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BOUNDARIES OF THE INITIAL MELTED AREA OF A SEMICONDUCTOR FILM FORMED BY FLOATING-ZONE MELTING

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Stationary hydrodynamic and temperature fields near the upper triple point of the floating-zone melting process are analyzed. Regularities determining the angular position and shape of the initial melted area as functions of thermal conditions on solid and liquid surfaces in the immediate vicinity of the triple point are established in the form of four analytical relations.

1. The floating-zone technique employing high-frequency currents of a plate inductor was described, as applied to semiconductor materials, for instance, in [1], where results of a numerical study were also reported. The theoretical investigation of this process involves a number of difficulties, in particular, those resulting from unknown interacting boundaries involved in the problem. The goal of the present work is to elucidate regularities that relate local (near the triple point) geometric parameters of the unknown boundaries with the thermal conditions on them.

We consider a stationary planar statement of the problem schematically represented in Fig. 1a. The solid phase (polycrystal) shown in this figure as a dashed area travels downward with a velocity v_0. As the solid phase passes through the boundary γ_s, it transforms into a melt, which drains down forming a film with a free boundary γ_l; the boundaries γ_s and γ_l are unknown (the subscripts s and l here refer to the solid phase and the melt, respectively). The problem is considered in the vicinity of the upper triple point of the floating-zone refining procedure [1], where the interface γ_s between the phases and the free surface γ_l cross the vertical plane boundary of the polycrystal γ. It should be emphasized that the melt film was not modeled numerically in [1].

In the experiment, the sample melts due to high-frequency currents generated by a plate inductor. In the present theoretical statement of the problem, the inductor is not considered, and its action is replaced by surface heat release and magnetic pressure. The thermal power supplied to a unit area of the polycrystal and the melt is set in the form of the expansions

$$W_s = W_s^{(0)} + W_s^{(1)}\xi_s + W_s^{(2)}\xi_s^2 + \ldots, \qquad W_l = W_l^{(0)} + W_l^{(1)}\xi_l + W_l^{(2)}\xi_l^2 + \ldots, \tag{1.1}$$

where ξ_s is the distance from the triple point O to a point at the solid surface and ξ_l is the distance along the free surface.

In the problem under study, we have to find the hydrodynamic and temperature fields in the melted film, the temperature distributions in the polycrystal, and the positions and shapes of the boundaries γ_s and γ_l in the vicinity of the triple point O as functions of the parameters $W^{(0)}, W^{(1)}, \ldots$ that characterize the heat flux toward the boundaries. In the hydrodynamic part of the study, thermal convection is not considered (i.e., the buoyancy forces are ignored); as a result, the overall problem splits into purely hydrodynamic and thermal problems. The density ρ, specific heat capacity c, and heat conductivity λ in a small vicinity of the point O are assumed constant, and the Stokes approximation is used.

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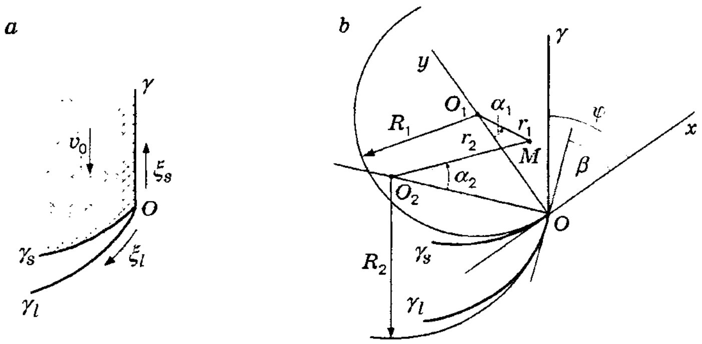

Fig. 1

It is convenient to treat the problem using two polar coordinate systems (r_1, α_1) and (r_2, α_2), whose origins lie at the points O_1 and O_2 (Fig. 1b). The positions of these points relative to the boundary γ and triple point O are described by angles φ and β and radii R_1 and R_2, respectively. From Fig. 1b, the following formulas that relate the coordinates of the center O_2 and those of an arbitrary point M can be derived:

$$x(O_2) = -R_2 \sin\beta = -[r_2 \sin(\beta + \alpha_2) - r_1 \sin\alpha_1],$$

$$y(O_2) = R_2 \cos\beta = R_1 - r_1 \cos\alpha_1 + r_2 \cos(\beta + \alpha_2).$$

From here, we have

$$r_1 = \sqrt{R_1^2 + R_2^2 + r_2^2 - 2R_1R_2\cos\beta + 2R_1r_2\cos(\beta+\alpha_2) - 2R_2r_2\cos\alpha_2}; \tag{1.2}$$

$$\tan\alpha_1 = \frac{-R_2\sin\beta + r_2\sin(\beta+\alpha_2)}{R_1 - R_2\cos\beta + r_2\cos(\beta+\alpha_2)}. \tag{1.3}$$

The coordinates of the point at the boundary γ are given by the following formulas:

$$r_{1*}(\alpha_1) = R_1 \frac{\cos\varphi}{\cos(\varphi - \alpha_1)} = R_1 - R_1\alpha_1 \tan\varphi + R_1(1 + 2\tan^2\varphi)\frac{1}{2}\alpha_1^2 + \ldots; \tag{1.4}$$

$$\xi_s = R_1 \frac{\sin\alpha_1}{\cos(\varphi - \alpha_1)} = R_1\Big(\frac{1}{\cos\varphi}\alpha_1 - \frac{\sin\varphi}{\cos^2\varphi}\alpha_1^2 + \ldots\Big). \tag{1.5}$$

