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EFFECT OF THERMOCAPILLARY FORCES ON THE INITIAL SECTION OF A MELT FILM

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The previous analysis of fields near the upper triple point of the floating-zone melting process is supplemented by the analysis of thermocapillary forces on the melt surface. It is shown that the effect of these forces is large in the general case, and a melt film with a macroscopic radius of curvature may be formed only if the temperature gradient over the melt surface and thermocapillary forces are small; in this case, the angular coordinates of the melt-film cross section are also small.

The geometric characteristics of the initial section of a stationary melt film formed in the floating-zone melting process were studied in [1]. Based on the analysis of local hydrodynamic and temperature fields near the triple point, relations between the angular coordinates and curvature radii of cross-sectional boundaries of the melt film and external heat fluxes are obtained. The hydrodynamic condition was the absence of shear stresses on the free surface of the film. It was found that different geometric configurations of the initial film section are possible under different thermal conditions.

Present paper is a continuation of [1] and contains results of studying the effect of thermocapillary forces. The same notation is used here, and the formulas borrowed from [1] are marked by an asterisk.

Thermal convection and thermocapillary forces taken into account, the global problem, generally speaking, is not divided into the hydrodynamic and thermal subproblems, as in [1], since the equation of motion has a term that describes buoyancy forces related to the temperature gradient. However, as noted in [1], hydrodynamic equations exert no effect on the local parameters of the melt film; thus, the latter are not affected by thermal convection. Thermocapillary forces affect one of the hydrodynamic boundary conditions on the free surface of the melt, which is related to shear stresses. Actually, this is the only difference induced by taking into account thermocapillary forces, since heat-conduction equations and all thermal boundary conditions remain unchanged; hence, the possibility of splitting the global problem remains valid.

The boundary condition for shear stresses on the free boundary of the melt taking into account thermocapillary forces has the following form [2]:

$$\Big(\sigma_{n\tau} - \frac{\partial\alpha}{\partial\tau}\Big)\Big|_{\gamma_l} = 0.$$

(The effect of the gas phase is neglected, as in [1].) Being projected onto a circle $r_2 = R_2$, this condition in the zero approximation reduces to

$$-\rho_l\nu\Big(\frac{1}{R_2^2}\,\frac{\partial^2\psi}{\partial\alpha_2^2} - \frac{\partial^2\psi}{\partial r_2^2} + \frac{1}{R_2}\,\frac{\partial\psi}{\partial r_2}\Big)\Big|_0 + \frac{d\alpha}{dT}\Big|_{T_0}\,\frac{\partial\theta_l}{\partial\alpha_2}\Big|_0\,\frac{1}{R_2} = 0. \qquad (1)$$

Here $d\alpha/dT\Big|_{T_0}$ is the derivative of the surface-tension coefficient with respect to the melting point and $(\partial\theta_l/\partial\alpha_2)\Big|_0$ is the derivative of the melt-surface temperature with respect to the angle α_2, taken at the

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point $\alpha_2 = 0$. The solution $\theta_l(r_1, \alpha_1)$ from [1] remains valid if thermocapillary forces are taken into account; from here, we obtain $\partial\theta_l(r_1, \alpha_1)/\partial\alpha_2 = (\partial\theta_l/\partial r_1)(\partial r_1/\partial\alpha_2) + (\partial\theta_l/\partial\alpha_1)(\partial\alpha_1/\partial\alpha_2)$ and, taking into account Eqs. (1.2)*, (1.3)*, (3.8)*, (3.11)*, and (3.14)*, we have

$$\frac{\partial\theta_l}{\partial\alpha_2}\Big|_0 = S_0'(R_1)(-R_2\sin\beta) = -\frac{W_l^{(0)} - \Lambda_l\theta_{l*}}{\lambda_l\cos\beta}\,R_2\sin\beta. \tag{2}$$

According to Eq. (2.13)*, the first term in brackets in Eq. (1) equals zero; the remaining terms are easily calculated from Eqs. (1.2)*, (1.3)*, (2.10)*, and (2.11)*. As a result, in view of (2), condition (1) is converted to the form

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

$$= \frac{1}{\rho_l\nu}\,\frac{d\alpha}{dT}\Big|_{T_0}\,\frac{W_l^{(0)} - \Lambda_l\theta_{l*}}{\lambda_l\cos\beta}\,R_2\sin\beta, \tag{3}$$

which differs from the corresponding relation in [1] only by the right part. Eliminating $\psi_0''(R_1)$ from Eqs. (3) and (2.15)*, we obtain the relation

$$\tilde{R}(1-\tilde{\rho})\cos(\varphi+2\beta) - \cos 2\beta\,\frac{\cos\varphi}{\cos\beta} + \frac{1}{\rho_l\nu}\,\frac{d\alpha}{dT}\Big|_{T_0}\,\frac{R_2}{v_0}\,\frac{W_l^{(0)} - \Lambda_l\theta_{l*}}{\lambda_l\cos\beta}\,\sin^3\beta = 0,$$

