NUMERICAL SOLUTION OF A THREE-DIMENSIONAL STEFAN PROBLEM

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A method is described, and the results are presented for the solution of the problem of directed crystallization of an ingot. A three-dimensional model of the process is examined.

The process of directed crystallization of an ingot, whose model can be represented schematically as follows, is considered.

Within a cylindrical radiator of radius R (muffle resistance furnace), a homogeneous ingot moves forward at the constant velocity v. The ingot is a half-cylinder of radius r whose axis coincides with the muffle axis (see Fig. 1). Some stationary temperature distribution $T_2(x)$, characterizing the process, is given on the muffle. In our case

$$T_2(x)=\begin{cases} T_{\text{over}} & \dots\quad x<0,\\ T_{\text{over}}+kx & \dots\quad 0\leqslant x<a,\\ T_{\text{over}}+ka & \dots\quad x\geqslant a,\end{cases}$$

where T_{over} is some overheating temperature. Such a temperature distribution on the muffle is characteristic for the directed crystallization process. The melted ingot crystallizes as it advances into the cold part. Such a problem was examined in [1] in a two-dimensional treatment, i.e., when axial symmetry is present. Here, as is seen from the sketch, the three-dimensional problem is considered. In such a formulation, a detailed investigation for different materials and different furnace modes is associated with an extremely high expenditure of machine time. Hence, the main idea herein is to study the influence of the given ingot shape on the shape of the isothermal surface $T = T_{\text{sur}}$ and the temperature field in the ingot. The stabilized (quasistationary) state of the ingot is of main interest here.*

Let $(\bar\rho, \bar\varphi, \bar z)$ be a cylindrical coordinate system connected with the moving ingot, and $\bar t$ the time. It follows from Lambert's law that the flux density at some point M on the XZ plane of the ingot which arrives from the muffle surface is

$$J_3=\varepsilon^*\sigma_0\int\limits_{-\infty}^{\infty}d\zeta\int\limits_{0}^{\pi}T_2^4(\zeta)\frac{\cos\alpha'\cos\beta}{\pi l_1^2}Rd\bar\varphi. \tag{1}$$

It can be shown that

$$f_3(\zeta)=\int\limits_0^{\pi}\frac{\cos\alpha'\cos\beta}{\pi l_1^2}Rd\bar\varphi=\frac{1}{\pi}\int\limits_0^{\pi}\frac{\sin\bar\varphi\,(R-\bar\rho\cos\bar\varphi)}{[R^2-2R\bar\rho\cos\bar\varphi+\bar\rho^2+\zeta^2]^2}d\bar\varphi$$
$$=\frac{1}{4\pi\bar\rho}\ln\left[1+\frac{4R\bar\rho}{(R-\bar\rho)^2+\zeta^2}\right]+\frac{R}{\pi}\,\frac{R^2-\bar\rho^2-\zeta^2}{[(R-\bar\rho)^2+\zeta^2][(R+\bar\rho)^2+\zeta^2]}.$$

*A state which is stationary in a moving coordinate system connected with the ingot is quasistationary.

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If M is on the cylinder $\bar{\rho} = r$, then the flux per unit surface of the ingot at the point M is

$$J = \varepsilon^* \sigma_0 \int_{-\infty}^{\infty} d\zeta \int_{\varphi_1}^{\varphi_2} T_2^4(\zeta) \frac{\cos \alpha_1' \cos \beta}{\pi l_1^2} R d\bar{\varphi} = \varepsilon^* \sigma_0 \int_{-\infty}^{\infty} T_2^4(\zeta) f(\zeta) d\zeta. \tag{2}$$

Here

$$f(\zeta) = \frac{1}{\pi r} \left\{ -\operatorname{arctg} \sqrt{\frac{R-r}{R+r}} + \frac{r\sqrt{R^2-r^2}\,(R^2-r^2+\zeta^2)}{[(R-r)^2+\zeta^2][(R+r)^2+\zeta^2]} \right\}$$

$$+ \left(R^2 + r^2 + \zeta^2 - \frac{8R^2 r^2 \zeta^2}{[(R-r)^2+\zeta^2][(R+r)^2+\zeta^2]} \right) \frac{\operatorname{arctg} \sqrt{\dfrac{R-r}{R+r} \cdot \dfrac{(R+r)^2+\zeta^2}{(R-r)^2+\zeta^2}}}{\sqrt{[(R-r)^2+\zeta^2][(R+r)^2+\zeta^2]}} .$$