The unknown boundaries in the vicinity of O are given by the expressions

$$\gamma_s\colon \quad r_{1s} = R_1 + R_1K_s\alpha_1^3 + O(\alpha_1^4); \tag{1.6}$$

$$\gamma_l\colon \quad r_{2l} = R_2 + R_2K_l\alpha_2^3 + O(\alpha_2^4). \tag{1.7}$$

Hence, φ is the angle between the tangent line to the interface between the phases at the point O and the solid boundary, β is the wedge angle at the initial point of the melted film, and R_1 and R_2 are the curvature radii of the boundaries γ_s and γ_l, respectively. The deviation of these boundaries from perfect circumferences is taken into account by the second terms in the right-hand parts of Eqs. (1.6) and (1.7), where K_s and K_l are some indefinite constants.

2. The hydrodynamic problem for the stream function $\psi(r_1, \alpha_1)$ and pressure $p(r_1, \alpha_1)$ is given by the equations

$$\Delta\Delta\psi(r_1, \alpha_1) = 0; \tag{2.1}$$

$$\operatorname{grad} p(r_1, \alpha_1) = \mu\Big[\frac{1}{r_1}\frac{\partial\Delta\psi}{\partial\alpha_1}\boldsymbol{e}_{r_1} - \frac{\partial\Delta\psi}{\partial r_1}\boldsymbol{e}_{\alpha_1}\Big] + \rho_l\boldsymbol{g}, \quad \boldsymbol{v} = \frac{1}{r_1}\frac{\partial\psi}{\partial\alpha_1}\boldsymbol{e}_{r_1} - \frac{\partial\psi}{\partial r_1}\boldsymbol{e}_{\alpha_1}, \tag{2.2}$$

where μ is the dynamic viscosity, $\boldsymbol{g}$ is the free-fall acceleration, and $\boldsymbol{e}_{r_1}$ and $\boldsymbol{e}_{\alpha_1}$ are the corresponding unit vectors, and also by certain boundary conditions.

At the boundary γ_s, the mass flux is constant and the tangent velocity is continuous. Hence, the velocity of the melt at the boundary γ_s is

$$v\Big|_{\gamma_s} = v_0 - (1-\tilde{\rho})(v_0 \cdot n)n, \tag{2.3}$$

where n is the unit vector of the normal directed out of the solid phase into the melt and $\tilde{\rho} = \rho_s/\rho_l$ is the ratio of the densities of the two phases. The difference between the velocity of the liquid at the boundary γ_s and the velocity v_0 is caused by the change in the density of the substance during the phase transition. Since for boundary (1.6) we have

$$n\Big|_{\gamma_s} = [1-(9/2)K_s^2\alpha_1^4 + O(\alpha_1^5)]\, e_{r_1} + [-3K_s\alpha_1^2 + O(\alpha_1^3)]\, e_{\alpha_1}, \tag{2.4}$$

condition (2.3) can be used at the boundary $r_1 = R_1$. It can be represented as an expansion in terms of powers of α_1:

$$\begin{aligned} v_{r_1}\Big|_{r_1=R_1} &= \tilde{\rho}v_0\sin\varphi - \tilde{\rho}v_0\alpha_1\cos\varphi - v_0[(1/2)\tilde{\rho}\sin\varphi + (1-\tilde{\rho})3K_s\cos\varphi]\alpha_1^2 + O(\alpha_1^3), \\ v_{\alpha_1}\Big|_{r_1=R_1} &= -v_0\cos\varphi - v_0\alpha_1\sin\varphi + v_0[(1/2)\cos\varphi + (1-\tilde{\rho})3K_s\sin\varphi]\alpha_1^2 + O(\alpha_1^3). \end{aligned} \tag{2.5}$$

At the free boundary γ_l, which is a streamline passing through the triple point, the kinematic condition

$$\psi\Big|_{\gamma_l} = \psi[r_{2l}(\alpha_2), \alpha_2] = \psi_*(\alpha_2) = \text{const}$$

is satisfied, which, for a local solution, is equivalent to the condition

$$\frac{d\psi_*(\alpha_2)}{d\alpha_2}\Big|_{\alpha_2=0} = 0, \qquad \frac{d^2\psi_*(\alpha_2)}{d\alpha_2^2}\Big|_{\alpha_2=0} = 0, \ldots \tag{2.6}$$

(subsequent approximations are not used). The dynamic conditions of continuity of the stress-tensor components are also valid at this boundary:

$$\sigma_{nn}\Big|_{\gamma_l} = -(p_0 + p_m), \qquad \sigma_{n\tau}\Big|_{\gamma_l} = 0.$$

