

RADIATIVE-CONDUCTIVE HEAT TRANSFER IN A CYLINDRICAL MONOCRYSTAL GROWN BY THE VERTICALLY ORIENTED CRYSTALLIZATION METHOD

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The steady-state two-dimensional problem of the radiative-conductive heat transfer in a cylindrical monocrystal is solved. The solution is obtained numerically by the time-independent technique. Convergence of the iteration process is achieved by including the relation between the intensity of the nonlinear source in the energy equation and the desired temperature field at a particular time step. An algorithm for calculating the intensity field and the nonlinear source is given. In calculating the first approximation of the temperature distribution, the method of moments is used. The results obtained are given.

The vertical directed crystallization (VDC) method is widely used for growing high-temperature monocrystals. This method is used to grow monocrystals from a melt in a thin-walled metal container, mounted on a heat-removing rod, at a rate of 1.5-8.0 mm/h (Fig. 1). The quality of the crystals grown depends substantially on thermal conditions in the growing device and the temperature distribution in the crystal.

The problem of radiative-conductive heat transfer in a crystal will be formulated as a steady-state and two-dimensional one. The problem statement is illustrated by the scheme in Fig. 2. The mathematical formulation of the problem has the form

$$\frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left(\lambda r \frac{\partial T}{\partial r} \right) - W_r(z, r) = 0, \quad (1)$$

$$T(L, r) = T_L, \quad (2)$$

$$\left. \frac{\partial T}{\partial r} \right|_{z,0} = 0, \quad (3)$$

$$-\lambda \left. \frac{\partial T}{\partial r} \right|_{z,r_0} + q_{rr} = \epsilon_{\text{red}} (T^4(z, r_0) - T_s^4(z)), \quad (4)$$

$$-\lambda \left. \frac{\partial T}{\partial z} \right|_{0,r} + q_{rz}(0, r_0) = \frac{1}{R_{\text{th},r}} (T_{\text{sb}} - T(0, r)), \quad (5)$$

$$\frac{dJ}{ds} = -kJ + kB(s), \quad (6)$$

$$J(L, r, s) = B(L, r), \quad (7)$$

$$J(z, r_0, s) = (1 - R_m(T)) B(z, r_0) + R_m(T) J(z, r_0, s^*), \quad (8)$$

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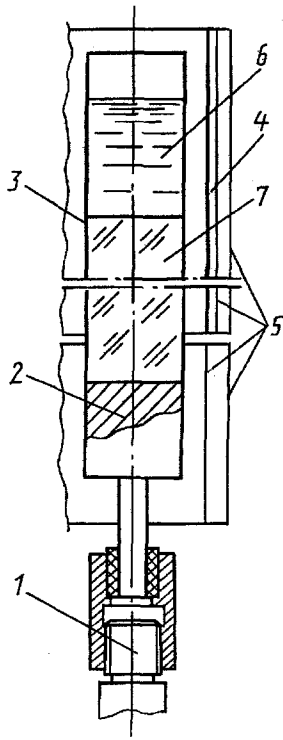


Fig. 1. The commercial set-up. 1) water-cooled rod; 2) substrate; 3) container; 4) heater; 5) screens; 6) melt; 7) crystal.

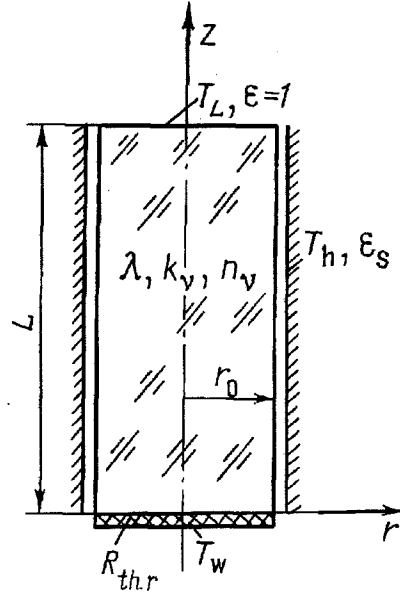


Fig. 2. Illustration of the problem formulation.