which is an extension of Eq. (2.16)* to the case of thermocapillary forces taken into account. Using the parameters $q_l^{(0)}$ and P^l (introduced in [1]) and the dimensionless parameter

$$\mathrm{Ma} = \frac{1}{\rho_l\nu}\Big(-\frac{d\alpha}{dT}\Big|_{T_0}\Big)\frac{\tilde{Q}}{c_l v_0}, \tag{4}$$

the relation considered acquires the form

$$\tilde{R}(1-\tilde{\rho})\cos(\varphi+2\beta) - \cos 2\beta\,\frac{\cos\varphi}{\cos\beta} - R_2P^{(l)}\tilde{\rho}q_l^{(0)}\mathrm{Ma}\,\frac{\sin^3\beta}{\cos\beta} = 0 \tag{5}$$

and, with thermocapillary forces taken into account, replaces the former "universal" dependence (4.3)*; relation (4.4)* remains unchanged. Thus, the system of linear equations (5) and (4.4)* for the dimensionless variables $\tilde{R}$ and $R_2P^{(l)}$ defined the sought radii of curvature. We rewrite Eq. (4.4)* in the form

$$R_2P^{(l)} = (\tilde{R}B + q_l^{(0)}\tan\beta)/D, \tag{6}$$

where

$$D = \Big(q_l^{(1)} + \frac{\cos 2\beta}{\cos 2\varphi}\,q_s^{(1)}\Big) - q_l^{(0)}\tan\beta(\sin\beta\cos\varphi + \chi_l) + q_s^{(0)}\tilde{P}\,\frac{\cos 2\beta}{\cos 2\varphi}\,(\sin^2\varphi + \chi_s\tan\varphi),$$

$$B = \frac{q_s^{(0)}}{\cos\varphi}\,\frac{\sin 2(\varphi-\beta)}{\cos\varphi} + \cos(\varphi+2\beta).$$

Resolving Eqs. (5) and (6) with respect to $\tilde{R}$ and $R_2P^{(l)}$, we obtain

$$R_2P^{(l)} = \frac{(1-\tilde{\rho})q_l^{(0)}\cos(\varphi+2\beta)\sin\beta + B\cos 2\beta\cos\varphi}{D(1-\tilde{\rho})\cos\beta\cos(\varphi+2\beta) - \tilde{\rho}\mathrm{Ma}\,q_l^{(0)}B\sin^3\beta}, \tag{7}$$

$$\tilde{R} = \frac{D\cos 2\beta(\cos\varphi/\cos\beta) + \tilde{\rho}\mathrm{M\ a}(q_l^{(0)}\sin^2\beta/\cos\beta)^2}{D(1-\tilde{\rho})\cos(\varphi+2\beta) - \tilde{\rho}\mathrm{Ma}\,(q_l^{(0)}/\cos\beta)B\sin^3\beta}.$$

It should be noted that the dimensionless parameter Ma (4) is large. (For example, under the conditions of [3], Ma is of the order of $5\cdot 10^6$ for silicon.) As a result, if the coefficients at Ma in formulas (7) are other than zero and finite, the sought quantities are of the order of $R_2P^{(l)} = O(1/\mathrm{Ma})$ and $\tilde{R} = O(1)$. Taking into account that $P^{(l)} \approx 1/50\ \mathrm{cm}^{-1}$ (see [1]), we find that R_2 and R_1 are of the order of $50(5\cdot 10^6)^{-1}$ cm $= 10^{-5}$ cm $= 0.1\ \mu$m.

We assume that the curvature radii of this microscopic size are of no interest in the process considered and find the conditions where these radii acquire macroscopic values of the millimeter range and the dimensionless parameter $R_2 P^{(l)}$ reaches, for instance, finite values

$$R_2 P^{(l)} \sim 10^{-2}. \tag{8}$$

For the relation $\tilde{R} = R_2/R_1 = O(1)$ to be valid, as it follows from (5), the following condition should be satisfied:

$$(q_l^{(0)}/\cos\beta)\sin^3\beta \ll 1. \tag{9}$$

It is satisfied in the following cases:

(a) $q_l^{(0)}/\cos\beta \ll 1$ for a finite $\sin^3\beta$;
(b) $\sin^3\beta \ll 1$ for a finite $q_l^{(0)}/\cos\beta$;
(c) both factors considered are small.

