ANALYTIC AND NUMERICAL SOLUTION OF FUSION AND CRYSTALLIZATION PROBLEMS OF A THIN METAL SURFACE LAYER

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The process of fusion and subsequent crystallization is examined for a thin surface layer of a massive specimen subjected to an impulsive thermal load.

Fusion of metals by powerful thermal fluxes permits different microstructures to be obtained for thin surface layers, including fine-crystalline and amorphous [1, 2]. Obtaining a definite surface layer microstructure is due primarily to the thermophysical aspects of the action of radiation on a metal. Determination of the temperature field during the melting and subsequent crystallization is a nonlinear problem even in the one-dimensional case with constant thermophysical material characteristics because of the presence of a moving phase interface. The temperature distribution in the liquid i = 1 and the solid phase i = 2 is described by the equations

$$\frac{\partial^2 T_i}{\partial x^2} = \frac{1}{a_i} \frac{\partial T_i}{\partial t}. \tag{1}$$

During the action of a pulse $t \leqslant \tau$ on a surface x = 0 a constant heat flux of density q is given

$$-\lambda_1 \left(\frac{\partial T_1}{\partial x} \right)\Big|_{x=0} = q. \tag{2}$$

The following heat balance holds on the phase interface

$$-\lambda_1 \left(\frac{\partial T_1}{\partial x} \right)\Big|_{x=y} = Q_0 \rho \frac{dy}{\partial t} - \lambda_2 \left(\frac{\partial T_2}{\partial x} \right)\Big|_{x=y}. \tag{3}$$

We have the temperature field

$$T_2(x,\ t_0) = T_{\text{к}} \left\{ \exp\left(-\frac{x^2}{4at_0} \right) - \frac{1}{2} \left(\frac{\pi}{at_0} \right)^{1/2} \operatorname{erfc} \left(\frac{x}{2\sqrt{at_0}} \right) \right\} \tag{4}$$

at the initial instant of melting t_0($T_2(0,\ t_0) = T_k$) in the solid phase. The temperature of the phase interfacial surface is constant during melting and equals T_k and there is no heat flux at infinity

$$T_1|_{x=y} = T_2|_{x=y} = T_{\text{к}},\ \frac{\partial T_2}{\partial x}\Big|_{x=\infty} = 0,\ T_2|_{x=\infty} = 0. \tag{5}$$

After termination of the melting the velocity of interphasal boundary motion depends on the instantaneous temperature T_c on the crystallization front, which varies in time because of the variable supercooling [5, 6]

$$\begin{gathered} T_1|_{x=y} = T_2|_{x=y} = T_c(t), \\ \frac{dy}{\partial t} = -\nu_0 d \exp(-U/kT_c)\,[1 - \exp(-\Delta G/kT_c)]. \end{gathered} \tag{6}$$

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Difficulties associated with satisfying the stability criterion occurs in solving the melting problem by difference methods [2, 4, 7]. We use the method of solving ablation problems based on the method of lines [4] and we extend it to two-phase domains. We go over to the dimensionless quantities $F_i=T_i/T_\text{к}$, $\Phi=T_c/T_\text{к}$, $Q=Q_0/cT_\text{к}$, $\xi=t/\tau$, $\xi_0=t_0/\tau$, $\Delta G/kT_\text{к}=h(1-\Phi)$, $u=U/kT_\text{к}$, $\varkappa=x/l$, $\zeta=y/l$, $l=2\sqrt{ma\tau}$, where m is the normalization constant introduced for convenience in solving problems on an electronic computer so that the characteristic depth of heat penetration $2\sqrt{at}$ would not exceed l which permits taking the solution of the problem (1)-(6) from the interval $0\leqslant x\leqslant\infty$ over to the interval $0\leqslant x\leqslant 1$. We introduce the coordinates r and p as follows $r=\varkappa/\zeta$ and $p=(1-\varkappa)/(1-\zeta)$. This substitution determines the position of the boundary $\varkappa=\zeta$ at the point r = p = 1, and the boundary coordinates $\varkappa$ = 0 and $\varkappa$ = 1 go over into r = 0 and p = 0. In conformity with the method of lines, we divide the planes r, ξ and p, ξ into N subdomains by means of the lines $r=n\Delta r$ and $p=n\Delta p$ $(n=0,\ 1,\ \ldots,\ N,\ \Delta r=\Delta p=1/N)$. Writing the spatial derivatives with respect to the new coordinates r and p in difference form, and the time derivatives along the corresponding lines, we arrive from (1)-(6) at the following system

$$\frac{\partial F_{1,n}}{\partial\xi}=\frac{1}{4m}\,\frac{a_1N^2}{a_2\zeta^2}\,(F_{1,n+1}-2F_{1,n}+F_{1,n-1})+\frac{n}{2\zeta}\,\frac{d\zeta}{d\xi}\,(F_{1,n+1}-F_{1,n-1}),\tag{7}$$

$$\frac{\partial F_{2,n}}{\partial\xi}=\frac{1}{4m}\left(\frac{N}{1-\zeta}\right)^2(F_{2,n+1}-2F_{2,n}+F_{2,n-1})\quad-\frac{n}{2(1-\zeta)}\,\frac{d\zeta}{d\xi}\,(F_{2,n+1}-F_{2,n-1}),\tag{8}$$