Here p_0 is the external pressure, constant over the surface, that also includes surface tension and p_m is the magnetic pressure (which is not always constant). It is assumed that electromagnetic forces have no tangent components, and the temperature dependence of the surface tension is ignored. Since

$$\sigma_{nn} = \sigma_{rr}n_r^2 + \sigma_{\alpha\alpha}n_\alpha^2 + 2\sigma_{r\alpha}n_r n_\alpha, \quad \sigma_{n\tau} = (\sigma_{\alpha\alpha} - \sigma_{rr})n_r n_\alpha + \sigma_{\alpha r}(n_r^2 - n_\alpha^2),$$

and n_r and n_α are given by a formula obtained from (2.4) with α_1 and K_s replaced by α_2 and K_l, the above dynamic boundary conditions can be transferred onto the circumference $r_2 = R_2$ and be represented in the form

$$\sigma_{\alpha r} - (\sigma_{\alpha\alpha} - \sigma_{rr})3K_l\alpha_2^2\Big|_{r_2=R_2} = O(\alpha_2^3); \tag{2.7}$$

$$\sigma_{rr} - 6\sigma_{r\alpha}K_l\alpha_2^2\Big|_{r_2=R_2} = -(p_0 + p_m)\Big|_{r_2=R_2}. \tag{2.8}$$

The components of the stress tensor entering relations (2.7) and (2.8) can be expressed in terms of the stream function and pressure in the melt:

$$\sigma_{rr} = -p + 2\mu\frac{\partial}{\partial r_2}\Big(\frac{1}{r_2}\frac{\partial\psi}{\partial\alpha_2}\Big), \qquad \sigma_{r\alpha} = \mu\Big(\frac{1}{r_2^2}\frac{\partial^2\psi}{\partial\alpha_2^2} - \frac{\partial^2\psi}{\partial r_2^2} + \frac{1}{r_2}\frac{\partial\psi}{\partial r_2}\Big), \tag{2.9}$$

$$\sigma_{\alpha\alpha} = -p + 2\mu\Big(-\frac{1}{r_2}\frac{\partial^2\psi}{\partial r_2\,\partial\alpha_2} + \frac{1}{r_2^2}\frac{\partial\psi}{\partial\alpha_2}\Big).$$

We consider the local solution of the hydrodynamic problem in the form of an expansion in terms of powers of α_1:

$$\psi(r_1,\alpha_1) = \psi_0(r_1) + \psi_1(r_1)\alpha_1 + \psi_2(r_1)\alpha_1^2 + \dots,$$
$$p(r_1,\alpha_1) = p_0(r_1) + p_1(r_1)\alpha_1 + p_2(r_1)\alpha_1^2 + \dots \tag{2.10}$$

It should be noted that the fourth-order system of differential equations for the functions $\psi_i(r_1)$ which is obtained by substitution of (2.10) into Eq. (2.1) is not given here since, to determine the local behavior of the solution, only several first terms in the expansion in the vicinity of the triple point are required:

$$\psi_0(r_1) = c_0 + \psi_0'(R_1)(r_1 - R_1) + (1/2)\psi_0''(R_1)(r_1 - R_1)^2 + \dots,$$
$$\psi_1(r_1) = \psi_1(R_1) + \psi_1'(R_1)(r_1 - R_1) + (1/2)\psi_1''(R_1)(r_1 - R_1)^2 + \dots,$$
$$\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots$$

(c_0 is a constant). These terms can be found from the boundary conditions. From condition (2.5), we have

$$\psi_1(R_1) = R_1\tilde{\rho}v_0\sin\varphi, \qquad 2\psi_2(R_1) = -R_1\tilde{\rho}v_0\cos\varphi,$$
$$3\psi_3(R_1) = -R_1v_0[(1/2)\tilde{\rho}\sin\varphi + (1-\tilde{\rho})3K_s\cos\varphi], \tag{2.11}$$
$$\psi_0'(R_1) = v_0\cos\varphi, \quad \psi_1'(R_1) = v_0\sin\varphi, \quad \psi_2'(R_1) = -v_0[(1/2)\cos\varphi + (1-\tilde{\rho})3K_s\sin\varphi].$$

The first of the kinematic conditions (2.6) at the free boundary yields the relation

$$\frac{\partial\psi}{\partial r_2}\Big|_0 \frac{dr_{2l}}{d\alpha_2}(0) + \frac{\partial\psi}{\partial\alpha_2}\Big|_0 = 0.$$

Here the subscript 0 shows that the derivatives are calculated at the point $r_2 = R_2$, $\alpha_2 = 0$. Since $(dr_{2l}/d\alpha_2)\Big|_0 = 0$, the requirement

$$\frac{\partial\psi}{\partial\alpha_2}\Big|_0 = 0 \tag{2.12}$$

arises. In a similar manner, from the second condition of (2.6) and in view of the condition $(d^2r_{2l}/d\alpha_2^2)\Big|_0 = 0$, we have

$$\frac{\partial^2\psi}{\partial\alpha_2^2}\Big|_0 = 0. \tag{2.13}$$

Stream function (2.10) is set in variables (r_1 and α_1) [see (1.2)–(1.5)]. Let us use formulas (1.2) and (1.3), and derive some corollaries of requirements (2.12) and (2.13). From (2.12), it follows that

$$-\psi_0'(R_1)R_2\sin\beta + \psi_1(R_1)\tilde{R}\cos\beta = 0,$$

where $\tilde{R} = R_2/R_1$, which, in view of (2.11), results in the first condition,

$$\tan\beta = \tilde{\rho}\tan\varphi \tag{2.14}$$

among those governing the geometry of the liquid film. The relation between the wedge angle β and the deflection angle of the tangent line to the interface from the vertical gives the law of refraction of streamlines at the interface for the streamline passing through the triple point.