Furthermore, let us note that the theoretical model of the process is based on the following assumptions:

1) the heat in the ingot is propagated only by heat conduction†;
2) the melting and crystallization of the materials occur at the constant temperature $T = T_{sur}$;
3) we neglect the influence of the ingot surface temperature on the given temperature distribution $T_2(x)$ on the muffle.

Let D denote the domain

$$D = \{0 < \bar{\rho} < r; \quad -\pi < \bar{\varphi} < 0; \quad -\infty < \bar{z} < \infty\},$$

and Γ the boundary of this domain. Then, under the assumptions made the ingot temperature T is described by the following conditions:

$$\frac{1}{\bar{\rho}} \frac{\partial}{\partial \bar{\rho}} \left(\lambda(T) \bar{\rho} \frac{\partial T}{\partial \bar{\rho}} \right) + \frac{1}{\bar{\rho}^2} \frac{\partial}{\partial \bar{\varphi}} \left(\lambda(T) \frac{\partial T}{\partial \bar{\varphi}} \right) + \frac{\partial}{\partial \bar{z}} \left(\lambda(T) \frac{\partial T}{\partial \bar{z}} \right) - c\gamma \frac{\partial T}{\partial \bar{t}} = 0, \tag{3_1}$$

$$(\bar{\rho}, \bar{\varphi}, \bar{z}) \in D, \quad \bar{t} > 0, \quad T \neq T_{sur}$$

$$-\lambda(T) \frac{\partial T}{\partial n} \bigg|_{\Gamma} = \varepsilon \sigma_0 T^4 |_{\Gamma} - \varepsilon \varepsilon^* \sigma_0 \Phi, \tag{3_Γ}$$

$$(\bar{\rho}, \bar{\varphi}, \bar{z}) \in \Gamma, \quad \bar{t} > 0,$$

$$\alpha\gamma \frac{\partial F_3}{\partial \bar{t}} + ([\lambda(T) \operatorname{grad} T], \operatorname{grad} F_3) = 0, \tag{3_2}$$

$$(\bar{\rho}, \bar{\varphi}, \bar{z}) \in D, \quad \bar{t} > 0, \quad T = T_{sur}$$

Here

$$\lambda(T) = \begin{cases} \lambda_1 = \text{const} & \ldots \quad T < T_{sur} \\ \lambda_2 = \text{const} & \ldots \quad T > T_{sur} \end{cases}$$

It follows from (1) and (2) that the boundary condition (3_Γ) given on the whole surface Γ is equivalent to the conditions

$$-\lambda(T) \frac{\partial T}{\partial \bar{\rho}} \bigg|_{\bar{\rho}=r} = \varepsilon \sigma_0 T^4 |_{\bar{\rho}=r} - \varepsilon \varepsilon^* \sigma_0 \int_{-\infty}^{\infty} T_2^4(\xi) f(\xi - \bar{x}) d\xi,$$

$$\bar{x} = \bar{z} + v\bar{t}; \quad \{-\pi < \bar{\varphi} < 0, \quad -\infty < \bar{z} < \infty\}, \quad \bar{t} > 0, \tag{3_3}$$

† Convection, whose influence is taken into account by the introduction of an effective coefficient of heat conduction, takes part in heat transfer in the liquid phase.