$$\frac{d\zeta}{d\xi}=-\frac{N}{4Qm}\left\{\frac{\Phi-F_{2,N-1}}{1-\zeta}+\frac{\lambda_1}{\lambda_2\zeta}(\Phi-F_{1,N-1})\right\}\ ,\tag{9}$$

$$F_{1,-1}=F_{1,1}+\frac{2\zeta\lambda_2}{N\lambda_1}\sqrt{\frac{\pi m}{\xi_0}}\,H(1-\xi),\tag{10}$$

$$F_{1,N}=F_{2,N}=\Phi(\xi),\ F_{2,-1}=F_{2,1}=F_{2,0}=0,\tag{11}$$

$$F_2(p,\ \xi_0)=\exp\left\{-\frac{(1-p)\,2m}{\xi_0}\right\}-\sqrt{\frac{\pi m}{\xi_0}}\,(1-p)\operatorname{erfc}\left\{(1-p)\sqrt{\frac{m}{\xi_0}}\right\},\tag{12}$$

$$\exp\left(-\frac{u}{\Phi}\right)\left\{1-\exp\left[-h\,\frac{1-\Phi}{\Phi}\right]\right\}=\frac{N}{Qm\nu_0d}\sqrt{\frac{a}{\tau}}\left\{\frac{\Phi-F_{2,N-1}}{1-\zeta}+\frac{\lambda_1}{\lambda_2\zeta}(\Phi-F_{1,N-1})\right\}\cdot\tag{13}$$

For Φ = 1 the equations (7)-(12) describe the melting process. At the time ξ_0 a very thin liquid phase layer $\zeta_0\ll 1$ appears. The temperature distribution in this layer can be considered linear $F_1(r,\ \xi_0)=1+\zeta_0\lambda_2(1-r)\sqrt{\pi/\xi_0}/\lambda_1$. Given ζ_0 or the overheating $\Delta F_0=F_1(0,\ \xi_0)-1=\lambda_2\zeta_0\sqrt{\pi/\xi_0}/\lambda_1$, we obtain the initial temperature distribution in the liquid phase. We took ΔF_0 = 10^{-2}-10^{-3} in performing the numerical computations. Termination of the pulse occurs at the time ξ_1 = 1, however, the melting continues until the time ξ_2 corresponding to the disappearance of the velocity of the phase interface motion $\zeta(\xi_2)=0$. The crystallization rate for $\xi>\xi_2$ is governed by the quantity $\Phi(\xi)$, which we can find by using (13). The solution of the system of differential equations (7)-(9) with conditions (10)-(13) taken into account is carried out on the ES-1060 electronic computer.

We find the analytic solution of the problem (1)-(6) by the method of Biot [4]. The temperature distribution for $\xi_0\leqslant\xi\leqslant 1$ is approximated as follows

$$F=\begin{cases}F_1=f\Big/\left\{1+\dfrac{\varkappa}{\zeta}(f-1)\right\},\ 0\leqslant\varkappa\leqslant\zeta,\\[2ex] F_2=\left(1-\dfrac{\varkappa-\zeta}{s}\right)^2,\ \zeta\leqslant\varkappa\leqslant\zeta+s.\end{cases}\tag{14}$$

Here $f=F_1|_{\varkappa=0}$, $\zeta+s$ is the depth of heat penetration in the metal in the time ξ . In place of the heat-conduction equation (1) we write the variational equation and energy conservation law

$$4\dot{\zeta}+\frac{13}{7}\dot{s}=\frac{21}{8}\frac{1}{s}, \tag{15}$$

$$\beta\frac{f\zeta}{f-1}\ln f+Q_1\zeta+\frac{s-s_0}{3}=\frac{1}{4}\sqrt{\frac{\pi}{\xi_0}}(\xi-\xi_0), \tag{16}$$

where $\beta=c_1\rho_1/c_2\rho_2$, $Q_1=1-\beta+Q$, $s_0=0{,}75\sqrt{\pi\xi_0}$ is the depth of heat penetration at the time ξ_0. The boundary condition (2) takes the form

$$\zeta=\frac{\lambda_1}{\lambda_2}\sqrt{\frac{\xi_0}{\pi}}f(f-1), \tag{17}$$

while taking (17) into account the Eq. (3) on the interphasal boundary becomes

$$4Q\dot{\zeta}=\frac{1}{f^2}\sqrt{\frac{\pi}{\xi_0}}-\frac{2}{s}. \tag{18}$$

The boundary conditions (5) are satisfied automatically by selecting the temperature distribution in the form (14) and the initial condition (4) is approximated with good accuracy by the expression $(1-\varkappa/s_0)^2$.

