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CONTROL OF THE SHAPE OF PHASE TRANSITION FRONTS DURING ZONE MELTING

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In order to prepare single crystals there is extensive use of the method of zone melting in which a long specimen is drawn through a heater [1, 2]. As a result of this, a molten zone occurs between the rod of polycrystalline material being consumed and the single crystal formed. Variants of the method differ in the way of heating and cooling, and also whether the specimen is contained in a crucible or not. The quality of the crystal obtained depends on the shape of the phase transition surfaces arising, which is determined by the boundary regime at the ingot surface. The problem of determining the boundary regime providing a specified (optimum in the sense of any criterion) shape of these surfaces is important. Apparently for many substances a flat shape is the optimum from the point of view of the quality of the single crystal obtained.

In this work the most simple model of the zone-melting process is considered ignoring convective heat transfer in the liquid phase. Use of this model is only valid in the case of very slow specimen movement when there is greatest interest in studying the steady-state process. It is assumed that the size of the ingot, parameters of the remelted substance, drawing rate, width of the liquid zone, and heating schedule are known. The cooling schedule is sought which provides a flat shape for the melting and crystallization fronts.

1. Statement of the Problem. Let an ingot be drawn through a heater at constant velocity v. We choose a Cartesian coordinate system (x_1, x_2, x_3) connected with the heater so that axis x_1 coincides with the direction of specimen movement. It is assumed that heat exchange is known at the boundary of the region G' which does not move in this coordinate system. The temperature field $T'(x_1, x_2, x_3)$, which is steady in the selected system, and the position of the melting Σ_1 and crystallization Σ_2 fronts are determined from the conditions

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Fig. 1

$$\Delta T' + v\chi^{-1}(T') T'_{x_1} = 0 \text{ with } X \in G'; \tag{1.1}$$

$$T' = T_0 \text{ with } X \in \Sigma'_1 \cup \Sigma'_2; \tag{1.2}$$

$$\left[\varkappa(T')\partial T'/\partial n_{\Sigma'_{i}}\right] = \Lambda' v n_{\Sigma_{i}} \text{ with } X \in \Sigma'_{i}, \ i = 1, \ 2;$$
(1.3)

$$\Phi_i(\partial T'/\partial n_{\Gamma_i}, T', X) = f_i(X) \text{ with } X \in \Gamma_i$$
(1.4)

Here T_0 is melting temperature; Λ' is latent heat of melting; n_{Γ} and n_{Σ} are unit vectors normal to surfaces Γ and Σ ; $\chi(T')$ and $\kappa(T')$ are thermal diffusivity and thermal conductivity coefficient, and

$$\chi(T') = \begin{cases} \chi_1 \text{ with } T' > T_0, \\ \chi_2 \text{ with } T' < T_0, \end{cases} \quad \varkappa(T') = \begin{cases} \varkappa_1 \text{ with } T' > T_0, \\ \varkappa_2 \text{ with } T' < T_0; \end{cases}$$

 $X = (x_1, x_2, x_3), \Phi_i(\partial T'/\partial n, T', X)$ are prescribed functions characterizing the type of heat exchange at the boundaries of the ingot and depending on heater construction and on the method of cooling the crystal; Φ_i may be different in different parts of the boundary of region G'. Normally, it is assumed that Φ_i is either linear for the first argument, or has the form

$$\Phi = \partial T' / \partial n + \alpha T'^4 + g(X), \tag{1.5}$$

where α is a known value; g(X) is a known function. Linear conditions (1.4) are typical for remelting processes in a crucible, but (1.5) with substitution in (1.4) gives the Stefan-Boltzmann radiation condition [1] and it is used to describe processes of crucibleless zone melting.

The problem of finding T'(X) and f(X) in parts of the boundary of region G' satisfying (1.1)-(1.4) with prescribed Σ_1 , Σ_2 , and f(X) in the remaining parts of the boundary relates to an inverse problem of the Stefan type or to a problem of controlling crystallization processes [3]. Applied to this problem, these terms are of equal importance. The last one is used below.

A considerable number of works have been devoted to the problem of controlling crystallization processes. A review of the results and detailed bibliography are given in [3, 4]. The most marked success has been achieved in studying the nonsteady-state problem with one spatial variable. The planar and axisymmetric problem has been previously solved approximately. In Eq. (1.1) the term $T'_{X_1X_1}$ [1, 5] or vT'_{X_1} [6] was ignored.

In this work the multidimensional quasisteady-state problem of zone melting is solved in a precise arrangement for the case when Σ_1 and Σ_2 are planes perpendicular to axis x_1 .