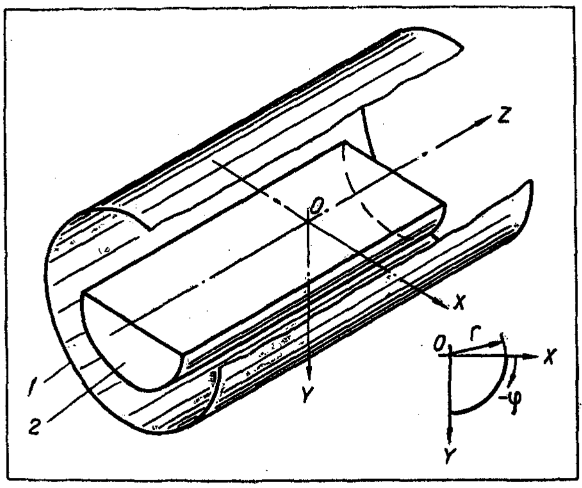

Fig. 1. Schematic model of directed crystallization of an ingot. 1) Radiator; 2) ingot.

$$-\lambda(T)\frac{1}{\bar{\rho}}\frac{\partial T}{\partial \bar{\varphi}}\Big|_{\bar{\varphi}=0} = \varepsilon\sigma_0 T^4|_{\bar{\varphi}=0} - \varepsilon\varepsilon^*\sigma_0 \times \int_{-\infty}^{\infty} T_2^4(\xi) f_3(\xi-\bar{x})\,d\xi, \qquad (3_4)$$

$$\bar{x}=\bar{z}+v\bar{t};\quad \{0<\bar{\rho}<r,\ -\infty<\bar{z}<\infty\},\quad \bar{t}>0,\quad \lim_{\bar{z}\to\pm\infty} T<\infty, \qquad (3_6)$$

where $\bar{x} = \bar{z} + v\bar{t}$ is the coordinate connected to the fixed muffle.

Let us note that condition (3) is not posed on the edge $\bar{\rho} = r$, $\bar{\varphi} = 0$ since the normal direction is not defined on this edge.

Since the domain D is symmetric relative to the plane $\bar{\varphi} = -\pi/2$, half of it can be considered by conserving the symmetry condition

$$\frac{\partial T}{\partial \bar{\varphi}}\Big|_{\bar{\varphi}=-\frac{\pi}{2}} = 0 \ \ldots\ \{0<\bar{\rho}<r,\ -\infty<\bar{z}<\infty\},\ \bar{t}>0. \qquad (3_5)$$

Let us introduce the dimensionless variables

$$\rho=\frac{\bar{\rho}}{r};\quad x=\frac{\bar{x}}{r};\quad t=\frac{\lambda_1\bar{t}}{c\gamma r^2};\quad \varphi=\bar{\varphi};\quad w=\frac{1}{k(w)}\,\frac{T-T_{sur}}{T_{sur}-T_1},$$

where T_1 is the initial ingot temperature and

$$k(w)=\begin{cases}1 & \ldots\ w<0,\\ \dfrac{\lambda_1}{\lambda_2} & \ldots\ w>0.\end{cases}$$

Let us assume

$$\Phi(rx)=\int_{-\infty}^{\infty} T_2^4(\xi) f(\xi-x)\,d\xi,$$

$$\Phi_3(rx)=\int_{-\infty}^{\infty} T_2^4(\xi) f_3(\xi-x)\,d\xi,$$

$$\mu=\frac{c\gamma vr}{\lambda_1},\quad \delta=\delta_3=\frac{T_{sur}}{T_{sur}-T_1},$$

$$A=\frac{\varepsilon\sigma_0 r(T_{sur}-T_1)^3}{\lambda_1},\quad B=\frac{\varepsilon\varepsilon^*\sigma_0 r}{\lambda_1(T_{sur}-T_1)},$$

$$A_3=\frac{\varepsilon\sigma_0\rho r(T_{sur}-T_1)^3}{\lambda_1},\quad B_3=\frac{\varepsilon\varepsilon^*\sigma_0\rho r}{\lambda_1(T_{sur}-T_1)}, \qquad (4)$$

$$b=\frac{\alpha}{c(T_{sur}-T_1)},\quad d=\frac{vr}{\lambda_1(T_{sur}-T_1)}.$$

Then (3_1)-(3_3) is written as

$$\Delta w = k(w)\frac{\partial w}{\partial t} + \mu k(w)\frac{\partial w}{\partial x},$$