In a similar way, from (2.13) the relation

$$\psi_0''(R_1)R_2\sin^2\beta + (1-\tilde{\rho})v_0(\cos\varphi\cos^2\beta - \sin\varphi\sin 2\beta) - v_0(\cos\varphi\cos\beta + \tilde{\rho}\sin\varphi\sin\beta) = 0 \tag{2.15}$$

results, which contains the second-order derivative $\psi_0''(R_1)$.

We consider now the dynamic boundary conditions. From the zeroth approximation for condition (2.7) $\sigma_{\alpha r}\Big|_0 = 0$, taking into account (2.13), we obtain

$$\Big(\frac{\partial^2\psi}{\partial r_2^2} - \frac{1}{R_2}\frac{\partial\psi}{\partial r_2}\Big)\Big|_0 = 0.$$

In view of (1.2), (1.3), and (2.11), this condition can be rewritten as

$$\psi_0''(R_1)R_2\cos^2\beta + \tilde{R}(1-\tilde{\rho})v_0(\cos\varphi\sin^2\beta + \sin\varphi\sin 2\beta) - v_0(\cos\varphi\cos\beta + \tilde{\rho}\sin\varphi\sin\beta) = 0.$$

Adding together the above equality and (2.15) and taking into account that, according to (2.14), $\cos\varphi\,\cos\beta + \tilde{\rho}\sin\varphi\,\sin\beta = \cos\varphi/\cos\beta$, we obtain the second-order derivative $\psi_0''(R_1)$ that supplements conditions (2.11):

$$\psi_0''(R_1)R_2 = [-\tilde{R}(1-\tilde{\rho})\cos\varphi + 2\cos\varphi/\cos\beta]v_0.$$

Substituting this expression into (2.15), we obtain a second important [along with (2.14)] relation,

$$\tilde{R}(1-\tilde{\rho}) = \frac{\cos 2\beta}{\cos(\varphi+2\beta)}\,\frac{\cos\varphi}{\cos\beta}, \tag{2.16}$$

which gives the ratio of the curvature radii for the unknown boundaries of interest. Here, it is pertinent to note that the above relation is rather universal. The value of $\tilde{R}$ does not depend on the constants K_s and K_l, which enter (1.6) and (1.7), and also on the conditions at the free boundary, except for the conditions of absence of external shear stresses at the free surface of the melt. Note also that, to obtain (2.16), one has to take into account the change in the density during the phase transition.

The zeroth approximation of boundary condition (2.8),

$$\sigma_{rr}\Big|_0 = -p\Big|_0 + 2\mu\Big(-\frac{1}{R_2^2}\frac{\partial\psi}{\partial\alpha_2}\Big|_0 + \frac{1}{R_2}\frac{\partial^2\psi}{\partial r_2\,\partial\alpha_2}\Big|_0\Big) = -p_0 - p_m\Big|_0,$$

simplified using (2.12), after calculation of the second derivative leads to the following expression for the pressure in the liquid at the triple point:

$$p\Big|_0 = p_0 + p_m\Big|_0 + \frac{\mu v_0}{R_2}\,\frac{\sin 2\varphi}{\cos(\varphi+2\beta)\cos\beta}.$$

The pressure distribution in the vicinity of this point is described by Eq. (2.2).

Consideration of the first approximations for the dynamic boundary conditions (2.7) and (2.8) together with the kinematic condition

$$\frac{d^3\psi_*}{d\alpha_2^3}\Big|_{\alpha_2=0} = 0$$

allows us to determine the values of the derivatives $\psi_0'''(R_1)$ and $\psi_1''(R_1)$ and establish the relation between the parameters K_s and K_l, which characterize the deflection of the boundaries of interest from exact circumferences with the radii R_1 and R_2, respectively. A simple "universal" relation (2.16) was obtained for $\tilde{R}$, whereas the relation between K_s and K_l is too cumbersome — it contains the parameter $(dp_m/d\alpha_2)\Big|_0$ that characterizes the effect of external conditions and, for this reason, this relation is not given here.

3. The thermal part of the problem is described by heat-conduction equations, which in the coordinates $(r_1,\,\alpha_1)$ have the form

$$\Delta\theta_s = P^{(s)}\Big[\frac{\partial\theta_s}{\partial r_1}\sin(\varphi-\alpha_1) - \frac{1}{r_1}\frac{\partial\theta_s}{\partial\alpha_1}\cos(\varphi-\alpha_1)\Big]; \tag{3.1}$$

$$\Delta\theta_l = \frac{P^{(l)}}{v_0}\Big(\frac{1}{r_1}\frac{\partial\psi}{\partial\alpha_1}\frac{\partial\theta_l}{\partial r_1} - \frac{1}{r_1}\frac{\partial\psi}{\partial r_1}\frac{\partial\theta_l}{\partial\alpha_1}\Big); \tag{3.2}$$

$$\Delta = \frac{1}{r_1}\frac{\partial}{\partial r_1}\Big(r_1\frac{\partial}{\partial r_1}\Big) + \frac{1}{r_1^2}\frac{\partial^2}{\partial\alpha_1^2}, \qquad P^{(s)} = \frac{\rho_s c_s v_0}{\lambda_s}, \qquad P^{(l)} = \frac{\rho_l c_l v_0}{\lambda_l}.$$

Here θ_s and θ_l are the excess temperatures of the solid and liquid phases over the melting point T_0.