We are interested in the melting modes for which evaporation from the surface can be neglected, i.e., when f is substantially below the melting point. We will consider the overheating $\delta = f - 1 < 1$ and we represent s in the form $s = s_0(1 + w)$. We substitute (17) into (16) and limiting ourselves to square terms in δ, we obtain

$$\left(\frac{3}{2}\beta+Q_1\right)\delta^2+(\beta+Q_1)\delta-\frac{1}{3}\sqrt{\frac{\pi}{\xi_0}}\left\{\frac{3}{4}\sqrt{\frac{\pi}{\xi_0}}(\xi-\xi_0)-s_0w\right\}=0. \tag{19}$$

Combining (15) and (18) we have

$$\frac{1}{Q}\frac{1}{(1+\delta)^2}\sqrt{\frac{\pi}{\xi_0}}+\frac{13}{7}s_0\dot{w}=\left(\frac{21}{8}+\frac{2}{Q}\right)\frac{1}{s_0(1+w)}. \tag{20}$$

The combined solution of (19) and (20) is performed by successive approximations by first linearizing (20) as follows

$$\frac{1}{Q}\frac{1}{(1+\bar{\delta}_j)^2}\sqrt{\frac{\pi}{\xi_0}}+\frac{13}{7}s_0\dot{w}_j=\left(\frac{21}{8}+\frac{2}{Q}\right)\frac{(1-w_j)}{s_0}, \tag{21}$$

$$\bar{\delta}_j=\frac{1}{(1-\xi_0)}\int_{\xi_0}^{1}\delta_j(\xi)\,d\xi. \tag{22}$$

Here δ_j is the magnitude of the overheating in the j-th approximation. In the zeroth approximation $\delta_0 = 0$. We find from (21)

$$w_j=\frac{b_j}{B}\{1-\exp[-B(\xi-\xi_0)]\}, \tag{23}$$

where

$$B=\frac{7}{13}\left(\frac{21}{8}+\frac{2}{Q}\right)\frac{1}{s_0^2};\ b_j=B-\frac{7}{13}\frac{1}{Qs_0}\sqrt{\frac{\pi}{\xi_0}}\frac{1}{(1+\bar{\delta}_j)^2}.$$

To simplify the calculation $\bar{\delta}_j$ we introduce the mean velocity $v_{mj} = w_j(\xi_1)/\eta_1$, $\eta_1 = 1 - \xi_0$, then $w_j(\xi) = v_{mj}(\xi - \xi_0)$ and substituting this last relationship into (19), we obtain

$$\delta_{j+1}=\frac{A}{2}\{[1+g_j(\xi-\xi_0)]^{1/2}-1\}, \tag{24}$$

where

$$A=\frac{\beta+Q_1}{1{,}5\beta+Q_1},\ g_j=\frac{4}{3}\sqrt{\frac{\pi}{\xi_0}}\frac{1{,}5\beta+Q_1}{(\beta+Q_1)^2}\left(\frac{3}{4}\sqrt{\frac{\pi}{\xi_0}}-s_0v_{mj}\right).$$

Rewriting (22) with (24) taken into account, we have

$$\overline{\delta}_{j+1} = \frac{A}{2}\left\{\frac{2}{3g_j\eta_1}[(1+g_j\eta_1)^{3/2}-1]-1\right\}. \tag{25}$$

Therefore, by finding g_0 in the zeroth approximation, we obtain δ_1 from (25). We then determine g_1 and continue this process until the necessary accuracy $|(\overline{\delta}_{j+1}-\overline{\delta}_j)/\overline{\delta}_j|\ll 1$ is achieved. From (24) we find the final value for $\delta(\xi)$, (17) yields the position of the phase boundary $\xi(\xi)$, and (14) yields the temperature distribution.

Melting continues a certain time $\eta_2 = \xi_2 - 1$ after termination of the pulse because of the energy stored in the liquid phase. The surface temperature f is hence reduced. At the time ξ_2 the velocity of interphasal boundary motion vanishes and melting ceases. Then $\dot{\zeta}$ and s can be described for $1\leqslant\xi\leqslant\xi_2$ in the form

$$\dot{\zeta} = \dot{\zeta}_1[1-(\xi-1)/\eta_2], \quad s = s_1(1+\alpha),$$

where

$$\alpha = (\xi-1)(\omega_0 - 14\dot{\zeta}/13s_1), \quad \omega_0 = 7(21/8s_1 - 2\dot{\zeta}_1)/13s_1;$$

$$\eta_2 = \beta\zeta_1\left\{\frac{\delta_m}{2}s_1\left(1-\frac{\delta_m}{3}\right)-\frac{2}{3}\frac{\zeta_1\lambda_2}{\lambda_1}\right\}\Big/\left\{\dot{\zeta}_1\left[\frac{s_1}{2}(\beta+Q_1)+\right.\right.$$
$$\left.\left.+\frac{2}{3}\frac{\beta\zeta_1\lambda_2}{\lambda_1}\right]+\frac{\omega_0}{2}\left[\frac{2}{3}s_1-\beta\zeta_1\delta_m(1-\delta_m/3)\right]\right\}, \quad \delta_m = f(\xi_1)-1.$$

We approximate the temperature distribution during crystallization $\xi\geqslant\xi_2$ as follows

$$F = \begin{cases} F_1 = f-(f-\Phi)\varkappa^2/\zeta^2, & 0\leqslant\varkappa\leqslant\zeta, \\ F_2 = \Phi\{1-(\varkappa-\zeta)/s\}^2, & \zeta\leqslant\varkappa\leqslant\zeta+s. \end{cases} \tag{26}$$