$$\left\{0<\rho<1,\ -\frac{\pi}{2}<\varphi<0,\ -\infty<z<\infty\right\},\quad t>0,\ w\neq 0, \qquad (5_1)$$

$$-\frac{\partial w}{\partial \rho}\Big|_{\rho=1} = A[k(w)w+\delta]^4 - B\Phi(rx),$$

$$x = z + vt, \quad \left\{-\frac{\pi}{2} < \varphi < 0, \quad -\infty < z < \infty\right\}, \quad t > 0, \tag{5$_2$}$$

$$-\left.\frac{\partial w}{\partial \varphi}\right|_{\varphi=0} = A_3 [k(w) w + \delta_3]^4 - B_3 \Phi_3 (rx),$$

$$x = z + vt, \quad \{0 < \rho < 1, \quad -\infty < z < \infty\}, \quad t > 0, \tag{5$_3$}$$

$$\left.\frac{\partial w}{\partial \varphi}\right|_{\varphi = -\frac{\pi}{2}} = 0, \tag{5$_4$}$$

$$b \frac{\partial F_3}{\partial t} + d \frac{\partial F_3}{\partial x} + ([\mathrm{grad}\, w], \mathrm{grad}\, F_3) = 0,$$

$$\left\{0 < \rho < 1, \quad -\frac{\pi}{2} < \varphi < 0, \quad -\infty < z < \infty\right\}, \quad w = 0, \quad t > 0. \tag{5$_5$}$$

Here

$$\Delta = \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial x^2}.$$

The problem (5) is solved below by using the method of Kamenomostskaya and Oleinik. In conformity with [2], (5_1) is written as

$$\Delta w = \frac{\partial a(w)}{\partial t} + \mu \frac{\partial a(w)}{\partial x}, \tag{6}$$

where

$$a(w) = \begin{cases} \int\limits_0^w k_1(\xi)\, d\xi & w < 0, \\ \int\limits_0^w k_2(\xi)\, d\xi + b & w > 0. \end{cases}$$

The Stefan condition (5_5) written thus turns out to be taken into account automatically since a δ-function appears in the differentiation in (6). Furthermore, following Oleinik [3], a(w) is smoothed, which permits treatment of (6) as an ordinary quasilinear equation with continuous coefficients. In our case we can take as a(w)

$$a(w) = w, \qquad w \leqslant -L,$$

$$a(w) = \frac{\lambda_1}{\lambda_2} w + b, \quad w \geqslant L.$$

Here a(w) "is smoothed" in the interval $-L < w < L$ by some polynomial. Experience shows that it is sufficient to take a third degree polynomial. The coefficients of this polynomial are found from the zeroth and first-order conjugate conditions. Then

$$\alpha(w) = a'(w) = \begin{cases} 1 & w \leqslant -L \\ \alpha_1 (w - L)^2 + \alpha_2 (w - L) + \frac{\lambda_1}{\lambda_2} & |w| < L \\ \frac{\lambda_1}{\lambda_2} & w \geqslant L, \end{cases} \tag{7}$$

where

$$\alpha_1 = -\frac{3b}{4L^3}; \quad \alpha_2 = \frac{1}{2L}\left(\frac{\lambda_1}{\lambda_2} - 1 - \frac{3b}{L}\right)$$

Therefore, (5_1) becomes

$$\Delta w = \alpha(w)\frac{\partial w}{\partial t} + \mu\alpha(w)\frac{\partial w}{\partial x},$$
$$\left\{0<\rho<1, \quad -\frac{\pi}{2}<\varphi<0, \quad -\infty<z<\infty\right\}, \quad t>0. \tag{8_1}$$