$$J(0, r, s) = (1 - R_m(T)) B(0, r) + R_m(T) J(0, r, s^*). \quad (9)$$

Here $W_r(z, r)$, $q_{rr}(z, r_0)$, and $q_{rz}(0, r)$, are the source describing the contribution of radiation to the heat balance of an element of the medium, and the densities of the net radiation fluxes at the respective boundaries. The dependence of these quantities on the temperature field and the field of the spectral radiation intensity is defined by the expressions

$$W_r(z, r) = \int_0^\infty k \left[4\pi B(z, r) - \int_{4\pi} J(z, r, s) d\omega_s \right] dv, \quad (10)$$

$$q_{rr}(z, r_0) = \int_0^\infty \int_0^{2\pi} (1 - R_m(T)) [J(z, r_0, s) - B(z, r_0)] \cos(\hat{n}s) d\omega_s dv, \quad (11)$$

$$q_{rz}(0, r) = \int_0^\infty \int_0^{2\pi} (1 - R_m(T)) [B(0, r) - J(0, r, s)] \cos(\hat{n}s) d\omega_s dv. \quad (12)$$

The problem (1)-(12) can be solved numerically using the time-independent technique. In a finite difference approximation of equation (1), its differential terms are usually expressed following the implicit scheme, and the source $W_r(z, r)$ is calculated from the temperature field of the preceding time step. In this case, the computational process does not involve any basic difficulties since with the known value of $W_r(z, r)$ Eq. (1) is an ordinary heat transfer equation with a prescribed right-hand side. Methods of its numerical calculation have been developed and are known [1]. However, convergence of the solution can be ensured under the condition that the temperature field is formed mainly by heat conduction. When heat is transferred largely by radiation (as is the case here), the solution is unstable or even diverges.

In the solution of this problem, convergence of the iteration process was provided by including the approximate dependence of the source $W_r(z, r)$ on the desired temperature distribution at a given time, i.e., by expressing the source in an implicit form.

With account of the general integral of radiation transfer equation (6), the expression for $W_r(z, r)$ is reduced to the form

$$W_r(z, r) = F(z, r) - \int_0^\infty \frac{4\pi}{3k} \left[\frac{\partial^2 B}{\partial z^2} + \frac{1}{r} \frac{\partial B}{\partial r} + \frac{\partial^2 B}{\partial r^2} \right] dv, \quad (13)$$

where

$$F(z, r) = \int_0^\infty k \int_{4\pi} \left\{ \left[B(z^*, r^*) - \frac{1}{k} \frac{\partial B}{\partial s} \Big|_{z^*, r^*} + \right. \right. \\ \left. \left. + \frac{1}{k^2} \frac{\partial^2 B}{\partial s^2} \Big|_{z^*, r^*} - \frac{1}{k^3} \frac{\partial^3 B}{\partial s^3} \Big|_{z^*, r^*} - J_0(z^*, r^*, s) \right] \exp(-ks) - \right. \\ \left. - \frac{1}{k^3} \int_0^s \frac{\partial^4 B}{\partial s^4} \Big|_s \exp[-k(s-s')] ds' \right\} d\omega dv. \quad (14)$$

It can be shown that the function $F(z, r)$ describing radiation coming to the considered point z, r from the boundaries and the remote elements of the medium does not change substantially when the temperature field changes by one time step. This allows the desired implicit expression of $W_r(z, r)$ in the energy equation to be written as

$$W_r^{p+1}(z, r) = W_r^p(z, r) + \Delta W_r(z, r) = W_r^p(z, r) + \\ + \int_0^\infty \frac{4\pi}{3k} \left\{ \left[\frac{\partial^2 B}{\partial z^2} + \frac{1}{r} \frac{\partial B}{\partial r} + \frac{\partial^2 B}{\partial r^2} \right]^p - \left[\frac{\partial^2 B}{\partial z^2} + \frac{1}{r} \frac{\partial B}{\partial r} + \frac{\partial^2 B}{\partial r^2} \right]^{p+1} \right\} dv. \quad (15)$$