The variational equation, energy conservation law, and heat-balance equation take the form

$$13\dot{s}/7s + 15\dot{\Phi}/14\Phi + 4\dot{\zeta}/s = 21/8s^2, \tag{27}$$

$$\beta\frac{\zeta}{3}(\Phi+2f)+\Phi s/3 + Q_1\zeta = \frac{1}{4}\sqrt{\pi/\xi_0}, \tag{28}$$

$$\lambda_1(f-\Phi)/\lambda_2\zeta = 2Q\dot{\zeta} + \Phi/s. \tag{29}$$

Introducing the mean cooling rate at the crystallization front $\Phi = 1 - \varepsilon\eta$, $\eta = \xi-\xi_2$ for small overcoolings, we obtain from (6)

$$\dot{\zeta} = -\nu_1\varepsilon u\eta\exp(-\varepsilon u\eta), \tag{30}$$

where

$$\nu_1 = \nu_0 d\sqrt{\tau/ah}\exp(-u)/2u.$$

Integrating (30), we find

$$\zeta = \zeta_2 - \zeta_\text{к}\{1-(1+u\varepsilon\eta)\exp(-u\varepsilon\eta)\}. \tag{31}$$

It follows from (31) that for $\zeta_\text{к}/\zeta_2<1\,(\zeta_\text{к}=\nu_1/\varepsilon u)$ the interphasal boundary does not emerge on the surface, i.e., either a thin amorphous layer or a finely crystalline coating is formed because of homogeneous generation. The rate of heterogeneous crystallization grows with the pulse duration.

In the case $\zeta_\text{к}/\zeta_2<1$ we introduce the mean velocity of interphasal boundary motion v by using (31) as follows

$$\int_0^\infty(1+u\varepsilon\eta)\exp(-u\varepsilon\eta)\,d\eta = \int_0^{\eta_0}(1-\eta/\eta_0)\,d\eta, \tag{32}$$

where $\eta_0 = \zeta_к/v$ yields the time of crystallization termination $\xi_c = \xi_2 + \eta_0$, $\zeta = \zeta_2 - v\eta$. From (32) we have $\eta_0 = 4\zeta_к/\nu_1$, i.e., $v = \nu_1/4$. Writing the change in surface temperature in the form $f = f_2 - \gamma\eta$, we determine the time ξ_3, at which equilibration of the temperature in the liquid phase occurs $f(\xi_3) \simeq \Phi(\xi_3) : \xi_3 = \xi_2 + \eta_3$, where $\eta_3 = \zeta_2/s_2(\gamma - \varepsilon)$. Rewriting the system (27)-(29), we find

$$\gamma = \omega_2/s_2 + \varepsilon\omega_3, \; s = s_2 + v_2\eta, \tag{33}$$

$$\varepsilon = \left\{v_1 - \frac{\nu_1\beta}{4}(1 + 2f_2 + 3Q_1/\beta) - \beta\,\frac{2\omega_2\zeta_2}{s_2}\right\} \Big/ \left\{\zeta_2\beta(1 + 2\omega_3) + \frac{11}{26}\,s_2\right\}, \tag{34}$$

where

$$\omega_1 = \frac{15}{26}s_2, \; v_1 = \frac{7}{13}\left(\frac{21}{8s_2} + \nu_1\right), \; v_2 = v_1 + \omega_1\varepsilon;$$

$$\omega_2 = \frac{v_1\zeta_2}{s_2} + \frac{\nu_1}{4}\left[1 + 2Qs_2\left(\frac{v_1\zeta_2}{s_2} - \frac{\nu_1}{4}\right)\right];$$

$$\omega_3 = 1 + \left(\frac{41}{26}\frac{\zeta_2}{s_2} + \frac{15}{52}Q\nu_1\zeta_2\right)\lambda_2/\lambda_1.$$

For $\xi \geqslant \xi_c$, $\dot{\zeta}(\xi) = 0$ and the combined solution of (27) and (28) yields

$$\Phi = \Phi_c s_c/s, \; \Phi_c = \Phi(\xi_c) = 1 - 4/u, \; s_c = s(\xi_c) = s_2 + v_2\eta_0; \tag{35}$$

$$s = \left\{s_c^2 + \frac{147}{22}(\xi - \xi_c)\right\}^{1/2}. \tag{36}$$

Thus, for $\zeta_к/\zeta_2 < 1$ an amorphous or fine-crystalline coating of thickness $\zeta_c = \zeta_2 - \zeta_к$ is formed on the surface.