Let Σ_1 be plane $x_1 = \alpha$, and Σ_2 be plane $x_1 = 0$. We state the control problem assuming that the heating schedule is specified, but the cooling schedule is sought. We introduce dimensionless variables, selecting as a scale for length the value of α , for velocity v, for temperature T_0 . Let

$$T = (T' - T_0)/T_0, \ y = (y_1, \ y_2) = (\pi x_2/a, \pi x_3/a), z = \pi x_1/a, x = (z, y_1, y_2).$$

It is assumed that region G is a cylinder $(-l_2, \pi + l_1) \times \Omega$, where $l_1 > 0$, $l_2 > 0$, Ω is a singly-connected region in plane (y_1, y_2) . Region G is divided into three parts: G_1 , G_2 , G_3 , and boundary Γ of region G is divided into five parts: Γ_1 , i = 1, ..., 5, as shown in Fig. 1. We consider the problem

$$\Delta T + 2b_1 T_z = 0 \text{ with } \mathbf{x} \in G_1; \tag{1.6}$$

$$\Delta T + 2b_2 T_z = 0 \text{ with } \mathbf{x} \in G_2 \cup G_3; \tag{1.7}$$

$$T = 0 \qquad \text{with } \mathbf{x} \in \Sigma_1 \cup \Sigma_2; \tag{1.8}$$

$$[k(z) T_z]_{\Sigma_i} = \Lambda \quad \text{with } x \in \Sigma_i, \ i = 1, 2, \tag{1.9}$$

Here

$$b_i = va/(2\pi\chi_i); \quad \Lambda = \Lambda' T_0 \chi_1/\varkappa_1; \quad \Sigma_1 = \{\mathbf{x} : z = 0, \quad \mathbf{y} \in \Omega\}; \quad \Sigma_2 = \{\mathbf{x} : z = \pi, \quad \mathbf{y} \in \Omega\};$$

$$k(z) = \begin{cases} k_1 = \pi\chi_1/(av) \text{ with } z \in (0, \pi), \\ k_2 = k_1\varkappa_2/\varkappa_1 \text{ with } z \in (0, \pi). \end{cases}$$

Condition (1.4) is fulfilled at boundary Γ .

It is assumed that functions Φ_i (i = 1,..., 5), $f_1(x)$ and all of the numerical parameters are prescribed, and T(x), $x \in G$, and $f_i(x)$ with $x \in \Gamma_i$, i > 1 are sought. The problem thus stated is reduced to three successively solved problems: boundary problem (1.6), (1.4), (1.8) in region G_1 and two Cauchy problems (1.7)-(1.9) in regions G_2 and G_3 . Boundary problems of type (1.6), (1.4), and (1.8) have been satisfactorily studied, and in [7] it is possible to find sufficient conditions for existence of their smooth solutions.

The Cauchy problem for elliptical equations is not generally speaking correct, but, as will be shown below, if the Cauchy data has the form (1.8), (1.9), then it is clearly resolvable in cylinders G_2 and G_3 , and if T(x), $x \in G_1$ is known, its solution is constructed in explicit form.

It is noted that solution of (1.6)-(1.9), (1.4) after a changeover to physical variables does not always give a solution of the original Stefan problem (1.1)-(1.4), but only in that case when the inequalities

$$T > 0 \text{ with } \mathbf{x} \in G_1, \ T < 0 \text{ with } \mathbf{x} \in G_2 \cup G_3 \tag{1.10}$$

are fulfilled.

On the other hand, any solution of problem (1.1)-(1.4) with planes Σ_1 ' and Σ_2 ' after a changeover to dimensionless variables satisfies (1.6)-(1.10) and, therefore, infringement of inequality (1.10) in order to solve problems (1.6)-(1.9), (1.4) means nonexistence of a solution for (1.1)-(1.4) with given $f_1(x)$, α , v, ℓ_1 , ℓ_2 , χ_1 , χ_2 , κ_1 , κ_2 in planes Σ_1 ' and Σ_2 '.

The main content of the present work consists of constructing solutions for (1.6)-(1.9) and obtaining the satisfactory and necessary conditions for fulfilling (1.10), i.e., solvability of the original control problem. These conditions have the form of inequalities in geometric characteristics of the ingot, thermophysical parameters of the remelted substance, and heater characteristics.

2. Solution of the Supplementary Problem. First we consider problem (1.6)-(1.9), (1.4) without troubling to fulfill (1.10). The following statements occur.