The boundary conditions can be written under the assumption that the heat transfer from the surface is radiative and the heat supply rate is given by relations (1.1). The expression for the radiative heat flux, $\varepsilon\sigma_0[(T_0+\theta)^4 - T_*^4]$ (σ_0 is the Stefan–Boltzmann constant), after linearization acquires the form $\Lambda_s(\theta_s+\theta_{s*})$ or $\Lambda_l(\theta_l+\theta_{l*})$ for the polycrystal or the melt, respectively. Here $\Lambda_s = \varepsilon_s\sigma_0(T_0+T_{s*})(T_0^2+T_{s*}^2)$ and $\Lambda_l =$

$\varepsilon_l \sigma_0 (T_0 + T_{l*})(T_0^2 + T_{l*}^2)$, $\theta_{s*} = T_0 - T_{s*}$ and $\theta_{l*} = T_0 - T_{l*}$ are constants, and T_* and ε are the ambient temperature and the emissivity, which, generally speaking, are different for the polycrystal and for the melt. Thus, the temperature boundary conditions are

— at the boundary γ_s: $\theta_s = 0$, $\theta_l = 0$, and $\lambda_l(\partial\theta_l/\partial n) - \lambda_s(\partial\theta_s/\partial n) = \rho_s v_{0n}[Q_0 + (c_l - c_s)T_0]$ (Q_0 is the specific melting heat);

— at the boundary γ_l: $\lambda_l(\partial\theta_l/\partial n) + \Lambda_l\theta_l = W_l(\xi_l) - \Lambda_l\theta_{l*}$;

— at the boundary γ: $\lambda_s(\partial\theta_s/\partial n) + \Lambda_s\theta_s = W_s(\xi_s) - \Lambda_s\theta_{s*}$.

(Note that, in the above form, the boundary conditions also admit other heat-exchange mechanisms, apart from the Joule heating and radiative heat release considered here.) The boundaries γ_s and γ_l are given by relations (1.6) and (1.7). We transfer the corresponding boundary conditions onto the circumferences and rearrange them with indication of a reliable term of the expansion in terms of powers of the small angle α_1:

$$\Big(\theta_s + \frac{\partial\theta_s}{\partial r_1} R_1 K_s \alpha_1^3\Big)\Big|_{r_1=R_1} = O(\alpha_1^4); \tag{3.3}$$

$$\Big(\theta_l + \frac{\partial\theta_l}{\partial r_1} R_1 K_s \alpha_1^3\Big)\Big|_{r_1=R_1} = O(\alpha_1^4); \tag{3.4}$$

$$\Big[\lambda_l \frac{\partial\theta_l}{\partial r_1} - \lambda_s \frac{\partial\theta_s}{\partial r_1} - \Big(\lambda_l \frac{\partial\theta_l}{\partial\alpha_1} - \lambda_s \frac{\partial\theta_s}{\partial\alpha_1}\Big)\frac{3K_s}{R_1}\alpha_1^2\Big]\Big|_{r_1=R_1}$$

$$= \rho_s v_0 \tilde{Q}\Big[\sin\varphi - \alpha_1\cos\varphi + \Big(3K_s\cos\varphi - \frac{1}{2}\sin\varphi\Big)\alpha_1^2\Big] + O(\alpha_1^3); \tag{3.5}$$

$$\Big[\lambda_l\Big(\frac{\partial\theta_l}{\partial r_2} - \frac{1}{R_2}\frac{\partial\theta_l}{\partial\alpha_2} 3K_l\alpha_2^2\Big) + \Lambda_l\theta_l\Big]\Big|_{r_2=R_2} = W_l^{(0)} - \Lambda_l\theta_{l*} - W_l^{(1)} R_2\alpha_2 + W_l^{(2)} R_2^2\alpha_2^2 + O(\alpha_2^3). \tag{3.6}$$

In relation (3.5), we have $\tilde{Q} = Q_0 + (c_l - c_s)T_0$. For the boundary γ, the unit vector of the normal is

$$\boldsymbol{n} = \cos(\varphi - \alpha_1)\,\boldsymbol{e}_{r_1} + \sin(\varphi - \alpha_1)\,\boldsymbol{e}_{\alpha_1},$$

and the corresponding boundary condition acquires the form

$$\Big\{\lambda_s\Big[\frac{\partial\theta_s}{\partial r_1}\cos(\varphi - \alpha_1) + \frac{1}{r_1}\frac{\partial\theta_s}{\partial\alpha_1}\sin(\varphi - \alpha_1)\Big] + \Lambda_s\theta_s\Big\}\Big|_{r_1=r_{1*}(\alpha_1)} = W_s(\xi_s) - \Lambda_s\theta_{s*} \tag{3.7}$$

[see also (1.4) and (1.5)].