In the case of rapid crystallization $\zeta(\xi_c) = 0$, $\eta_c/\xi_c = (\xi_c - \xi_2)/\xi_c \ll 1$ the velocity of phase interface motion (30) can be written as $\dot{\zeta} = -\nu_1 u\varepsilon\eta$ and the solution of the problem (27)-(29) becomes

$$\zeta = \zeta_2\{1 - (\eta/\eta_c)^2\}, \; \eta_c = (\zeta_2/\nu_1\varepsilon u)^{1/2}; \tag{37}$$

$$s = s_2 + (s_c - s_2)\eta/\eta_c, \; s_c = \frac{3}{4}\sqrt{\frac{\pi}{\xi_0}} \Big/ (1 - \varepsilon\eta_c); \tag{38}$$

$$\gamma = \zeta_2/s_2\eta_c + \varepsilon, \; \varepsilon = \frac{4\nu_1 u}{\zeta_2}\left\{\frac{1 - \lambda_1 \ln 2/\lambda_2}{1 + 2Q\nu_1 u s_2}\right\}^2. \tag{39}$$

For $\xi \geqslant \xi_c$ the depth of heat penetration is described by (36) while the surface temperature equals $f = 3\sqrt{\pi/\xi_0}/4s$.

Results of computations on the basis of the analytical expressions are presented by dashes in Figs. 1-4 while the numerical solution executed on the ES 1060 is presented by solid lines for steel [5]: $\lambda_1 = \lambda_2 = 0{,}233$ W/cm·℃, $c_1 = c_2 = 0{,}672$ J/g·℃, $a_1 = a_2 = 0{,}0463$ cm^2/sec, $Q_0 = 27$ J/g, $T_к = 1400$ ℃, $\nu_0 = 10^{13}$ c^{-1}, $d = 3\cdot 10^{-8}$ cm, $U = 30\,000$ cal/mole.

The velocity of the interphasal boundary motion (Fig. 1a) and the rate of surface heating (Fig. 2) are maximal at the initial instant of melting and equal, respectively, $\dot{y}_0 = q(1 - 8/3\pi)/\rho Q_0$ and $(\partial T/\partial t)|_{t=t_0} = q\dot{y}_0/\lambda_1$. Where the position of the curves corresponding to the melting are determined by the quantity $t_0/\tau \sim 1/q^2\tau$ in Fig. 1a and 2, i.e., by the combination of radiation parameters q and τ. The growth of q or τ results in an increase in the depth of melting and the surface temperature at the time of pulse termination (Fig. 3). Still a certain time $\tau < t < t_2$ after pulse termination melting proceeds (see Fig. 1) but the surface temperature diminishes abruptly (Fig. 2). The cooling rate during crystallization decreases, exactly as the heating during melting, with both depth and time (Fig. 2). However, the growth of the quantity q results in an increase in the heating rate but a diminution in the cooling rate. The surface heating rate at the beginning of melting is independent of τ, while the cooling rate at the time of pulse termination drops abruptly with the growth of $t_0/\tau = 0.5$,

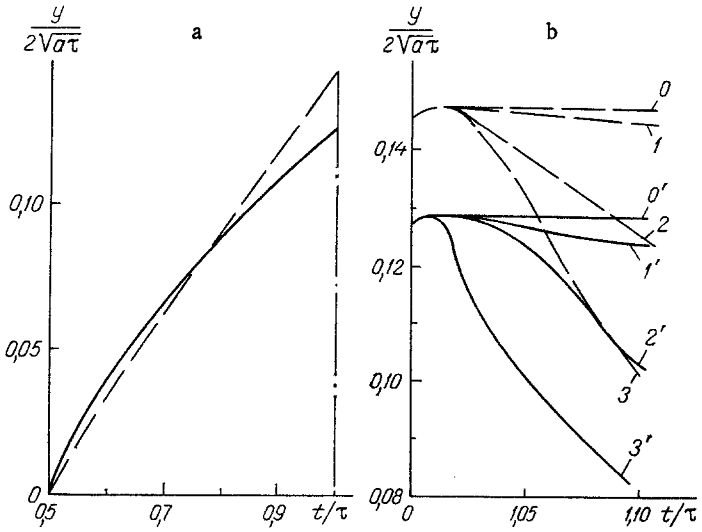

Fig. 1. Position of the phase interface: a) during action of the pulse $t_0 \leqslant t \leqslant \tau$; b) after pulse termination $t > \tau$, 0 and 0' — $\tau = 10^{-6}$ sec; 1 and 1' — 10^{-4} sec; 2 and 2' — 10^{-2} sec; 3 and 3' — 1 sec.

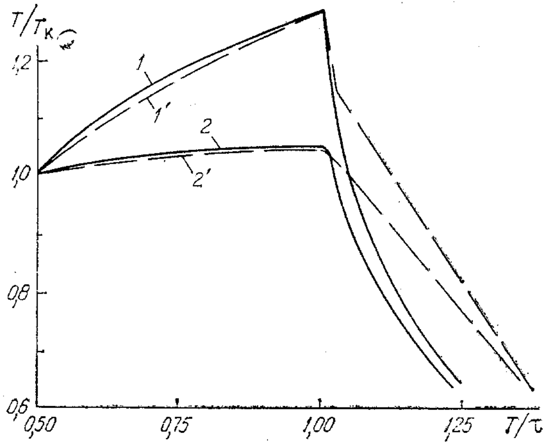

Fig. 2. Temperature change on the surface (1 and 1') and in the depth of the melt x/y = 0.8 (2 and 2') during melting and crystallization ($\tau = 10^{-6}$ sec).

where this latter exceeds the former substantially in magnitude, thus, by an order for (Fig. 4). Consequently, the position of the phase interface during crystallization depends strongly on the pulse duration (see Fig. 1b). As it diminishes the cooling rate grows and heterogeneous crystallization encloses a still smaller part of the melted layer, thus for $\tau = 10^{-6}$ sec it is practically nonexistent.

