CALCULATION OF THE THERMAL STRESSES IN A SOLIDIFYING CRUST

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The equation for the thermoelastic displacement potential in the quasi-steady approximation is refined by taking the body force potential into account. The equation is solved for bodies of simple shape. The optimal law of solidification ensuring minimum temperature stresses in the crust is determined for an infinite slab.

The equation of thermoelasticity written in displacements for the quasi-steady approximation has the form [1]

$$\mu\nabla^2 \mathbf{U} + (\lambda + \mu)\,\mathrm{grad\,div}\,\mathbf{U} - (3\lambda + 2\mu)\alpha\ \mathrm{grad}\,T + \mathbf{F} = 0. \tag{1}$$

When this equation is used to solve problems of thermoelasticity associated with the heating or cooling of bodies without phase transformations and in the absence of external forces, the body force vector **F** is taken equal to zero. Neglecting it leads to a paradoxical result: the calculations give nonzero thermal stresses at the crystallization from. At the same tim [2], new layers forming dimensions corresponding to the crust of the ingot at the time of their formation. Therefore there should be no stresses at the crystallization front.

As will be seen in what follows, taking the body force vector into account in Eq. (1) makes it possible to eliminate this paradox.

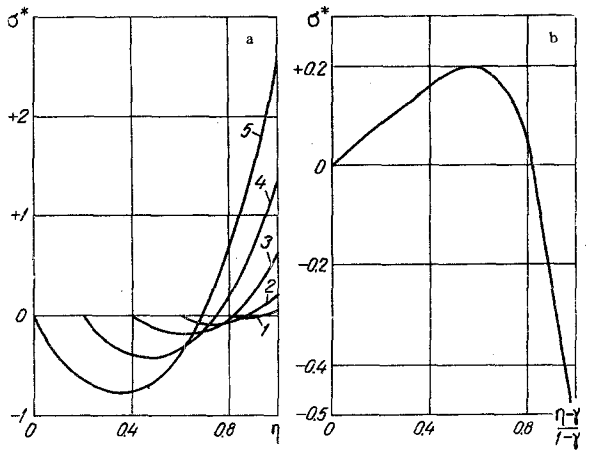

Fig. 1. Stress distribution over thickness of crust for an infinite slab solidifying according to the laws; a) $\xi = 1 - 2\mathrm{Fo}$ (the figures on the curves represent Fo × 10); b) $\xi = 1 - \sqrt{\mathrm{Fo}}$.

Using (with minor changes) the method developed in [3, 4], we introduce the thermoelastic displacement potential Φ satisfying the condition

$$\mathbf{U} = \mathrm{grad}\,\Phi. \tag{2}$$

We also introduce the quantity $\varphi(x_i)$ proportional to the body force potential and depending only on the coordinates x_i:

$$\mathbf{F} = -(3\lambda + 2\mu)\alpha\,\mathrm{grad}\,\varphi. \tag{3}$$

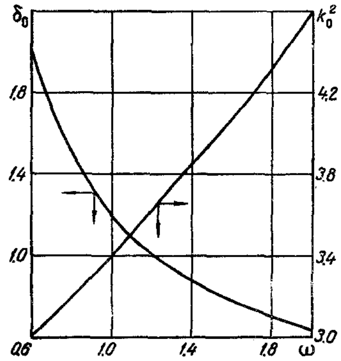

Fig. 2. Parameters k_0 and δ_0 of the optimum law of solidification as functions of the average rate of solidification ω_{av}.

Then from Eq. (1)

$$(\lambda + 2\mu)\,\mathrm{grad}\,(\nabla^2\Phi) = (3\lambda + 2\mu)\,\alpha\,\mathrm{grad}\,(T + \varphi). \tag{4}$$

Integrating with respect to the coordinates x_i and assuming that α = const, we obtain

$$\nabla^2\Phi = \frac{3\lambda + 2\mu}{\lambda + 2\mu}\,\alpha\,[T + \varphi(x_i) + D(\tau)], \tag{5}$$

where D is a constant of integration which can depend only on time τ.