THEOREM 1. Let Φ_1 , f_1 be such that a single solution exists

$$T_1(x) \Subset C^{2+\alpha}$$
 (G₁) $\cap C^1(\overline{G}_1)$

for problem (1.6), (1.8), (1.4). Then

$$T_i(x) \in C^{2+\alpha}(G_i) \cap C^1(\overline{G}_i), \ i = 2, \ 3,$$

is found satisfying in G_i Eq. (1.7), and in Σ_1 and Σ_2 satisfying conditions (1.8), (1.9). Function T(x), $x \in G$ is such that T = T_i(x) with $x \in G_i$ and

$$f_j(\mathbf{x}) = \Phi_j \left(\frac{\partial T}{\partial n_{\Gamma_j}}, T, \mathbf{x} \right), \ \mathbf{x} \in \Gamma_j \ (j = 2, \ldots, 5)$$

will apparently, with solution of (1.6)-(1.9), (1.4), be determined in part 1. With given f_1 , Φ_1 , solution of (1.6)-(1.9), (1.4) is unique.

<u>Note 1</u>. Conditions specifying clear solvability of problems (1.6)-(1.9), (1.4) postulated in the condition of Theorem 1 are given in [7]. They have the form of requirement for evenness for f_1 and conditions for agreement of (1.4) and (1.8).

The uniqueness of the solution follows from the uniqueness of the solution for the boundary problem in G_1 and the Cauchy problems in G_2 and G_3 [8]. Its existence is substantiated below by constructing in explicit form functions T_2 and T_3 in terms of known function T_1 .

<u>Proof</u>. First we find a solution of (1.6)-(1.9) depending only on one variable z. Function $\overline{T(z)}$ should satisfy the equations

$$T'' + 2b_1T' = 0 \text{ with } z \in (0, \pi),$$

$$T'' + 2b_2T' = 0 \text{ with } z \in (0, \pi)$$

and conditions

$$T(0) = T(\pi) = 0,$$

$$k_1 T'(+0) - k_2 T'(-0) = k_2 T'(\pi + 0) - k_1 T'(\pi - 0) = \Lambda,$$

which govern function T(z) in a unique way:

$$T = T^{0}(z) = \begin{cases} \Lambda [1 - \exp(-2b_{2}z)]/(2b_{2}k_{2}) & \text{with } z \leq 0, \\ 0 & \text{with } z \equiv (0, \pi), \\ \Lambda [1 - \exp(2b_{2}\pi - 2b_{2}z)]/(2b_{2}k_{2}) & \text{with } z \geq \pi_{z} \end{cases}$$

 $T^{0}(z)$ does not satisfy (1.10) and the dimensional function corresponding to it is not consequently a solution of (1.1)-(1.4).

We shall seek a solution of (1.6)-(1.9) in the form

$$T(x) = \begin{cases} T^{0}(z) + k_{2}^{-1} \exp(-b_{2}z) u(x) & \text{with } z \leq 0, \\ k_{1}^{-1} \exp(-b_{1}z) u(x) & \text{with } z \equiv (0, \pi), \\ T^{0}(z) + k_{2}^{-1} \exp(b_{2}\pi - b_{2}z) u(x) & \text{with } z \geq \pi_{x} \end{cases}$$

where u(x) is a solution of the problem

$$\Delta u = b_1^2 u \quad \text{with } \mathbf{x} \in G_1; \tag{2.1}$$

$$\Delta u = b_2^2 u \quad \text{with } \mathbf{x} \in G_2 \cup G_3; \tag{2.2}$$

$$[u_{z}]_{z=0} = [u_{z}]_{z=\pi} = 0 \quad \text{with } y \in \Omega;$$
(2.3)

$$u(0, \mathbf{y}) = u(\pi, \mathbf{y}) = 0 \text{ with } \mathbf{y} \in \Omega;$$
(2.4)

$$F\left(\frac{\partial u}{\partial n_{\Gamma_1}}, u, \mathbf{x}\right) \equiv \Phi_1\left(k_1^{-1} \exp\left(-b_1 z\right) \frac{\partial u}{\partial n_{\Gamma_1}}\right)$$
(2.5)

$$T^{0}(z) + k_{1}^{-1} \exp(-b_{1}z) u, \mathbf{x} = f_{1}(\mathbf{x})$$
 with $\mathbf{x} \in \Gamma_{1}$.