The simplified relation, obtained from) by linearization, was used in the calculations:

$$W_r^{p+1}(z, r) = W_r^p(z, r) + \frac{4\pi}{3} \left\{ \left[\frac{\partial^2 T}{\partial z^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} \right]_{z,r}^p - \right. \\ \left. - \left[\frac{\partial^2 T}{\partial z^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial r^2} \right]_{z,r}^{p+1} \right\} \int_0^\infty \frac{1}{k} \frac{dB}{dT} \Big|_{z,r}^p dv. \quad (16)$$

It can be easily seen that (16) does not introduce any basic complications into the method for numerical solution of equation (1), and the accuracy of the final result depends only on the accuracy of evaluating $W_r^p(z, r)$. The value of $W_r^p(z, r)$ is found using the known temperature distribution. This is the most complicated stage in the solution and requires bulky computation. Zonal methods [2], usually employed in determining the parameters of the radiation field, reduce the integration of the radiation intensity over the solid angle to summation of the radiation incident on the point considered from the individual volume elements of the medium. These methods employ complex algorithms for calculating the geometrical optical coefficients and determining the radiative interaction of volume and surface zones, and involve ill-posed assumptions that result in errors that cannot be corrected in principle. Meanwhile, modern calculation methods allow the researchers to use more accurate quadrature formulas

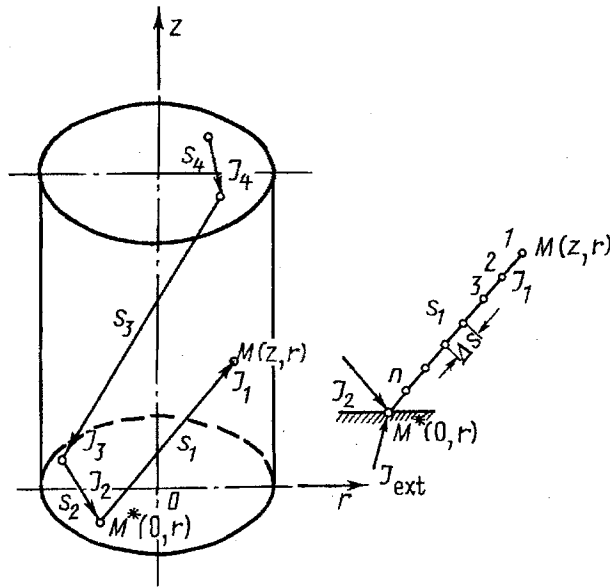


Fig. 3. Determination of the spectral radiation intensity.

for integration over the solid angle in (10). The Gauss quadrature formula was used in our calculations, and the calculation complexity was reduced to computation of the spectral radiation intensity at the point considered for directions determined by the points of the quadrature formula.

The desired quantity $J(z, r, s)$ was calculated from the relation obtained from solution of radiation transfer equation (6) in the form:

$$J(z, r, s) = [J_0(z^*, r^*, s) - B_{N+1}] \exp\left(-\frac{s}{N} \sum_{i=1}^{i=N} k_i\right) + B_1 - \sum_{i=1}^{i=N} \frac{N}{k_i s} (B_i - B_{i+1}) \left[1 + \exp\left(-k_i \frac{s}{N}\right)\right] \exp\left(-\frac{s}{N} \sum_{j=1}^{j=i-1} k_j\right). \quad (17)$$