We search for the local solutions in the form

$$\theta_s(r_1,\alpha_1) = t_0(r_1) + t_1(r_1)\alpha_1 + \ldots, \quad \theta_l(r_1,\alpha_1) = s_0(r_1) + s_1(r_1)\alpha_1 + s_2(r_1)\alpha_1^2 + \ldots . \tag{3.8}$$

For two extra conditions [in addition to (2.14) and (1.16)] required to determine the parameters φ, β, R_1, and R_2, which specify the unknown boundaries γ_s and γ_l, it suffices to determine the zeroth expansion terms of Eqs. (3.1) and (3.2):

$$t_0''(r_1) + \frac{1}{r_1}t_0'(r_1) + \frac{2}{r_1^2}t_2(r_1) = P^{(s)}\Big[t_0'(r_1)\sin\varphi - \frac{1}{r_1}t_1(r_1)\cos\varphi\Big]; \tag{3.9}$$

$$s_0''(r_1) + \frac{1}{r_1}s_0'(r_1) + \frac{2}{r_1^2}s_2(r_1) = \frac{P^{(l)}}{v_0}\Big[\frac{1}{r_1}\psi_1(r_1)s_0'(r_1) - \frac{1}{r_1}\psi_0'(r_1)s_1(r_1)\Big]. \tag{3.10}$$

Boundary conditions (3.3) and (3.4) yield the relations

$$t_0(R_1) = t_1(R_1) = t_2(R_1) = 0, \qquad s_0(R_1) = s_1(R_1) = s_2(R_1) = 0. \tag{3.11}$$

From the expressions for the zeroth and first terms of the expansion of boundary condition (3.5), we obtain

$$\lambda_l s_0'(R_1) - \lambda_s t_0'(R_1) = \rho_s v_0\tilde{Q}\sin\varphi; \tag{3.12}$$

$$\lambda_l s_1'(R_1) - \lambda_s t_1'(R_1) = -\rho_s v_0\tilde{Q}\cos\varphi. \tag{3.13}$$

In order to obtain the zeroth and first terms of expansion (3.6) in terms of powers of the variable α_2, we have to use the geometric relations $r_1(r_2, \alpha_2)$ and $\alpha_1(r_2, \alpha_2)$ [see (1.2)–(1.5)]. These expansion terms, in view of (2.10) and (2.11), yield the equalities

$$\lambda_l s_0'(R_1)\cos\beta = W_l^{(0)} - \Lambda_l \theta_{l*}; \tag{3.14}$$

$$\lambda_l s_0'(R_1)\sin\beta[(2\tilde{R} - P^{(l)}R_2\tilde{\rho}\sin\varphi)\cos\beta - 1 - (\Lambda_l/\lambda_l)R_2] + \lambda_l s_1'(R_1)\tilde{R}\cos 2\beta = -R_2 W_l^{(1)}. \tag{3.15}$$

From boundary condition (3.7), with allowance for geometric relations (1.4) and (1.5), we obtain the equalities

$$\lambda_s\Big(\cos\varphi\frac{\partial\theta_s}{\partial r_1} + \sin\varphi\frac{1}{R_1}\frac{\partial\theta_s}{\partial\alpha_1} + \frac{\Lambda_s}{\lambda_s}\theta_s\Big)\Big|_0 = W_s^{(0)} - \Lambda_s\theta_{s*},$$

$$\lambda_s\Big[\cos\varphi\Big(\frac{\partial^2\theta_s}{\partial r_1^2}A_1 + \frac{\partial^2\theta_s}{\partial r_1\,\partial\alpha_1} - \frac{1}{R_1}\frac{\partial\theta_s}{\partial\alpha_1}\Big) + \sin\varphi\Big(-\frac{1}{R_1^2}\frac{\partial\theta_s}{\partial\alpha_1}A_1 + \frac{1}{R_1}\frac{\partial^2\theta_s}{\partial r_1\,\partial\alpha_1}A_1$$

$$+\frac{1}{R_1}\frac{\partial^2\theta_s}{\partial\alpha_1^2} + \frac{\partial\theta_s}{\partial r_1}\Big) + \frac{\Lambda_s}{\lambda_s}\Big(\frac{\partial\theta_s}{\partial r_1}A_1 + \frac{\partial\theta_s}{\partial\alpha_1}\Big)\Big]\Big|_0 = \frac{R_1}{\cos\varphi}W_s^{(1)}, \quad A_1 = -R_1\tan\varphi,$$

wherefrom, using (3.8), (3.9), and (3.11), we have

$$\lambda_s t_0'(R_1)\cos\varphi = W_s^{(0)} - \Lambda_s\theta_{s*}; \tag{3.16}$$

$$\lambda_s\Big\{\Big[\sin\varphi(2 - P^{(s)}R_1\sin\varphi) - \frac{\Lambda_s}{\lambda_s}R_1\tan\varphi\Big]t_0'(R_1) + \frac{\cos 2\varphi}{\cos\varphi}t_1'(R_1)\Big\} = \frac{R_1}{\cos\varphi}W_s^{(1)}. \tag{3.17}$$

Substituting the expressions $t_0'(R_1)$ and $s_0'(R_1)$ given by (3.14) and (3.16) into (3.12), we obtain the first condition required for the unknown boundaries to be determined:

$$\frac{W_l^{(0)} - \Lambda_l\theta_{l*}}{\cos\beta} - \frac{W_s^{(0)} - \Lambda_s\theta_{s*}}{\cos\varphi} = \rho_s v_0 \tilde{Q}\sin\varphi.$$