If Φ_1 and f_1 satisfy the conditions of Theorem 1, then problem (2.1), (2.4), (2.5) has in G_1 a unique solution $u_1(x) \Subset C^{2+\alpha}(G_1) \cap C^1(\overline{G}_1)$. It is presented in the form of a Fourier series

$$u_1(x) = \sum_{n=1}^{\infty} \psi_n(y) \sin nz \text{ with } \mathbf{x} \in G_{1s}$$
(2.6)

where

$$\psi_n(y) = \pi^{-1} \int_0^{\pi} u_1(x) \sin nz \, dz.$$

It is noted that $\psi_n(y)$ satisfies with $y \in \Omega$ the equation

$$\Delta \psi_n = (t_1^2 + n^2) \psi_{n^*}$$

If Φ_1 is linear for the first two arguments, then representation $f_1(x)$ determines for each of functions ψ_n boundary conditions at $\partial \Omega$. Equation (2.6) is in this case a clear solution of problem (2.1), (2.4), (2.5) in G_1 .

Let $b_2^2 - b_1^2 < 1$, or, in dimensional variables,

$$\chi_2^2 - \chi_1^2 < 4\pi^2/(av)^2. \tag{2.7}$$

We define u with z < 0 and $z > \pi$ in the following way:

$$u = \sum_{n=1}^{\infty} n \left(b_1^2 - b_2^2 + n^2 \right)^{-1/2} \psi_n(\mathbf{y}) \sin \left(\sqrt{(b_1^2 - b_2^2 + n^2)} z \right)$$
with $z < 0$, $\mathbf{y} \in \Omega$;
(2.8)

$$u = \sum_{n=1}^{\infty} n \left(b_1^2 - b_2^2 + n^2 \right)^{-1/2} \psi_n(\mathbf{y}) \times \sin \left[\sqrt{(b_1^2 - b_2^2 + n^2)} (\pi - z) \right] \text{with } z > \pi, \ \mathbf{y} \in \Omega.$$
(2.9)

Convergence of series (2.8) and (2.9) in corresponding spaces follows from convergence of series (2.6). Equalities (2.3) and (2.4) are fulfilled termwise. Thus, Theorem 1 is proven.

<u>Note 2</u>. For the majority of substances, $\chi_1 < \chi_2$ and inequality (2.7) is fulfilled. If it is not infringed, then in series (2.8) and (2.9) the final number of terms changes form. In fact, if $b_1^2 + n^2 < b_2^2$, $\sin \sqrt{(b_1^2 - b_2^2 + n^2)}z$ is exchanged for $\sinh \sqrt{(b_2^2 - b_1^2 - n^2)}z$, and if $b_1^2 + n^2 = b_2^2$, then for linear function z. This in no way affects the convergence of series (2.8), (2.9), but the qualitative properties of the solution may changed markedly.

<u>Note 3</u>. The construction provided above makes sense not only for cylindrical regions of G, but also when $G_1 \supseteq (0, \pi) \times \Omega$, $G_2 \subseteq (-\ell_2, 0) \times \Omega$, $G_3 \subseteq (\pi, \pi + \ell_1) \times \Omega$. An example of a region of this type is shown by a dotted line in Fig. 1. Similar regions occur in describing processes of crucibleless zone melting. Theorem 1 is also true for them, and if Γ_1 does not have common points with $(0, \pi) \times \partial\Omega$, then in the conditions of the theorem it is possible go give up the requirement $u_1 \subseteq C^1(G_1)$.

<u>3. Accurate Solutions</u>. The uniqueness of the solution for the original control problem follows from Theorem 1. For existence of a solution for this problem it is necessary and sufficient that the solution of the supplementary problem satisfies inequality (1.10), of, what is the same, solution of problem (2.1)-(2.5) satisfies the equations

$$u > 0 \qquad \qquad \text{with } \mathbf{x} \in G_1; \tag{3.1}$$

$$b_2 u < +\Lambda \operatorname{sh}(b_2 z) = b_2 \varphi_2(z) \qquad \text{with } x \in G_2; \tag{3.2}$$

$$b_2 u < \Lambda \text{ sh} \left(b_2 \pi - b_2 z \right) = b_2 \varphi_3(z) \quad \text{with } \mathbf{x} \in G_3. \tag{3.3}$$

We construct an example of exact solution of problem (2.1)-(2.4) satisfying (3.1)-(3.3). Let (2.7) be fulfilled. It is assumed that

$$u^{1}(\mathbf{x}) = \begin{cases} \beta b^{-1}\psi_{1}(y)\sin bz & \text{with } z \leqslant 0, \ \mathbf{y} \in \Omega, \\ \beta \sin z\psi_{1}(y) & \text{with } z \in (0, \pi), \ \mathbf{y} \in \Omega, \\ \beta b^{-1}\psi_{1}(y)\sin b(\pi - z) & \text{with } z \geqslant \pi, \ \mathbf{y} \in \Omega. \end{cases}$$

Here, $b = (b_1^2 - b_2^2 + 1)^{1/2}$, and $\psi_1(y)$ is a solution of the problem

$$\Delta \psi_1 = (b_1^2 + 1) \psi_1 \text{ with } \mathbf{y} \in \Omega,$$

$$\psi_1 = a(\mathbf{y}) \quad \text{with } \mathbf{y} \in \partial\Omega.$$

Function $\alpha(y)$ is prescribed such that $0 < \alpha_0 \leq \alpha(y) \leq 1$ with $y \in \partial \Omega$; $u^1(x)$ is a solution of problem (2.1)-(2.5), where condition (2.5) has the form

$$u(\mathbf{x}) = \beta a(\mathbf{y}) \sin z$$
 with $\mathbf{y} \in \partial \Omega, \ z \in (0, \pi)$.