The graphs presented display a good correspondence between the analytical expressions obtained by the Biot method and the numerical solution of the problem on the electronic computer. However, utilization of the averaging (22) in solving the melting problem (14)-(18) by the Biot method as well as giving the initial condition in the liquid phase in the numerical solution on an electronic computer does not permit consideration of the most initial stage of the melting, the emergence of the velocity of the phase boundary motion on the maximal value $\dot{y}_0$. The initial stage of the melting was examined in [8] on the basis of an approximate variational solution of the ablation problem, however its description can be developed by starting from the exact solution of the heat conduction equation [9]

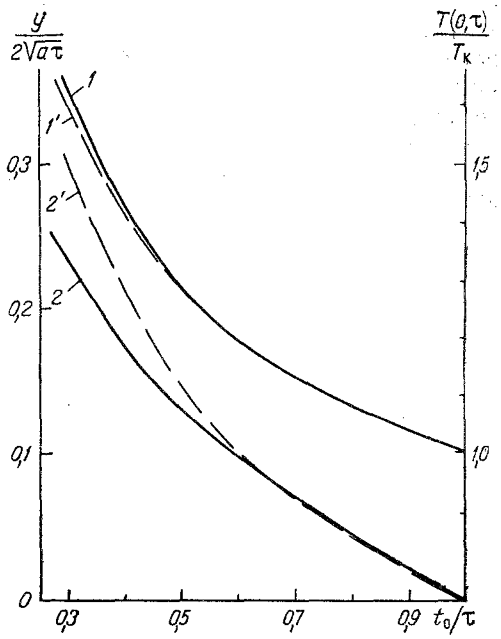

Fig. 3. Surface temperature (1 and 1') and depth of melting (2 and 2') at the time of pulse termination.

$$T(x,\ t)=\frac{q}{\lambda}\left\{2\sqrt{\frac{at}{\pi}}\exp\left(-\frac{x^2}{4at}\right)-x\,\mathrm{erfc}\left(\frac{x}{2\sqrt{at}}\right)-\right.$$
$$-2\sqrt{\frac{a(t-\tau)}{\pi}}\exp\left(-\frac{x^2}{4a(t-\tau)}\right)+x\,\mathrm{erfc}\left(\frac{x}{2\sqrt{a(t-\tau)}}\right)- \tag{40}$$
$$\left.-\frac{Q_0}{2c\sqrt{\pi a}}\int\limits_{t_0}^{t}\frac{\dot{y}(\xi)\,d\xi}{\sqrt{t-\xi}}\left\{\exp\left[-\frac{(x-y(\xi))^2}{4a(t-\xi)}\right]+\exp\left[-\frac{(x+y(\xi))^2}{4a(t-\xi)}\right]\right\}\right\}.$$

The expression (40) is an equation to find the position of the interphasal boundary for x = y(t). Let us introduce the dimensionless quantities: $\theta=(t-t_0)/t_0$, $\psi=(t-\tau)/t_0$, $\eta=(t-t_2)/t_0$, $z=y/2\sqrt{at_0}$; θ, ψ, η, $z\ll 1$, and we seek the quantity z governing the position of the phase interface in the form of the series $z=\varphi_0/Q+\varphi_1/Q^2+\varphi_2/Q^3+\ \ldots$

In the melting case we have from (40) to the accuracy of linear terms in z

$$\sqrt{1+\theta}-\sqrt{\pi}\,z-\frac{2Q}{\sqrt{\pi}}\int\limits_0^\theta\frac{\dot{z}(\xi)\,d\xi}{\sqrt{\theta-\xi}}=1.$$

Collecting coefficients of identical powers of Q^{-1} we obtain a system of integrodifferential equations

$$\sqrt{1+\theta}-\frac{2}{\sqrt{\pi}}\int\limits_0^\theta\frac{\dot{\varphi}_0 d\xi}{\sqrt{\theta-\xi}}=1,$$
$$\varphi_{i-1}+\frac{2}{\pi}\int\limits_0^\theta\frac{\dot{\varphi}_i d\xi}{\sqrt{\theta-\xi}}=0,\ i=1,\ 2. \tag{41}$$

We carry out the solution of the system (41) by using the Laplace–Carson integral transform [10]. After appropriate manipulations we obtain from the first equation of the system

$$\varphi_0(\theta)=\frac{1}{2\sqrt{\pi}}\left\{(\theta+1)\ \mathrm{arctg}\sqrt{\theta'}-\sqrt{\theta}\right\}\simeq\frac{\theta^{3/2}}{3\sqrt{\pi}}\,. \tag{42}$$

Applying the Laplace–Carson transform to the second equation of the system i = 1 and using the solution (42) for φ_0, we find