For the stresses σ_{ik} we have [3]

$$\sigma_{ik} = 2\mu\left(\frac{\partial^2\Phi}{\partial x_i \partial x_k} - \nabla^2\Phi\,\delta_{ik}\right). \tag{6}$$

As boundary conditions it is convenient to assign the following:

1) at the outer surface of the body

$$U_i|_{\Pi} \equiv \left.\frac{\partial\Phi}{\partial x_i}\right|_{\Pi} = f_i(x_k, \tau), \tag{7}$$

2) on the contour of the solidification front

$$\sigma_{ik}|_{\Gamma} = 0. \tag{8}$$

In the particular case of bodies of simple shape (infinite slab, infinite cylinder, sphere) Eq. (5) may be simplified and written in the following dimensionless form:

$$\frac{\partial^2 P}{\partial \eta_1^2} + \frac{m}{\eta_1} \frac{\partial P}{\partial \eta_1} = b[\theta + \psi(\eta_1) + \gamma(\text{Fo})], \tag{9}$$

$$1 \geqslant \eta_1 \geqslant \zeta(\text{Fo}).$$

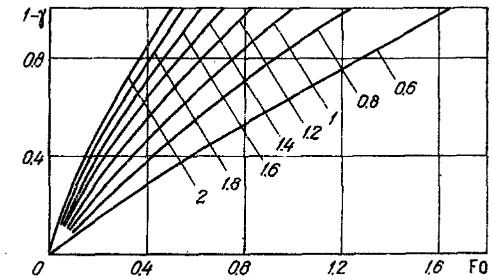

Fig. 3. Optimal law of crust growth in an infinite slab. Figures on the curves are values of ω_{av}.

The expressions for the dimensionless stresses are

$$\sigma_{11}^* = -\frac{1}{b} \frac{m}{\eta_1} \frac{\partial P}{\partial \eta_1}, \tag{10}$$

$$\sigma_{22}^* = -\frac{1}{b}\left[\frac{m(m-1)}{2} \frac{1}{\eta_1} \frac{\partial P}{\partial \eta_1} + \frac{\partial^2 P}{\partial \eta_1^2}\right], \tag{11}$$

$$\sigma_{33}^* = -\frac{1}{b}\left[\frac{m(3-m)}{2} \frac{1}{\eta_1} \frac{\partial P}{\partial \eta_1} + \frac{\partial^2 P}{\partial \eta_1^2}\right]. \tag{12}$$

As the boundary condition at the outer surface it is convenient to take the zero-displacement condition

$$\left.\frac{\partial P}{\partial \eta_1}\right|_{\eta_1=1} = 0. \tag{13}$$

Using (10)–(12), we can write the condition of zero stresses at the crystallization front in the form

$$\left.\frac{\partial P}{\partial \eta_1}\right|_{\eta_1=\zeta} = 0, \tag{14}$$

$$\left.\frac{\partial^2 P}{\partial \eta_1^2}\right|_{\eta_1=\zeta} = 0. \tag{15}$$

Integrating (9) with respect to η_1 with allowance for condition (14), we obtain

$$\frac{\partial P}{\partial \eta_1} = \frac{b}{\eta_1^m} \int_\zeta^{\eta_1} [\theta + \psi(\eta_1) + \gamma(\text{Fo})]\, \eta_1^m d\eta_1. \tag{16}$$

From (9)

$$\frac{\partial^2 P}{\partial \eta_1^2} = -\frac{mb}{\eta_1^{m+1}} \int_\zeta^{\eta_1} [\theta + \psi(\eta_1) + \gamma(\text{Fo})]\, \eta_1^m d\eta_1 + b[\theta + \psi(\eta_1) + \gamma(\text{Fo})]. \tag{17}$$

To satisfy condition (15) it is enough that

$$\gamma(\text{Fo}) = -\theta_\Gamma - \psi(\zeta). \tag{18}$$

Here, $\theta\Gamma$ is the dimensionless crystallization temperature, a constant, and by definition

$$\psi(\zeta) = \psi(\eta_1)|_{\eta_1=\zeta}.$$

Finally, from (13), using (16), we obtain

$$\int_\zeta^1 [\theta + \psi(\eta_1) + \gamma(\text{Fo})]\, \eta_1^m d\eta_1 = 0. \tag{19}$$

Using (18), we get

$$\int_\zeta^1 [\psi(\eta_1) - \psi(\zeta)]\, \eta_1^m d\eta_1 = \int_\zeta^1 (\theta_\Gamma - \theta)\, \eta_1^m d\eta_1. \tag{20}$$

Differentiating (20) with respect to ζ and using the fact that θ may be regarded as a function of η_1 and ζ, we have

$$\frac{1}{m+1}(1 - \zeta^{m+1}) \frac{d\psi(\zeta)}{d\zeta} = \int_\zeta^1 \frac{\partial\theta}{\partial\zeta} \eta_1^m d\eta_1$$

