temperature of a crustal, $^{\circ}$C; $T_s^{(1)}$, $T_s^{(2)}$, temperatures of the upper edges of screens, $^{\circ}$C; T_0, temperature of the upper edge of a crystal, $^{\circ}$C; V_0, pulling speed, m/sec; x, y, z, current coordinates; $\varepsilon_j^{(i)}$ (i = 1, 2; j = 1, 2, 3), emissivities; μ, ν, ξ, current coordinates; ρ, density of a crystal, kg/m^3. Subscripts: m, melt; s, crystal.

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