Since we are interested in the influence of the absence of cylindrical symmetry, let us pose the problem for deviations of the solution of the three-dimensional problem from a similar problem in the case of an ingot of cylindrical shape. The selection of such an approach is explained by the fact that it can a priori be expected that the solution of the problem in the three-dimensional formulation will differ slightly from the corresponding solution of the two-dimensional problem, and hence, the error of the computation method in solving the problem in the two- or three-dimensional formulation separately may turn out to be of the same order of magnitude as the deviations themselves. Furthermore, let us note that the conditions which the dimensionless temperature u satisfies in the case of cylindrical symmetry agree with the conditions (5_1), (5_2), (5_5) and the conditions (5_3), (5_4) are replaced by the conditions

$$\left.\frac{\partial u}{\partial \varphi}\right|_{\varphi=0} = 0,$$
$$\{0<\rho<1, \quad -\infty<z<\infty\}, \quad t>0, \tag{9}$$
$$\left.\frac{\partial u}{\partial \varphi}\right|_{\varphi=-\frac{\pi}{2}} = 0.$$

This problem was solved by one of the implicit numerical methods also by using the method of Kamenomostskaya and Oleinik [1]. Hence, the equation

$$\Delta u = \alpha(u)\frac{\partial u}{\partial t} + \mu\alpha(u)\frac{\partial u}{\partial x} \tag{10}$$

is analogous to (8_1). Let us put

$$v(x, \rho, \varphi, t) = w(x, \rho, \varphi, t) - u(x, \rho, \varphi, t). \tag{11}$$

Then

$$\alpha(w)\frac{\partial w}{\partial t} - \alpha(u)\frac{\partial u}{\partial t} = \alpha(u+v)\frac{\partial(u+v)}{\partial t} - \alpha(u)\frac{\partial u}{\partial t} = [\alpha(u+v)-\alpha(u)]\frac{\partial u}{\partial t} + \alpha(u+v)\frac{\partial v}{\partial t}.$$

Subtracting the corresponding equations of the three- and two-dimensional problems, we find that the perturbation v(x, ρ, φ, t) satisfies the following conditions:

$$\frac{\partial^2 v}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial v}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 v}{\partial \varphi^2} + \frac{\partial^2 v}{\partial x^2} = [\alpha(u+v)-\alpha(u)]\frac{\partial u}{\partial t}$$
$$+\alpha(u+v)\frac{\partial v}{\partial t} + \mu[\alpha(u+v)-\alpha(u)]\frac{\partial u}{\partial x} + \mu\alpha(u+v)\frac{\partial v}{\partial x}, \tag{12_1}$$
$$\left\{0<\rho<1, \quad -\frac{\pi}{2}<\varphi<0, \quad -\infty<x<\infty\right\}, \quad t>0,$$

$$\left.\frac{\partial v}{\partial \rho}\right|_{\rho=1} = -A\{[k(u+v)(u+v)+\delta]^4 - [k(u)u+\delta]^4\},$$
$$\left\{-\frac{\pi}{2}<\varphi<0, \quad -\infty<x<\infty\right\}, \quad t>0, \tag{12_2}$$

$$\left.\frac{\partial v}{\partial \varphi}\right|_{\varphi=0} = -A^3[k(u+v)(u+v)+\delta_3]^4 - B_3\Phi_3, \tag{12_3}$$

$$\left.\frac{\partial v}{\partial \varphi}\right|_{\varphi=-\frac{\pi}{2}} = 0, \quad \{0<\rho<1, \quad -\infty<x<\infty\}, \quad t>0. \tag{12_4}$$

Here u is considered known. Namely, let us take the quasistationary solution of the two-dimensional problem* as u. The problem (12_1)-(12_4) was solved by a mesh method. A finite ingot hence replaced the infinite ingot. The condition of zero flux is imposed at the left end of the ingot in both the two- and the three-dimensional case so that

$$\left.\frac{\partial v}{\partial x}\right|_{x=L_{\text{begin}}} = 0. \tag{12_5}$$

The temperature at the right endpoint was determined from the condition (5_2), where it was considered that

$$\left.\frac{\partial u}{\partial \rho}\right|_{x=L_{\text{begin}}} = 0 \ \ldots \ 0<\rho<1; \quad \left.\frac{\partial w}{\partial \rho}\right|_{x=L_{\text{begin}}} = 0 \ \ldots \ 0<\rho<1, \ -\frac{\pi}{2}<\varphi<0.$$