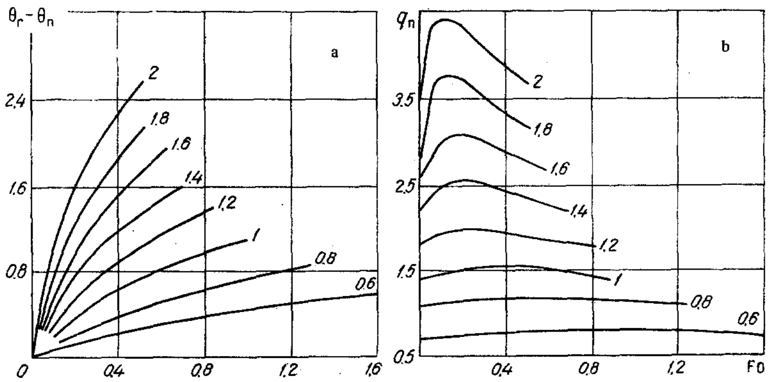

Fig. 4. Thermal conditions at outer surface of slab ensuring solidification according to the optimum law (figures on curves are values of ω_{av}): a) variation with time of the difference of the dimensionless crystallization and surface temperatures $\vartheta_\Gamma - \eta_{II}$; b) variation in time of the heat flow from the surface $q_{II} = -\partial\theta/\partial\eta_1|_{II}$.

and

$$\psi(\zeta) = (m+1)\int_1^{\zeta} \frac{d\zeta}{1-\zeta^{m+1}} \int_{\zeta}^{1} \frac{\partial\theta}{\partial\zeta}\,\eta_1^m\, d\eta_1 + N, \tag{21}$$

Where N is an arbitrary constant of integration. From the last expression, substituting η_1 for the upper limit of integration ζ into the second integral, by virtue of the fact that ψ depends on only one argument, we obtain

$$\psi(\eta_1) = (m+1)\int_1^{\eta_1} \frac{d\zeta}{1-\zeta^{m+1}} \int_{\zeta}^{1} \frac{\partial\theta}{\partial\zeta}\,\eta_1^m\, d\eta_1 + N. \tag{22}$$

Using (18), (21), and (22), we have

$$\theta + \psi(\eta_1) + \gamma(\mathrm{Fo}) = \theta - \theta_\Gamma + (m+1)\int_{\zeta}^{\eta_1} \frac{d\zeta}{1-\zeta^{m+1}} \int_{\zeta}^{1} \frac{\partial\theta}{\partial\zeta}\,\eta_1^m\, d\eta_1. \tag{23}$$

For the dimensionless stresses we obtain

$$\sigma_{11}^* = \frac{m}{\eta_1^{m+1}} \int_{\zeta}^{\eta_1} \Big\{\theta_\Gamma - \theta - (m+1) \times \int_{\zeta}^{\eta_1} \frac{d\zeta}{1-\zeta^{m+1}} \int_{\zeta}^{1} \frac{\partial\theta}{\partial\zeta}\,\eta_1^m\, d\eta_1\Big\}\,\eta_1^m\, d\eta_1, \tag{24}$$

$$\sigma_{22}^* = \frac{3-m}{2}\,\sigma_{11}^* + \theta_\Gamma - \theta - (m+1) \times \int_{\zeta}^{\eta_1} \frac{d\zeta}{1-\zeta^{m+1}} \int_{\zeta}^{1} \frac{\partial\theta}{\partial\zeta}\,\eta_1^m\, d\eta_1, \tag{25}$$

$$\sigma_{33}^* = \frac{m-1}{2}\,\sigma_{11}^* + \theta_\Gamma - \theta - (m+1) \times \int_{\zeta}^{\eta_1} \frac{d\zeta}{1-\zeta^{m+1}} \int_{\zeta}^{1} \frac{\partial\theta}{\partial\zeta}\,\eta_1^m\, d\eta_1. \tag{26}$$

From the written expressions it follows that the stresses in the ingot crust are equal to zero if

$$\theta - \theta_\Gamma + (m+1)\int_{\zeta}^{\eta_1} \frac{d\zeta}{1-\zeta^{m+1}} \int_{\zeta}^{1} \frac{\partial\theta}{\partial\zeta}\,\eta_1^m\, d\eta_1 = 0.$$

However, in accordance with (23), this condition is equivalent to the requirement

$$\theta = -\psi(\eta_1) - \gamma(\mathrm{Fo}).$$

This means that the temperature must be expressed as the sum of two functions, one of which depends only on the coordinate η_1, and the other only on time Fo. Such an expression for the temperature does not satisfy the heat-conduction equation and hence cannot be realized. Therefore the solidifying process must be accompanied by the appearance of temperature stresses. The authors of [2] arrive at a similar conclusion.