Relation (17) was obtained by substitution of the sum of N integrals over separate equal sections ($\Delta s = s/N$) of the paths for the integral over this path in the solution of the radiation transfer equation. For each section the absorption coefficient of the medium was assumed constant ($k_i = 1/\Delta T \int k(T) dt$, and the distribution $B(s)$ was assumed linear ($B(s) = B_i + (B_{i+1} - B_i) s/\Delta s$). The spectral intensity of the effective radiation of the boundaries $J_0(z^*, r^*, s)$ is found from the boundary conditions for the radiation transfer equation. In the present case, when the surfaces surrounding the monocrystal were assumed specular, the history of the beam incident on the point z, r was followed. According to the laws of geometric optics, the path of the beam is a spatial broken line with vertexes on the boundary surfaces (Fig. 3). For each j th section of the broken line the recurrence formula can be written

$$J_j = J_{med j} + \xi_j [J_{ext j} + R_j J_{j+1}]. \quad (18)$$

The spectral intensity of the radiation $J_{med j}$ of the medium along the j th section is calculated from (17). The quantity ξ_j includes attenuation of the radiation by the semitransparent crystal and is found from the relation

$$\xi_j = \exp\left(-\frac{s_j}{N} \sum_{i=1}^{i=N} k_i\right). \quad (19)$$

The quantities $J_{ext j}$, ξ_j , and $J_{med j}$ are calculated preliminarily at $j = 1, 2, 3, \dots$, starting from the considered point z, r (section $j = 1$) and passing from section to section. The radiation path should not be followed too far because

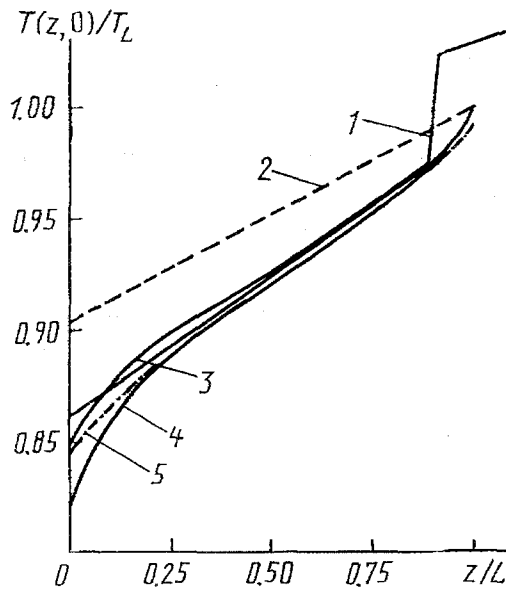


Fig. 4. Temperature distribution $T(z, 0)$ in the growing monocrystal: 1) temperature of external surfaces; 2) zero approximation; 3) temperature field obtained by the method of moments; 4) solution of the problem; 5) radiative temperature distribution.

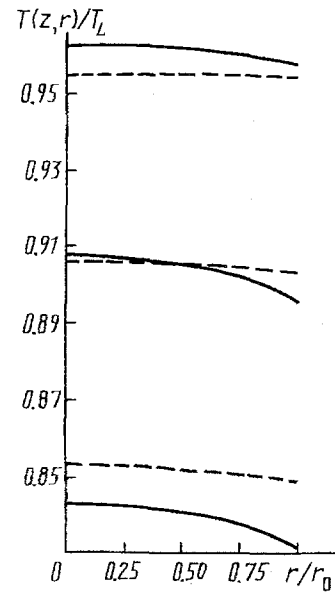


Fig. 5. Temperature distributions $T(0, 01, r)$, $T(0, 1, r)$, and $T(0, 18, r)$ in different sections of the growing monocrystal: solid curves) $T(z, r)$; dashed curves) $T_r(z, r)$.

it is attenuated by the medium and boundaries. For practice it is sufficient to take only the total optical thickness of the path passed by the beam equal to three ($\sum_1^n k_j s_j \geq 3$). With $J_{med j}$, ξ_j , and $J_{ext j}$ known from (18), we pass to the desired intensity $J_1 = J(z, r, s)$.

The algorithm developed for calculation of the field of spectral radiation intensities does not contain any limitations on the generality of the problem statement, and the accuracy of results depends mainly on the discretization of the initial equations.