The value of β characterizes the power of the heater.

From the maximal principle there follows existence of a number $\psi_m > 0$ such that $\psi_m \leq \psi_1(y) < 1$ with $y \in \Omega$. If we consider a plane or axisymmetric problem (most important for applications), then it is possible to assume that a(y) = 1 and to find the explicit form of $\psi_1(y)$. In the axisymmetric case condition $\psi_1(R) = 1$ satisfies the function

$$\psi_{1}(r) = I_{0}\left(\sqrt{\left(b_{1}^{2}+1\right)}r\right) / I_{0}\left(\sqrt{\left(b_{1}^{2}+1\right)}R\right),$$

where I_0 is the Bessel function of the imaginary argument; $r = \sqrt{y_1^2 + y_2^2}$. This function reaches its minimum value with r = 0,

$$\psi_m = 1/I_0 \left(\sqrt{\left(b_1^2 + 1 \right)} R \right).$$

The last equation illustrates the dependence of ψ_m on ingot thickness. So,

$$\psi_m = o\left(\exp\left(-\sqrt{(b_1^2+1)}R\right)\right)$$
 with $R \to \infty$.

It is evident that with $\beta \ge 0$ function $u^1(\mathbf{x})$ satisfies (3.1), and with $\beta \le 0$ it does not. For any solution of problem (2.1)-(2.4) of the form $\varphi(z)\psi(\mathbf{y})$, apart from $u^1(\mathbf{x})$, inequality (3.1) is infringed.

For any function u(x), continuously differentiated in G satisfying conditions (2.4) and (3.1), a necessary condition for fulfillment of (3.3) in a certain right-hand neighborhood Σ_1 is fulfillment of the inequality

$$\partial u/\partial z \leqslant -\Lambda = \varphi'_{3}(\pi) \text{ with } z = \pi - 0, \quad y \in \Omega,$$
 (3.4)

and the inequality

$$\partial u/\partial z \leqslant -(1+\varepsilon)\Lambda$$
 with $z = \pi - 0$, $y \in \Omega$

is sufficient with $\epsilon > 0$. In the particular case being considered, (3.4) is fulfilled simultaneously with

$$\beta > \Lambda \psi_m^{-1}. \tag{3.5}$$

Let $z_0 = \pi(1 + b^{-1})$. It is evident that $T^0(z_0) > 0$, $u^1(z_0) = 0$ and inequality (3.3) is infringed. Consequently, $\ell_1 < \ell_1^0 < \pi/b$, where ℓ_1^0 is the least positive root of the equation $\beta \psi_m \sin b(\pi + \ell_1^0) = b \phi_3(\ell_1^0 + \pi)$. On the other hand, $T^0(z) \le 0$, $u^1(x) < 0$ with $-\pi/b < z < 0$, and (3.2) is fulfilled. This means that solution of the control problem corresponding to $u = u^1$ exists with all $\ell_2 < \pi/b$.

Since $T^0(z) < 0$ also increases uniformly with z < 0, and u^1 is such that with z < 0, $y \in \Omega$, $u^1(z, y) = -u^1(-2n\pi/b - \pi + z, y)$, $n = 0, 1, \ldots$, inequality (3.2) may only be infringed with $z \in \left(-\frac{3\pi}{2b}, -\frac{\pi}{b}\right)$. If

$$\beta < b\varphi_2(3\pi/2b) = \Lambda bb_2^{-1} \operatorname{sh}(3\pi b_2/2b), \qquad (3.6)$$

then (3.2) is true with all z < 0 and l_2 may be chosen as large as one wishes. In the opposite case $l_2 < l_2^0$, where l_2^0 is the least positive root of the equation $b\varphi_2(l_2^0) = \beta \sin(bl_2^0)$. From the reasoning given it follows that $2\pi < 2bl_2^0 < 3\pi$.