Whence

$$v\big|_{x=L_{\text{begin}}} = 0. \tag{12_6}$$

Let us take the zero deviation of the three-dimensional from the two-dimensional solution

$$v\big|_{t=0} = 0 \tag{12_0}$$

as the initial state for the deviations $v(x, \rho, \varphi, t)$. A classical explicit difference scheme [4] was used to construct the difference analog of the problem (12). The solution at internal points on the $(k+1)$-th level is found by this scheme from the known solution at the internal and boundary points of the k-th time level. Then, by using the solution just found at the internal points and the boundary conditions (12_i) ($i = 2, 3, 4, 5, 6$), the value of the solution is found at the boundary points of the $(k+1)$-th level. All the nonlinear coefficients were "linearized" in such a way that the main terms were taken on the $(k+1)$-th level, and the rest were referred to the previous time level.

In constructing the difference analog of the problem (12), the domain

$$D_k = \left\{0<\rho<1, \quad -\frac{\pi}{2}<\varphi<0, \quad L_{\text{begin}}<x<L_{\text{end}}\right\}$$

is divided by several planes in φ, and each plane is divided by a rectangular mesh. The solution at the mesh nodes will be

$$v^k_{ijl} = v(x_l, \rho_i, \varphi_j, t_k),$$

where

$$\begin{aligned} x_l &= L_{\text{begin}} + \sum_{\xi} h_{\xi}, & l &= 1, \ldots, p, \\ \rho_i &= i\eta, & i &= 1, \ldots, n, \\ \varphi_j &= -\frac{\pi}{2} + j\theta, & j &= 1, \ldots, m, \\ t_k &= k\tau, & k &= 1, 2, \ldots, \end{aligned}$$

if h_ξ, η, θ, τ are the spacings in x, ρ, φ, t, respectively. Here nonuniform spacings are chosen in x, where the shallowest spacings are selected at places of the greatest change in the desired function. The spacings h_ξ and $h_{\xi+1}$ are inserted around the point x_ξ.

The computation was performed in a BÉSM-4 digital computer. Selected for the computation were $m = 5$, $n = 7$, where $p = 53$, $\theta = -\pi/8$, $\eta = r/6$, $\min h_\xi = r/3$, where h_ξ was increased as the endpoints of the ingot approached. The time spacing depends considerably on the "spreading" interval of the Stefan heat. Thus, if it were successful to calculate with $\min\tau = 0.002$ for $l = L = 0.125$, then for $l = L = 0.0025$ with the spacing $\min\tau = 0.0005$.

The spacing τ was varied for the selected l, L, during the computation. Namely, τ could be increased as the time t itself increased. The problem (12) was also calculated with a finer mesh: $m = 5$, $n = 13$, $p = 81$,

* Let us recall that the main problem is to determine the quasistationary temperature distribution.

where in the case of the coarser mesh η the spacing in ρ was doubled, and the mesh was unloaded in x so that the least spacing was retained in the expected region of the melting isotherm. A comparison between results of a computation with a mesh of $5 \times 7 \times 53 = 1855$ nodes and $5 \times 13 \times 81 = 5265$ nodes showed that the maximum relative error is from 1% to 10% for deviations of from 10^{-3} to 10^{-7} in absolute magnitude as the mesh spreads. The mentioned comparison permitted at least a ninefold increase in the time spacing τ which will naturally lead to a diminution in the expended machine time. Thus, if the optimal spacing is $\tau = 0.0002$ for a $81 \times 13 \times 5$ mesh, then it is successful to compute with a $\tau = 0.002$.

Let us note that in both the first and second case no egress has been made to the external memory. The final problem (12) was solved with a mesh of $5 \times 7 \times 53$ nodes. About 10 sec of machine time was expended at each time level. Naturally, the time of egress to the quasistationary depends on the initial approximation. This is precisely why the quasistationary solution of the two-dimensional problem is taken as the initial state. In this case the time needed for the solution of the problem (12) to become quasistationary, does not reflect the true time needed to build up the process.