For an infinite slab (m = 0) from (24)–(26)

$$\sigma_{11}^* = 0,$$

$$\sigma_{22}^* = \sigma_{33}^* = \sigma^* = \theta_\Gamma - \theta - \int_{\zeta}^{\eta_1} \frac{d\zeta}{1-\zeta} \int_{\zeta}^{1} \frac{\partial\theta}{\partial\zeta}\, d\eta_1. \tag{27}$$

We assume that solidification proceeds according to a linear law:

$$\zeta = 1 - \omega\,\mathrm{Fo}. \tag{28}$$

Using the Stefan solution [5] of the problem for the temperature field

$$\theta = \theta_\Gamma + 1 - \exp\left[\omega(\eta_1 - \zeta)\right], \tag{29}$$

we obtain

$$\sigma^* = \exp\left[\omega(\eta_1-\zeta)\right] - 1 - \int_{\omega(1-\eta_1)}^{\omega(1-\zeta)} \frac{1}{y}(\exp y - 1)\,dy = \exp\left[\omega(\eta_1-\zeta)\right] - 1 - \ln\left[(1-\zeta)/(1-\eta_1)\right] + \mathrm{Ei}^*\left[\omega(1-\eta_1)\right] - \mathrm{Ei}^*\left[\omega(1-\zeta)\right], \tag{30}$$

where

$$\mathrm{Ei}^*(z) = \int_{-\infty}^{z} \frac{1}{y}\exp y\,dy = C + \ln z + \sum_{n=1}^{\infty} \frac{z^n}{n\cdot n!}.$$

When $\eta_1 = 1$ (on the surface of the slab), using the series representation of the functions Ei*(z) and exp(z), we obtain

$$\sigma^*|_{\eta_1=1} = \sum_{n=1}^{\infty}\left(1-\frac{1}{n}\right)\frac{\left[\omega(1-\zeta)\right]^n}{n!}. \tag{31}$$

Since $\omega(1-\zeta) \geq 0$, it follows that $\sigma^*|_{\eta_1=1} \geq 0$.

Thus, for a linear law of solidification the stresses at the surface of an infinite slab are always tensile (plus sign).

We will specify a more general law of solidification:

$$\zeta = 1 + \delta - \sqrt{\delta^2 + k^2\mathrm{Fo}}. \tag{32}$$

When $\delta = 0$ it goes over into the familiar "square-root law"

$$\zeta = 1 - k\sqrt{\mathrm{Fo}}, \tag{33}$$

and when $\delta \to \infty$, $k^2 - \omega\delta$ it yields the linear law

$$\zeta = 1 - \omega\,\mathrm{Fo}.$$

It is easy to verify that the solution of the inverse problem of solidification with given law of solidification (32) will be

$$\theta = \theta_\Gamma - \frac{\sqrt{\pi}}{2}\,k\exp\frac{k^2}{4}\left\{\mathrm{erf}\left(\frac{k}{2}\right) - \right.$$

$$-\operatorname{erf}\left(\frac{k}{2}\ \frac{1-\eta_1+\delta}{1-\zeta+\delta}\right)\Bigg\}. \qquad (34)$$

When $\delta = 0$ this expression goes over into the Stefan solution [6] for law of solidification (33), and when $\delta \to \infty$, $k^2 - 2\omega\delta$ from (34) we obtain solution (29).

Using (34), from (27) we obtain we obtain

$$\sigma^* = \sqrt{\pi}\ \frac{k}{2} \exp\left(\frac{k^2}{4}\right) \times$$

$$\times\left[\operatorname{erf}\left(\frac{k}{2}\right) - \operatorname{erf}\left(\frac{k}{2}\ \frac{1-\eta_1+\delta}{1-\zeta+\delta}\right)\right] +$$

$$+\int\limits_{\zeta}^{\eta_1} \frac{1}{1-\zeta} \times$$

$$\times\left\{1-\exp\left[\frac{k^2}{4}\left(1-\frac{\delta^2}{(1-\zeta+\delta)^2}\right)\right]\right\} d\zeta. \qquad (35)$$

When $\delta = 0$ this expression is easily integrated:

$$\sigma^* = \sqrt{\pi}\ \frac{k}{2} \exp\left(\frac{k^2}{4}\right)\times$$

$$\times\left[\operatorname{erf}\left(\frac{k}{2}\right) - \operatorname{erf}\left(\frac{k}{2}\ \frac{1-\eta_1}{1-\zeta}\right)\right] +$$

$$+\left[\exp\left(\frac{k^2}{4}\right)-1\right]\ln\frac{1-\zeta_1}{1-\zeta}. \qquad (36)$$

Recalling that $\exp(k^2/4) - 1 > 0$ when $k \neq 0$ and that the first term in (36) is a bounded quantity, we obtain

$$\sigma^*|_{\eta_1=1} \to -\infty.$$

Thus, at the surface of an infinite slab solidifying according to law (33) infinitely large compressive stresses (with a minus sign) develop.