It is noted that conditions (3.5) and (3.6) may be fulfilled simultaneously only if ψ_m^{-1} is sufficiently small:

$$\psi_m^{-1} \leqslant b \, \text{sh} \, (3\pi b_2/2b)/(2b_2), \tag{3.7}$$

The hatched region in Fig. 2a, b gives values of parameters satisfying inequalities (3.5) and (3.6).

In the axisymmetric case, by using an explicit form of the dependence of ψ_m on the radius of the region and the value of b_1 , it is possible to write (3.7) in the form

$$\frac{\pi R'}{a} = R < (b_1^2 + 1)^{-1/2} I_0^{-1} \left[\frac{b}{2b_2} \operatorname{sh} \left(\frac{3\pi b_2}{2b} \right) \right] = R_0 (b_1, b_2)_2$$
(3.8)

where I_0^{-1} is an inverse function to I_0 ; R' is radius of a cylindrical specimen.

In modeling the process of crucibleless zone melting, it is desirable to fulfill the condition of hydrodynamic stability of the liquid zone, which for a round cylinder of length a and radius R' has the form [9]

$$2\pi R'/a > 1. \tag{3.9}$$



The question arises of whether conditions (3.8) and (3.9) are common. It is easy to show that (3.8) and (3.9) may be fulfilled simultaneously if b_1 and b_2 are quite small. In Fig. 3 is a hatched region in plane (b_1, b_2) , determined by the inequalities

$$V 1 + b_1^2 > b_2 > 0, \quad 2R_0 (b_1, b_2) > 1_s$$

i.e., the region of values of b_1 and b_2 for which there exists a solution of the u^1 type and inequalities (3.8) and (3.9) may be fulfilled simultaneously.

If inequality (2.7) is infringed, then solution of the problem (2.1)-(2.4) having with $x \in G_1$ the form $\beta \sin z \psi_1(y)$ with $x \in G_2 \cup G_3$ either linear for z (if $b_2^2 = b_1^2 + 1$), or proportional shb'z [if $b_2^2 > b_1^2 + 1$, b' = $(b_2^2 - b_1^2 - 1)^{1/2}$]. If $\beta > 0$, then these solutions satisfy (3.1) with $x \in G_1$ and (3.2) with all z < 0, $y \in \Omega$. In order to fulfill (3.3) in some neighborhood Σ_1 , it is sufficient to fulfill (3.5). Since b' $< b_2$, inequality (3.3) is infringed with quite large z. Therefore, ℓ_2 may be chosen as large as one wishes, and $\ell_1 < \ell_1^0$, where ℓ_1^0 is the least root of the equation $\beta \psi_m \operatorname{shb}^! \ell_1^0 = \mathrm{b}^! \varphi_3(\ell_1^0 + \pi)$, if $b_2^2 - b_1^2 > 1$, and the equation $\beta \psi_m \ell_1^0 = \mathrm{b}^! \varphi_3(\ell_1^0 + \pi)$, if $b_2^2 = b_1^2 + 1$. It is easy to see that $\ell_0^1 \to \infty$ with $\beta \to \infty$. Therefore, it is possible to aim for the existence of a solution of the problem with as large ℓ_1 as one wishes by selecting quite high power for the heater.

The example considered is a basis for suggesting that the case of $\chi_1 > \chi_2$ is more favorable from the point of view of obtaining high-quality single crystals by the zone melting method.

A solution in the form $u^1(x)$ of problem (2.1)-(2.5) exists with any values of b_1 and b_2 , but it requires special assignment of f_1 . Exact solutions of (2.1)-(2.5) are considered below with arbitrary f_1 existing with $b_1 = b_2$. The latter is true if v = 0 or $\chi_1 = \chi_2$

If $b_1 = b_2$, then from (2.8) and (2.9) it follows that u(x) is a 2π -periodic, antisymmetric function relative to planes z = 0 and $z = \pi$.

If v = 0, then $b_1 = b_2 = 0$ and $T^0(z) \equiv 0$. Therefore, if (3.1) is true with $x \in G_1$, then T > 0 is true with $z \in (2\pi, 3\pi)$ and $z \in (-2\pi, -\pi)$. Consequently, solution of the control problem exists with $\ell_1 \leq \pi$, $\ell_2 \leq \pi$, and it does not exist with infringement of even one of these conditions.

If $v \neq 0$, $b_1 = b_2$, then by repeating the reasoning given above for $u = u^1(x)$ it is easy to show that solution of the control problem with $\ell_2 < \pi$ and $\ell_1 > 0$ exists if (3.5) is fulfilled. It is possible to indicate sufficient conditions for existence of a solution with any $\ell_1 \leq \pi$ and for any $\ell_2 > 0$ in the form of inequalities for function $f_1(x)$.