Computations were carried out for two modifications of the parameters of GaAs. The following thermophysical characteristics were used:

$$v = 6.6 \cdot 16^{-6}\ \text{m/sec};\quad c = 431.24\ \text{J/kg}\cdot\text{deg};\quad \gamma = 5310\ \text{kg/m}^3;$$

$$\alpha = 6.07 \cdot 10^5\ \text{J/kg};\quad \sigma_0 = 5.65 \cdot 10^{-8}\ \text{W/m}^2\cdot\text{deg}^4;\quad T_{\text{det}} = 1513\ ^\circ\text{K};$$

$$T_1 = 300\ ^\circ\text{K};\quad \varepsilon = \begin{cases} 0.2 & \ldots\ T < T_{\text{det}} \\ 0.6 & \ldots\ T > T_{\text{det}} \end{cases}$$

Modification I:

$$\lambda_1 = 13.146\ \text{W/m}\cdot\text{deg}\quad \frac{\lambda_1}{\lambda_2} = 0.5;\quad l = L = 0.125;\quad R = 0.02\ \text{m};$$

$$r = 0.0075\ \text{M};\quad L\quad = 0.735\ \text{M};\quad k = -500\ \text{deg/m};\quad \varepsilon^* = 0.97;$$

$$T_2(x) = \begin{cases} 1530 & \ldots\ -\infty < x \leqslant 0.855, \\ -1.29293x^2 + 226.465x - 8381.1 & \ldots\ 0.855 < x \leqslant 0.9, \\ k(x - 90) + 1530 & \ldots\ 0.9 < x \leqslant 1.55, \\ 888 & \ldots\ 1.55 < x < \infty, \end{cases}$$

Modification II:

$$\lambda_1 = 12.56\ \text{W/m}\cdot\text{deg};\quad \frac{\lambda_1}{\lambda_2} = 0.3947368;\quad l = L = 0.0025;\quad R = 0.035\ \text{M};$$

$$r = 0.015\ \text{M};\quad L. \quad = -0.33\ \text{M};\quad k = -200\ \text{deg/m};\quad \varepsilon^* = 1;$$

$$T_2(x) = \begin{cases} 1520 & -\infty < x \leqslant 0, \\ 1520 + kx & 0 < x < \infty. \end{cases}$$

It is seen from an analysis of the temperature fields calculated in solving the two-dimensional axisymmetric problem [1] for modification I that the maximum change of the quantity $u(\rho, z)$ in ρ does not exceed 10^{-4}. Let us here recall that u has been normalized to 1. Consequently, in place of the two-dimensional solution $u(\rho, z, t)$, the average of u with respect to ρ can be inserted in the numerical solution of the problem (12):

$$\bar{u} = \frac{2}{r^2}\int_0^r \rho u(\rho,\ z,\ t)\, d\rho. \tag{13}$$

Then $\bar{u}$ is determined by the conditions

$$\frac{\partial}{\partial z}\left(\lambda(\bar{u})\frac{\partial \bar{u}}{\partial z}\right) - 2\lambda(\bar{u})\{A[k(\bar{u})\bar{u} + \delta]^4 - B\Phi(rz)\} = \alpha(\bar{u})\left(\frac{\partial \bar{u}}{\partial t} + \mu\frac{\partial \bar{u}}{\partial z}\right) \ldots L_{\text{begin}} < z < L_{\text{end}}\quad t > 0, \tag{14_1}$$

$$\left.\frac{\partial \bar{u}}{\partial z}\right|_{z = L_{\text{begin}}} = 0,\quad t > 0, \tag{14_2}$$

TABLE 1. Coordinates of the Isothermal Surface in the Case k = −500 deg/m

ρ	φ: 0	$-\frac{\pi}{8}$	$-\frac{\pi}{4}$	$-\frac{3\pi}{8}$	$-\frac{\pi}{2}$
0	91,907	91,907	91,907	91,907	91,907
0,125	91,907	91,915	91,920	91,923	91,923
0,25	91,906	91,921	91,931	91,935	91,935
0,375	91,902	91,926	91,937	91,941	91,941
0,5	91,898	91,929	91,941	91,944	91,944
0,625	91,893	91,930	91,942	91,945	91,945