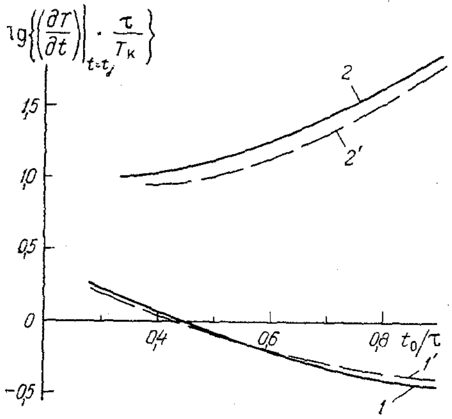

Fig. 4. Surface heating $t_j = t_0$ (1 and 1') and cooling $t_j = t_2$ (2 and 2') rates.

$$\varphi_1(\theta) = -\frac{\sqrt{\pi}}{6}\left\{(\theta+1)(\sqrt{1+\theta}-1) - \frac{\theta}{2}\right\} \simeq -\frac{\sqrt{\pi}}{16}\theta^2.$$

All subsequent terms φ_i are found analogously by using the value φ_{i-1}, obtained from the preceding step. We have for the first terms of the series expansion of $z(\theta)$

$$z(\theta) = \frac{1}{Q}\frac{\theta^{3/2}}{3\sqrt{\pi}} - \frac{1}{Q^2}\frac{\sqrt{\pi}}{16}\theta^2 + \frac{1}{Q^3}\frac{\sqrt{\pi}}{30}\theta^{5/2} - \frac{\pi^{3/2}}{192Q^4}\theta^3 + \ldots \tag{43}$$

Using the first term in the expansion (43), we find the duration of the initial stage of melting $\theta_H = [\pi(1-8/3\pi)/2]^2 \simeq 0{,}056$ from the conditions $z(\theta_H) = z_0$, $z_0 = \sqrt{\pi}(1-8/3\pi)/4Q$. For $\theta < \theta_H$ the series (43) converges sufficiently rapidly (the ratio of the absolute value of the fourth term to the first is 0.084), i.e., by limiting ourselves here to the first term in (43), we can speak about the law of interphasal boundary motion $z \sim \theta^{3/2}$. The initial stage of the melting acquires physical as well as mathematical meaning when the depth of melting in the interval $\theta_H(\theta_1 > \theta_H)$ substantially exceeds the interatomic spacing $d/y_0 \leqslant 0{,}1$, $y_0 = z(\theta_H)2\sqrt{at_0}$. In other words, the radiation power should be sufficient for the melting $q > q_c$, $q_c = T_K\lambda\sqrt{\pi/a\tau}/2$ is the energy flux density for which the melting temperature on the surface is reached at the time of pulse termination but does not exceed the maximal value $q < q_m$, $q_m = \lambda T_K\theta_H^{3/2}/30dQ$, otherwise the emergence of the velocity of phase interface motion at the magnitude $\dot{z}_0$ would occur so rapidly that the depth of melting after this time would be microscopic. The inequality $q_c < q_m$ yields the necessary condition for macroscopicity of the melting in the initial stage $\tau > \tau_m$, $\tau_m = (15dQ)^2\pi/\theta_H^3 a$, for steel $q_m \simeq 10^7$ W/cm^2 and $\tau_m \simeq 10^{-8}$ sec. If $\theta_1 < \theta_H$, i.e., $q < q_c(1+0{,}5\theta_H)$, then the melting process is described by the law $z \sim \theta^{3/2}$, and the depth of melting $z_1 = z(\theta_1)$ is macroscopic for $q > q_c(1+0{,}5\alpha)$, $\alpha = (15dQ\sqrt{\pi/a\tau})^{2/3}$. The condition $\theta_H > \alpha$ is equivalent to $\tau > \tau_m$

The position of the phase boundary during melting after pulse termination $\tau < t < t_2$ is determined according to (40) by the equation

$$1 = \sqrt{1+\theta} - \sqrt{\psi}\exp\left(-\frac{z^2}{\psi}\right) - \sqrt{\pi}z\,\mathrm{erf}\left(\frac{z}{\sqrt{\psi}}\right) - \frac{2Q}{\sqrt{\pi}}\int_0^{\theta_1}\frac{\dot{z}d\xi}{\sqrt{\theta-\xi}} - \frac{\theta}{\sqrt{\pi}}\int_0^{\psi}\frac{\dot{z}(\xi)d\xi}{\sqrt{\psi-\xi}}\left\{\exp\left[-\frac{(z(\psi)-z(\xi))^2}{\psi-\xi}\right] + \exp\left[-\frac{(z(\psi)+z(\xi))^2}{\psi-\xi}\right]\right\}. \tag{44}$$

Since an increase in the depth of melting after pulse termination is insignificant $(z_2-z_1)/z_1 \ll 1$, $z_2 = z(t_2)$, $z_1 = z(\tau)$ then to find φ_0 from (44) we can write

$$1 = \sqrt{1+\theta} - \sqrt{\psi}\exp\left(-\frac{z_1^2}{\psi}\right) - \frac{2}{\sqrt{\pi}}\int_0^{\theta_1}\frac{\dot{\varphi}_0 d\xi}{\sqrt{\theta-\xi}} - \frac{1}{\sqrt{\pi}}\int_0^{\psi}\frac{\dot{\varphi}_0 d\xi}{\sqrt{\psi-\xi}}. \tag{45}$$