The case (a) is excluded by the condition $q_s^{(0)} > 0$ of existence of the solid phase at the boundary γ [condition (3.19)*]. Indeed, as follows from Eq. (4.2)*, we have $q_s^{(0)}/\cos\varphi = (q_l^{(0)}/\cos\beta) - \sin\varphi$; for $q_l^{(0)}/\cos\beta \ll 1$, the condition $q_s^{(0)} > 0$ is satisfied at $\sin\varphi < q_l^{(0)}/\cos\beta \ll 1$, i.e., at $\sin\beta \ll 1$. Thus, for finite $\tilde{R}$ to exist for Ma $\sim 10^6$, condition (9) is supplemented by the condition

$$\beta = \tilde{\rho}\varphi \ll 1. \tag{10}$$

Conditions (9) and (10) being satisfied, the coefficient at Ma in Eq. (7) is also small, and it is possible to reduce the effect of this large parameter to obtain values of $R_2 P^{(l)}$ that satisfy condition (8). Hence, if thermocapillary forces are taken into account, curvature radii of macroscopic dimensions arise only under condition (10). In this case, we have

$$\tilde{R} = \frac{1 + \tilde{\rho} Ma (R_2 P^{(l)})\tilde{\rho}^3\varphi^3}{1-\tilde{\rho}} + O(\varphi^2),$$

$$R_2 P^{(l)} = \frac{1 + (1-\tilde{\rho})(\tilde{\rho} q_l^{(0)} + 2q_s^{(0)})\varphi}{[q_l^{(1)} + q_s^{(1)} + (\tilde{\rho} q_l^{(0)}\chi_l + \tilde{P} q_s^{(0)}\chi_s)\varphi](1-\tilde{\rho}) - \tilde{\rho}\mathrm{Ma}\, q_l^{(0)}\beta^3} + O(\varphi^2).$$

(In these formulas, terms proportional to $\mathrm{Ma}\,\varphi^3$ are retained because of the large coefficient at Ma in them.) In the limit $\beta = \varphi = 0$, we have $\tilde{R}\Big|_{\varphi=0} = (1-\tilde{\rho})^{-1}$ and $R_2 P^{(l)}\Big|_{\varphi=0} = [(q_l^{(1)} + q_s^{(1)})(1-\tilde{\rho})]^{-1}$, i.e., the curvature radius of the melt surface R_2 is an order of magnitude greater than the corresponding quantity R_1 for the phase interface, since $\tilde{\rho} \approx 0.9$, and R_2 depends on the velocity of heat-flux increase on the melt surface with distance from the triple point. To obtain $R_2 P^{(l)}$ of the order of 10^{-2}, the value of $q_l^{(1)} + q_s^{(1)}$ should be of the order of 10^3. It should be noted that the melt film with these limiting angular coordinates, apparently, is not formed. This is a consequence of the formulas for the temperature of a polycrystal at the boundary γ and the melt-surface temperature obtained from the solutions of [1] and valid for $\beta = \tilde{\rho}\varphi \ll 1$:

$$\begin{aligned} \theta_s\Big|_{\gamma} &= (\rho_s v_0 \tilde{Q} R_1/\lambda_s)(-q_s^{(0)}\varphi\alpha_1 + (q_s^{(0)}/2)\alpha_1^2) + O(\alpha_1^3), \\ \theta_l\Big|_{\gamma_l} &= (\rho_s v_0 \tilde{Q} R_2/\lambda_l)(-q_l^{(0)}\beta\alpha_2 + (q_l^{(0)}/2)(\tilde{R}-1)\alpha_2^2) + O(\alpha_2^3). \end{aligned} \tag{11}$$

For $\beta = \varphi = 0$, we have

$$\theta_s\Big|_{\gamma} = (\rho_s v_0 \tilde{Q} R_1/\lambda_s)(q_s^{(0)}/2)\alpha_1^2 + O(\alpha_1^3), \quad \theta_l\Big|_{\gamma_l} = (\rho_s v_0 \tilde{Q} R_2/\lambda_l)(q_l^{(0)}/2)(\tilde{R}-1)\alpha_2^2 + O(\alpha_2^3), \tag{12}$$

and condition (4.2)* reduces to the requirement $q_l^{(0)} = q_s^{(0)}$. Since the polycrystal-surface temperature should decrease with distance from the triple point, and the melt-surface temperature should be greater than the melting point, the variables (12) should satisfy the following conditions:

$$\theta_s\Big|_{\gamma} < 0 \quad \text{for} \quad \alpha_1 > 0, \qquad \theta_l\Big|_{\gamma_l} > 0 \quad \text{for} \quad |\alpha_2| > 0. \tag{13}$$

The solutions of (12) in combination with the requirement $q_l^{(0)} = q_s^{(0)}$ contradict the above conditions. Hence, the limiting angles $\varphi = \beta = 0$ cannot be obtained, and the angles $0 < \varphi \ll 1$ and $\beta = \tilde{\rho}\varphi$ are formed, i.e., the melt film begins from a small nonzero angle of the wedge. The main terms of expansions (11) show that conditions (13) are satisfied for $q_s^{(0)} > 0$ and $q_l^{(0)} = q_s^{(0)} + \varphi > 0$. In fact, the result obtained means that curvature radii of macroscopic dimensions arise only in the case of a low temperature on the melt surface, when thermocapillary forces are small.

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