4. Solution of the Control Problem in the General Case. Above, on the example of exact solutions, it has been demonstrated that although solvability of the problem (2.1)-(2.5) proceeds from the solvability of the boundary problem (2.1), (2.3), (2.5) in G₁, for existence of a solution to the control problem it is still necessary to fulfill conditions of the inequality type for values of ℓ_1 , ℓ_2 , and $f_1(\mathbf{x})$, Provided below is a summary of these results for the case of arbitrary values of b_1 and b_2 and arbitrary functions f_1 .

First let, at the melt boundary temperature distribution be specified

$$u = \beta f_1(\mathbf{x}) \text{ with } \mathbf{x} \in \Gamma_1,$$

$$\beta > 0, f_1(0, y) = f_1(\pi, y) = 0 \text{ with } \mathbf{y} \in \partial\Omega.$$

From the maximal principle it follows that (3.1) is fulfilled simultaneously with inequality $f_1(x) \ge 0$ with $x \in \Gamma_1$. In view of the continuous differentiability of function u(x) and the

continuity of $T^0(z)$, and also inequality $T^0(z) < 0$ with z < 0, fulfillment of (3.2) in a certain neighborhood Σ_2 flows from (3.1), and sufficient condition for fulfillment of (3.3) in a certain neighborhood Σ_1 will be equality (3.4), for whose verification in the general case it is necessary to solve the boundary problem in G_1 . If region Ω has a simple shape (e.g., a circle), then the problem is solved in explicit form. If the shape of Ω is more complex or G_1 is not a cylinder (see note 3), then it is possible to obtain sufficient conditions for fulfillment of (3.4) in the form of inequalities for β and $f_1(x)$. For this we consider a Dirichlet problem:

$$\Delta w = b_1^2 w \text{ with } \mathbf{x} \in G_1,$$

$$w = \beta f_1 - \beta_0 \psi_1(y) \sin z \text{ with } \mathbf{x} \in \Gamma_1,$$

$$w = 0 \text{ with } \mathbf{x} \in \Sigma_1 \cup \Sigma_2,$$

where β_0 satisfies (3.5). From the maximal principle it follows that if

$$\beta f_1(\mathbf{x}) > \beta_0 a(\mathbf{y}) \sin z, \tag{4.1}$$

then $w \ge 0$ with $x \in G_1$ and, therefore, $w_z \le 0$ with $z = \pi$. By assuming that $w = u - u^1$, we conclude that u satisfies (3.4). Condition (4.1) is not necessary, which is demonstrated by an example of the function

$$u^2(\mathbf{x}) = \beta \psi_1(\mathbf{y}) \sin z + \gamma \psi_2(\mathbf{y}) \sin 2z$$

If f_1 satisfies the condition of Theorem 1, and, in addition,

$$f_{1z}|_{z=0} > 0, f_{1z}|_{z=\pi} < 0, f_1(\mathbf{x}) > 0 \text{ with } \mathbf{x} \in \Gamma_1,$$

then fulfillment of (4.1) may be obtained by choosing sufficiently large β . On the other hand, if

$$\beta f_1(\mathbf{x}) < \beta_1 a(\mathbf{y}) \sin z, \tag{4.2}$$

where β_1 satisfies (3.6), then ℓ_2 may be as large as one wishes. Conditions for (4.1) and (4.2) may be fulfilled simultaneously only if $\beta_1 > \beta_0$. The necessary and satisfactory conditions for fulfilling the last inequality are given in part 3. Provided below in the form of a theorem is a summary of these results for the case of nonlinear boundary conditions.

<u>THEOREM 2.</u> Let $u^1(x)$, $x \in G_1$ be the function determined in part 3, β satisfies (3.5), then $\delta > 0$ is found such that, if functions Φ_1 and f_1 satisfy the condition of Theorem 1 and

$$||F(\partial u^1/\partial n_{\Gamma}, u^1, \mathbf{x}) - f_1(\mathbf{x})|| < \delta,$$

then solution of the problem (2.1)-(2.5) satisfies (3.1) with $x \in G_1$, (3.2) with $x \in (-\ell_2^0/2,0) \times \Omega$, and (3.3) with $x \in (\pi, \pi + \ell_1^0/2) \times \Omega$, where ℓ_1^0 and ℓ_2^0 are determined in part 3. In addition, if β satisfies (3.6) and δ is quite small, then (3.2) is fulfilled with all z < 0, $y \in \Omega$.

Confirmation of Theorem 2 flows from the continuous dependence of the solution of the boundary problem (2.1), (2.3), (2.5) on f_1 , representing a solution with z < 0, $z > \pi$, $y \in \Omega$ in the form of series (2.8), (2.9), and the properties of function $u^1(x)$ established in part 3.