The second condition can be found by substituting the value of $\lambda_l s_1'(R_1)$ found from (3.14) and (3.15) for $\cos 2\beta \neq 0$ and the value of $\lambda_s t_1'(R_1)$ found from (3.16) and (3.17) for $\cos 2\varphi \neq 0$ into expression (3.13). From here, we obtain

$$R_2 = \frac{1}{P^{(l)}}\frac{N}{D}, \tag{3.18}$$

where

$$N = \tilde{R}\cos 2\beta[\rho_s v_0\tilde{Q}\cos\varphi + (2\sin\varphi/\cos 2\varphi)(W_s^{(0)} - \Lambda_s\theta_{s*})] + (W_l^{(0)} - \Lambda_l\theta_{l*})(\tan\beta - 2\tilde{R}\sin\beta);$$

$$D = \frac{W_l^{(1)}}{P^{(l)}} + \frac{\cos 2\beta}{\cos 2\varphi}\frac{W_s^{(1)}}{P^{(l)}} - (W_l^{(0)} - \Lambda_l\theta_{l*})\tan\beta\Big(\sin\beta\cos\varphi + \frac{\Lambda_l}{\lambda_l P^{(l)}}\Big)$$

$$+ (W_s^{(0)} - \Lambda_s\theta_{s*})\frac{\cos 2\beta}{\cos 2\varphi}\Big(\sin^2\varphi\frac{P^{(s)}}{P^{(l)}} + \frac{\Lambda_s}{\lambda_s P^{(l)}}\tan\varphi\Big),$$

and $1/P^{(l)} = \lambda_l/(\rho_l c_l v_0)$ is a dimensional quantity that determines the linear scale. For instance, for silicon we have $\rho_l \simeq 2.5\text{g/cm}^3$, $c_l \simeq 0.91$ J/(g · K), and $\lambda_l \simeq 0.67$ J/(cm · sec · K), and for $v_0 = (2/3)\cdot 10^{-2}$ cm/sec, we obtain $1/P^{(l)} \simeq 50$ cm.

For $\cos 2\beta = 0$, the value of R_2 can be found from (3.14) and (3.15), whereas for $\cos 2\varphi = 0$ the curvature radius R_1 can be determined from (3.16) and (3.17). Note that these values can also be obtained from the general formula (3.18).

Below, we write the main terms of the expansion for the temperature of the polycrystal at the boundary γ and for the temperature of the melt surface (for $\varphi > 0$), which follow from (3.8), (3.14), and (3.16):

$$\theta_s\Big|_{\gamma} = \theta_s\Big|_{r_{1*}(\alpha_1)} = -\frac{W_s^{(0)} - \Lambda_s\theta_{s*}}{\lambda_s}\,\xi_s \tan\varphi + O(\xi_s^2),$$

$$\theta_l\Big|_{\gamma_l} = \theta_l\Big|_{r_2=R_2} = \frac{W_l^{(0)} - \Lambda_l\theta_{l*}}{\lambda_l}\,\xi_l \tan\beta + O(\xi_l^2).$$

Note that the required negative values of θ_s at the boundary γ are available only under the condition

$$W_s^{(0)} - \Lambda_s\theta_{s*} > 0, \tag{3.19}$$

for which the amount of heat released at the polycrystal surface exceeds the amount of heat that leaves it (in the main expansion term).

4. We rewrite the results obtained, introducing the dimensionless parameters for the energy quantities:

$$q_s^{(0)} = \frac{W_s^{(0)} - \Lambda_s\theta_{s*}}{\rho_s v_0 \tilde{Q}}, \quad q_l^{(0)} = \frac{W_l^{(0)} - \Lambda_l\theta_{l*}}{\rho_s v_0 \tilde{Q}}, \quad q_l^{(1)} = \frac{W_l^{(1)}}{P^{(l)}\rho_s v_0 \tilde{Q}}, \quad q_s^{(1)} = \frac{W_s^{(1)}}{P^{(l)}\rho_s v_0 \tilde{Q}}.$$

The dimensionless quantities $q_l^{(0)}$ and $q_s^{(0)}$ characterize the released heat minus the heat lost for heat exchange, immediately at the surface of the melt and at the solid surface, near the point O, respectively. The parameters $q_l^{(1)}$ and $q_s^{(1)}$ determine the rate of heat-release changes with distance from the triple point toward either the melt or the polycrystal.

Thus, we have the formulas

$$\tan\beta = \tilde{\rho}\tan\varphi, \tag{4.1}$$

$$\frac{q_l^{(0)}}{\cos\beta} - \frac{q_s^{(0)}}{\cos\varphi} = \sin\varphi, \tag{4.2}$$

which relate the angles φ and β with the energy parameters $q_l^{(0)}$ and $q_s^{(0)}$. From (3.19) and (4.2) it follows that, for a stationary process for $\varphi > 0$ to exist, the condition

$$0 < q_s^{(0)} < q_l^{(0)}$$

should be satisfied. Using (4.1), we can represent expression (4.2) in the form of a relation that yields the required value of $q_l^{(0)}$ for given $q_s^{(0)}$ and φ:

$$q_l^{(0)} = (1 + \tilde{\rho}^2\tan^2\varphi)^{-1/2}[q_s^{(0)}/\cos\varphi + \sin\varphi].$$