TABLE 2. Coordinates of the Isothermal Surface in the Case k = −200 deg/m

ρ	φ: 0	$-\frac{\pi}{8}$	$-\frac{\pi}{4}$	$-\frac{3\pi}{8}$	$-\frac{\pi}{2}$	two-dimensional isotherm
0	9,098	9,098	9,098	9,098	9,098	9,31
0,25	9,092	9,125	9,137	9,14	9,14	9,31
0,5	9,053	9,11	9,119	9,12	9,12	9,3
0,75	9,001	9,068	9,075	9,075	9,075	9,26
1,0	8,1	9,005	9,01	9,01	9,01	9,02
1,25	7,599	8,402	8,432	8,432	8,432	8,43

$$\bar{u}\Big|_{z=L_{\text{begin}}} = \frac{1}{k(\bar{u})}\left\{\sqrt[4]{\frac{B}{A}\Phi(rL_{\text{end}})} - \delta\right\}, \quad t>0, \tag{14_3}$$

$$\bar{u} = \frac{1}{k(\bar{u})}\left\{\sqrt[4]{\frac{B}{A}\Phi(rz)} - \delta\right\} \ldots L_{\text{begin}} < z < L_{\text{end}} \quad t=0. \tag{14_4}$$

The A, B, Φ(rz) entering here are the same as above. Taking $u(\rho, z, t) = \bar{u}(z, t)$ in this modification in the numerical solution of the problem (12),. we simplify the program considerably and diminish the computation time.

It is impossible to carry out the computations of modification II thus since it is characterized by the fact that a significant dependence of the solution on ρ is obtained in the two-dimensional case. Hence, the solution of the two-dimensional problem is taken as u in the solution of the problem (12). The computation is carried out until a monotonic diminution is achieved:

$$\Delta = \max_{i,j,l} |v_{ijl}^{k+1} - v_{ijl}^{k}|.$$

Compliance with the criterion

$$\Delta < 10^{-5} \approx 0.01\ ^\circ\text{K}$$

is considered the criterion for the solution to become quasistationary.

The computation was carried out to t = 27.6 sec for modification I, and to t = 24.8 sec for modification II.

The temperature field of the three-dimensional problem and its deviation from the two-dimensional field at the mesh nodes as well as the x coordinate of the isothermal surface $T = T_{\text{sur}}$ are printed out. The values of $x(\rho, \varphi)$ (in cm) are presented in Tables 1 and 2 for modifications I and II, respectively.

Coordinates of the melting isotherm for the axisymmetric problem are given for comparison in the right-hand column of Table 2.

Let us note that the maximum displacement (to the left) of the coordinates of the three-dimensional isotherm in the second modification as compared with the two-dimensional isotherm is ≈8 mm and in the first modification is ≈4 mm.

An analysis of the field of deviations of the three-dimensional from the two-dimensional solution in the modification I yields a maximum deviation of $\approx 2.8 \cdot 10^{-3} \approx 3.3$°K at the right end of the ingot, and

$\approx 10^{-4} \approx 0.1°K$ in the area of the isotherm. For the second modification, the maximum deviations are on both sides of the domain of the isotherm $T = T_{sur}$ and equal $\approx 10^{-3} \approx 1°K$.

Therefore, the computations conducted showed that it is possible to limit oneself to an examination of the axisymmetric problem for the investigation of the directional crystallization process in modes encountered in practice.

NOTATION

σ_0 is the Stefan–Boltzmann constant;
ε^* is the reduced radiation factor of the muffle;
ε is the relative radiativity of the ingot material;
γ is the density;
α is the specific latent heat of crystallization;
T is the temperature;
l_1 is the distance between a point M and an arbitrary point N on the muffle;
α' is the acute angle between the direction MN and the Y axis;
α_1' is the acute angle between the direction MN and the radius r;
β is the acute angle between the direction MN and the radius R of the muffle;
n is the normal direction to the surface Γ;
F_3 is the equation of the isothermal surface $T = T_{sur}$.

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