<u>Note 4</u>. Confirmation of Theorem 2 remains in force if in its condition $u^1(x)$ is substituted by any other exact solution of (2.1)-(2.5) satisfying (3.1)-(3.3), for example, $u^2(x)$ with appropriate β and γ .

Now we demonstrate that for any values of $b_1 > b_2 > 0$ and any functions f_1 , Φ_1 we find ℓ_1^0 such that with $\ell_1 > \ell_1^0$ a solution of the problem being considered does not exist.

In fact, in the opposite case this solution with $z > \pi$ would be presented in the form $T = T^{0}(z) + k_{2}^{-1} \exp(b_{2}\pi - b_{2}z)u(x)$, where u(x) satisfies (3.3) with $z > \pi$, whence

$$U(x) = b_2^{-2} \Lambda^{-1} \left| \int_{\pi}^{z} u(\zeta, \mathbf{y}) d\zeta \right| > \operatorname{ch} (b_2 z - b_2 \pi) - 2.$$

On the other hand, from the representation of $u(\mathbf{x})$ in the form of series (2.9) it follows that if $u_1 \in C^1(\overline{G}_1)$, then U uniformly for z is limited with $z > \pi$, $y \in \Omega$. The proof is demonstrated. It remains in force also in the case of $b_2 < b_1$. In this way U(\mathbf{x}) may grow linearly or exponentially, but more slowly than $\exp(b_2 z)$. Therefore, (3.3) is infringed with quite large z.

5. Other Arrangements of the Zone Melting Control Problem. Consideration was given above to the process of heat transfer in the region fixed in a coordinate system connected with the heater. In real processes the specimen has finite dimensions and at instant of time t it occupies the region $G_t = (-\ell_2' - vt, \alpha + \ell_1' - vt) \times \Omega'$. A molten zone of width a, enclosed between solid rods, may only exist for finite time $t_0 < \ell_1'/v$. If $G_t \subseteq G$ with all $t < t_0$, i.e., $\ell_1' < \ell_1^0 \alpha / \pi$, $\ell_2' + vt_0 < \ell_2^0 \alpha / \pi$, then construction of the solution above is determined in region $\{(X, t): t \in (0, t_0), X \in G_t\}$, but for its realization it is necessary to have maintained a complex essentially nonlinear cooling regime for the ingot ends. It is simplest to obtain a solution of type u^1 with linear equations at the ends. For this purpose it is necessary to specify functions f_4 and f_5 as follows:

$$f_i(x) = \psi_1(\mathbf{y})[\alpha \sin \pi (l_{i-3} - vt)/a + \beta \cos \pi (l_{i-3} - vt)/a]$$

with $X \in \Gamma_i, i = 4, 5$.

Choice of the cooling schedule as a control function makes it practically difficult to use the results obtained. In practice it is easier to control the heating schedule. Cooling is normally carried out by radiation, or blowing a gas, or by means of a liquid jet. From the uniqueness theorem for the problem being considered it follows that with an arbitrarily prescribed cooling schedule for both parts of the crystal it is not generally possible by selecting the heating schedule to make flat melting and solidification fronts. It is only possible to prescribe in an arbitrary way the cooling schedule for part of the crystal either ahead of the melting front or behind the crystallization front. The problem of providing a special cooling schedule for another part of the crystal remains. It is noted that from the results of this work it is clear that if the specimen movement rate differs from zero, then in prescribing an identical cooling schedule for two parts of the crystal it is impossible to provide a flat front for phase transitions.

It was demonstrated in part 4 that if $b_1 > b_2$, then solution of the problem of zone melting with flat melting and crystallization fronts only exists with $\ell_1 < \ell_1^0$, and in all of the examples considered $\ell_1^0 \le \pi$, whereas in carrying out production processes the length of the molten zone is normally much less than the length of the ingot. This limitation arose from the requirement for continuing the solution beyond the flat melting front. Dropping this require should not severely worsen the quality of the crystal obtained. The problem is therefore of interest of constructing a solution with a quite narrow molten zone and with a flat solidification front, but a curved melting front.

By using the methods of the present work, it is also possible to construct a broad class of accurate nonsteady-state solutions for zone melting with flat phase transition fronts. These solutions require specification of agreed starting data in the liquid and solid phases.

Under these conditions, when exact solutions of the stated problem do not exist or heattransfer schedules corresponding to them are impractical for any reason, a solution should be sought with a front shape close to flat using methods of optimum control theory. In [3, 4] this approach was applied to the problem of controlling crystallization processes in which the control functions were not connected with the shape of the phase transition.

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