The relations presented below give the curvature radius R_1 of the interface between the phases and that of the free surface of the melt R_2, i.e., the shape of the initial melted film:

$$\tilde{R} = \frac{R_2}{R_1} = \frac{1}{1-\tilde{\rho}}\,\frac{\cos 2\beta}{\cos(\varphi + 2\beta)}\,\frac{\cos\varphi}{\cos\beta}; \tag{4.3}$$

$$R_2 = \frac{1}{P^{(l)}}\,\frac{\tilde{R}\cos 2\beta(\cos\varphi + q_s^{(0)} 2\sin\varphi/\cos 2\varphi) + q_l^{(0)}(\tan\beta - 2\tilde{R}\sin\beta)}{q_{ls}^{(1)} - q_l^{(0)}\tan\beta(\sin\beta\cos\varphi + \chi_l) + q_s^{(0)}\tilde{P}(\sin^2\varphi + \chi_s\tan\varphi)\cos 2\beta/\cos 2\varphi}, \tag{4.4}$$

where $\chi_l = \Lambda_l/(\lambda_l P^{(l)})$, $\chi_s = \Lambda_s/(\lambda_s P^{(s)})$, and $\tilde{P} = P^{(s)}/P^{(l)}$ are dimensionless parameters, and $q_{ls}^{(1)} = q_l^{(1)} + q_s^{(1)}\cos 2\beta/\cos 2\varphi$.

The dependence $\tilde{R}(\varphi)$ specified by relations (4.3) and (4.1) for fixed $\tilde{\rho} = 0.91$, which corresponds to silicon, is shown in Fig. 2. In the interval $0 < \varphi < \pi/2$, there is a segment $\varphi_1 < \varphi < \varphi_2$, where $\tilde{R}$ acquires negative values. [The end points of the segment are determined by the conditions $\cos(\varphi + 2\beta) = 0$ (from here, we have $\tan\varphi_1 = (2\tilde{\rho} + \tilde{\rho}^2)^{-1/2}$) and $\cos 2\beta = 0$ ($\tan\varphi_2 = 1/\tilde{\rho}$).] Negative values of $\tilde{R}$ correspond to a configuration that differs from the configuration depicted in Fig. 1b, since the curvature centers O_1 and O_2 lie on different sides of the boundary γ_s. (This statement rests on an independent solution built on a modified configuration; in this case, the solution procedure is analogous to that given above.) For the floating-zone

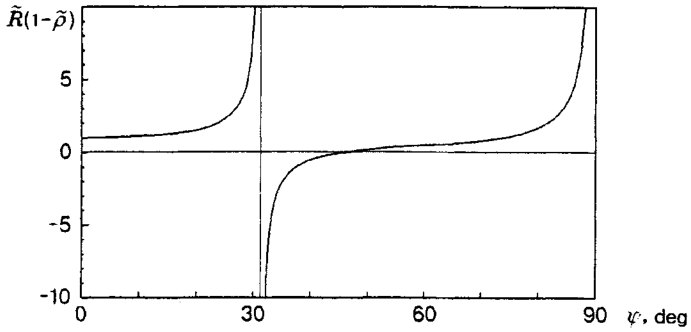

Fig. 2

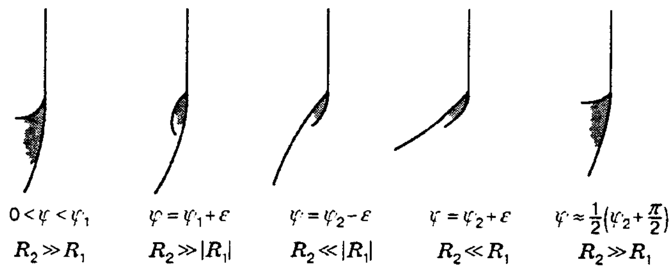

Fig. 3

technology, of importance is the case where the free surface of the melt has a boundary similar to that shown in Fig. 1b, i.e., $R_2 > 0$. [As follows from (4.4), for all φ, β, $q_s^{(0)}$, and $q_l^{(0)}$ that satisfy conditions (4.1) and (4.2), by means of the free parameters $q_l^{(1)}$ and $q_s^{(1)}$, the quantity R_2 can be adjusted so that its positiveness is ensured.) In this case, negative $\tilde{R}$ correspond to the geometry in which it is the center O_1 that lies on the other side of the boundary γ_s, i.e., outside the polycrystal. Thus, as follows from the dependence $\tilde{R}(\varphi)$, the initial part of the melted film may acquire one of the shapes shown in Fig. 3. (Here, it is the quantity $\varepsilon \ll 1$ that is positive.) The transition from one shape to another occurs at some critical angles φ, namely, at the above values φ_1 and φ_2.

It should be noted that only in a small vicinity of the value $\varphi = \varphi_2$ do we obtain $R_2 \ll |R_1|$. For the floating-zone technology, this condition is obviously a necessary one for the stability of the initial part of the melted film, which can be ensured by surface-tension forces. For $\varphi = \varphi_2$ ($\cos 2\beta = 0$), from (4.4) and (4.3) we have

$$R_{2*} = \frac{1}{P^{(l)}} \frac{q_l^{(0)}}{q_l^{(1)} - q_l^{(0)}((\sqrt{2}/2)\tilde{\rho}/(1+\tilde{\rho}^2)^{-1/2} + \chi_l)}.$$

Hence, for $R_{2*} \ll 1/P^{(l)}$ to be obtained, it is required that $q_l^{(1)} \gg q_l^{(0)}$ or, in other words, the heat-flux density at the surface of the melt should grow rather rapidly with distance from the triple point.

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