Although the algorithm proposed for computation of the radiative heat transfer seems to be relatively simple, like zonal methods it requires up-to-date computer methods. However, the computer time required to solve the problem is determined mainly by the necessity to carry out computations at each iteration step rather than by the method chosen for the computation of the parameters of the radiation field, i.e., this time depends directly on the number of iterations (the number of time steps). When the radiation mechanism of energy transfer dominates, the convergence the iteration process is slow.

The use of a rough estimate of $W_r(z, r)$ reduced substantially the amount of calculations at the initial stage of the solution. This estimate was obtained using a binomial approximation of the method of moments. It is convenient as it reduces the mathematical description of the radiative field to the differential equation for the zero-order moment, directly evaluating $W_r(z, r)$. In this case this equation has the form

$$\frac{\partial^2 B_r}{\partial z^2} + \frac{1}{r} \frac{\partial B_r}{\partial r} + \frac{\partial^2 B_r}{\partial r^2} = 3k^2 (B_r - B(z, r)), \quad (20)$$

where $B_r(z, r) = 1/4\pi \int_{4\pi} J d\omega$ is the zero-order moment.

In the adopted approximation the boundary conditions for (20) are prescribed on the external surfaces of the domain by the equation

$$B_r(M) = B(M) - \frac{1}{2k} \left. \frac{dB}{dl} \right|_M \frac{1+R}{1-R}, \quad (21)$$

where l is the normal to the considered boundary surface at the point M ; R is the reflectivity of the boundary.

The resultant set of equations is linear for the desired quantity $B_r(z, r)$ and can be solved at the present temperature distribution. The temperature field obtained in this way agrees quantitatively with the desired one and only a few iteration steps, with the field parameters calculated more accurately, following the algorithm considered above, are needed to refine it.

Calculations of temperature fields and heat fluxes in VDC growing of monocrystals were carried out for crystallization of sapphire (Al_2O_3). Thermophysical properties of this material are known quite well [3]. The shape of the absorptivity versus the radiation frequency curve of sapphire allowed the authors of [4] to distinguish a band (0.5-4.0 μm) in the absorption spectrum of sapphire, within which the absorptivity could be averaged at a given temperature. Outside this band sapphire was considered as a fully nontransparent material.

Results of the temperature field calculations in a growing sapphire monocrystal are shown in Figs. 4 and 5. Figure 4 shows the temperature distribution $T(z, 0)$ in a sapphire monocrystal with a diameter of 30 mm and a height of 200 mm. The linear temperature distribution along the crystal height was taken as a zero approximation. Distribution 3 was obtained, using the method of moments. This distribution agrees well with the final solution of the problem (line 4). A substantial difference is observed only at small z , when the final solution gives a lower temperature and a lower temperature gradient. Evidently, this can be ascribed to the fact that the method of moments based on averaging the space distribution of the radiation intensity cannot provide a sufficiently accurate description of the radiation field near the boundaries having a high reflectivity. Line 5 characterizes the radiation field in the growing monocrystal and presents the radiative temperature distribution

$$T_r = \sqrt{\left(\int_0^\infty \int_{4\pi} J d\omega d\nu / \sigma_0 n^2 \right)}.$$

That the curves $T(z, 0)$ and $T_r(z, 0)$ coincide throughout except the areas at the crystal butt-ends indicates clearly that the temperature field and heat fluxes are mainly formed here by the mechanism of radiative energy transfer. This is confirmed by the temperature distributions in crystal sections at different heights, shown in Fig. 5. In the monocrystal core the radiative and molecular temperatures are nearly equal. Slight changes of the radiative temperature along the crystal radius are typical here and can be explained by the high absorptivity of the container walls.

NOTATION

λ , thermal conductivity; k , spectral absorptivity; $J(z, r, s)$, spectral intensity of radiation at the point z, r , in the direction s ; R_m , reflectivity of molybdenum; $B(z, r)$, spectral intensity of blackbody radiation; ε_{red} , reduced emissivity of the container-screen system; R_{hr} , heat resistance of the substrate; ν , radiation frequency; $d\omega_s$ unit solid angle around the direction s ; p , number of the time step.

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