The nature of the stress distribution over the thickness of a slab solidifying according to laws (28) and (33) is illustrated in Fig. 1.

It should be noted that at a certain ratio of the parameters k^2 and δ solidification according to intermediate law (32) makes it possible to obtain a minimum (in a certain sense) state of stress in the crust.

As the parameter charcterizing the stress level in the slab we will take the stress at the outer surface ($\eta_1 = 1$) at the end of solidification ($\zeta = 0$). Then the minimum, in this sense, state of stress of the crust is determined by a zero value of the parameter $\sigma^*|_{\eta=1;\zeta=0}$.

We introduce the average rate of growth of solid phase $\omega = 1/\mathrm{Fo}^*$, which characterizes the rate of solidification for some law of crust growth. From (32), considering that $\zeta(\mathrm{Fo}^*) = 0$, we obtain

$$k^2 = \omega_{\mathrm{Av}}(1+2\delta). \qquad (37)$$

Using (35), we can write the condition of f minimum state of stress of the crust in the form

$$\frac{\sqrt{\pi}}{2}\sqrt{\omega_{\mathrm{av}}(1+2\delta)} \times$$

$$\times\exp\left[\frac{\omega_{\mathrm{av}}}{4}(1+2\delta)\right]\left\{\operatorname{erf}\left[\frac{1}{2}\sqrt{\omega_{\mathrm{av}}(1+2\delta)}\right] -\right.$$

$$\left.-\operatorname{erf}\left[\frac{\delta}{2(1+\delta)}\sqrt{\omega_{\mathrm{Av}}(1+2\delta)}\right]\right\} =$$

$$=\int\limits_0^1 \frac{1}{y}\left\{\exp\left[\omega_{\mathrm{av}}\, y\, \frac{(1+2\delta)(y+2\delta)}{4(y+\delta)^2}\right]-1\right\} dy. \qquad (38)$$

From this equation the optimum values of the parameter $\delta = \delta_0$ were determined numerically as a function of the given rate of solidification ω_{av} (Fig. 2). The same figure also contains the optimum values of k_0 calculated from (37)

Hence we find the optimum law of solidification for a given rate of solidification ω_{av} (Fig. 3)

The law of variation of the surface temperature or heat flow from the surface in time ensuring an optimum law of solidification can be obtained from (34). The results of the corresponding calculations are presented in Fig. 4.

NOTATION

X_i ($i = 1, 2, 3$) denote variable coordinates; $\tilde{X}$ is the characteristic dimension of the body; τ is time; $\mathbf{U}$ is the displacement vector; U_i -its components along the coordinate axes ($i = 1, 2, 3$); E is the modulus of elasticity; ν is Poisson's ratio; T is temperature; T_Γ is the crystallization temperature; α is the linear coefficient of thermal expansion; F is the body-force vector; Φ is the thermoelastic displacement potential; $\tilde{\Phi}$ is the fixed value of thermoelastic displacement potential; $D(\tau)$ is an arbitrary function of time obtained by integrating with respect to the coordinates; σ_{ik} is the stress tensor; δ_{ik} is the Kronecker delta (equal to 0 when $i \neq k$ and to 1 when $i = k$); m is the shape factor equal to 0 for the slab, 1 for the cylinder, 2 for the sphere; a is the thermal diffusivity; c is the specific heat; ρ is the specific latent heat of crystallization; $\lambda = \nu E/(1+\nu)(1-2\nu)$; $\mu = E/2(1+\nu)$ an Lamé constants; $\varphi(x_i)$ is the potential of the vector $\mathbf{F}/3\lambda + 2\mu)\alpha$, $\eta_i = x_i/\tilde{X}$ is a dimensionless variable coordinate; ζ is a dimensionless coordinate of crystallization front; $\mathrm{Fo} = at/\tilde{X}^2$ is dimensionless time; Fo^* is the dimensionless duration of total solidification; $P = \Phi/\tilde{\Phi}$ is the dimensionless thermoelastic displacement potential; $b = \Phi/\tilde{X}^2$; $\sigma^*_{ik}(\lambda + 2\mu)c/2\mu(3\lambda + 2\mu)\alpha\rho$ is the dimensionless stress tensor; $\theta = Tc/\rho$ is the dimensionless variable temperature; $\vartheta_\Gamma = T_\Gamma c/\rho$ is the dimensionless crystallization temperature; $\psi(\eta_1) = \varphi c/\rho$; $\lambda(\mathrm{Fo}) = Dc/\rho$.

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