Using (42) for φ_0 and rewriting the first integral in (45) and then applying the Laplace—Carson transform, we find

$$\varphi_0 = \varphi_0(\theta_1) + \frac{\theta_1^{1/2}\psi}{2\sqrt{\pi}} - \frac{\theta_1\psi^{3/2}}{3\sqrt{\pi}} - \frac{\sqrt{\pi}}{2}\left\{(\psi - 2z_1^2)\,\mathrm{erfc}\left(\frac{z_1}{\sqrt{\psi}}\right) + 2z_1\sqrt{\frac{\psi}{\pi}}\exp\left(-\frac{z_1^2}{\psi}\right)\right\}. \tag{46}$$

At the time of termination of the melting $t_2 = \tau + \psi_2 t_0$, $\dot{\varphi}_0(\psi_2) = 0$. Rewriting (46), we obtain an equation to determine ψ_2

$$\frac{\theta_1^{1/2}}{\pi}\left(1 - \frac{\theta_1^{1/2} z_1}{\omega}\right) = \mathrm{erfc}\,\omega + \frac{2}{\sqrt{\pi}}\,\omega\exp(-\omega^2), \tag{47}$$

where $\omega = z_1/\sqrt{\psi_2}$. The value of ω can be found graphically. Thus, for steel with $\theta_1 = 0.1$ we have $z_1 = 1.2 \cdot 10^{-2}$ and we find $\psi_2 = 4{,}7 \cdot 10^{-5}$ from (47). Since $\psi_2 \ll \theta_1 \ll 1$, then to find $\varphi_i(\psi)$, $i = 1, 2, \ldots$, there is no need to solve the complex integrodifferential equation (44) but by using the conditions $\varphi_i(\psi_2) = 0$ we can write $\varphi_i = \varphi_i(\theta_1)(1 - \psi/\psi_2)$, from which $\varphi_i(\psi) = \varphi_i(\theta_1) + \varphi_i(\theta_1)\psi(1 - \psi/2\psi_2)$, $i = 1, 2, \ldots$. To find $\varphi_0(\eta)$ crystallization $t > t_2$ we have from (40)

$$1 = \sqrt{1+\theta} - \sqrt{\psi} - \frac{2}{\sqrt{\pi}}\int_0^{\theta_1}\frac{\dot{\varphi}_0 d\xi}{\sqrt{\theta-\xi}} - \frac{1}{\sqrt{\pi}}\int_0^{\psi_2}\frac{\dot{\varphi}_0 d\xi}{\sqrt{\psi-\xi}} - \frac{2}{\sqrt{\pi}}\int_0^{\eta}\frac{\dot{\varphi}_0 d\xi}{\sqrt{\eta-\xi}}.$$

This equation is solved by an operator method by using the relationships (42) and (46), consequently we obtain

$$\varphi_0 = \varphi_0(\psi_2) - \frac{1}{2\sqrt{\pi}}\{(\eta + \psi_2)\,\mathrm{arctg}\,(\eta/\psi_2)^{1/2} - (\eta\psi_2)^{1/2}\}. \tag{48}$$

In the initial stage of crystallization $\eta < \psi_2$ we have from (48)

$$\varphi_0 = \varphi_0(\psi_2) - \eta^{3/2}/3(\pi\psi_2)^{1/2}.$$

The time of termination of crystallization $t_3 = t_2 + t_0\eta_3$ corresponds to the emergence of the phase boundary on the surface, i.e., $\varphi_0(\eta_3) = 0$. Rewriting (48) with $\eta_3 \gg \psi_2$ taken into account we obtain $\eta_3 = 4\varphi_0(\psi_2)/\sqrt{\pi} \approx 4\varphi_0(\theta_1)/\sqrt{\pi} = 4\theta_1^{3/2}/3\pi$. Since $\theta_1 < 1$, then $\eta_3 < \theta_1$, i.e., crystallization proceeds at a higher velocity than melting. For $\varphi_i(\eta)$, $i = 1, 2, \ldots$, by taking $\varphi_i(\eta_3) = 0$ into account we can write $|\varphi_i| = |\varphi_i(\psi_2)|(1 - \eta/\eta_3)$. To find the surface temperature $T(0, t)$ during the melting and subsequent crystallization we set $x = 0$ in (40) and going over to dimensionless parameters with $z \ll 1$ and $\psi_2 \ll \theta_1 \ll 1$, $x = 0$ taken into account we obtain

$$f = 1 + \sqrt{\pi}\,z\,\mathrm{erf}\,(z/\sqrt{\psi}) - \sqrt{\psi}\,(1 - \exp(-z^2/\psi)). \tag{49}$$

For $t_0 < t < \tau$ we have $f = 1 + \sqrt{\pi}\,z$ from (49) by limiting ourselves to the first term in the expansion of z: $f = 1 + \theta^{3/2}3Q$ or returning to dimensional quantities

$$T(0, t) = T_\text{к} + \frac{8q^3c}{3Q_0T_\text{к}\lambda^3}\left[\frac{a(t-t_0)}{\pi}\right]^{3/2}, \tag{50}$$

which describes the change in temperature in the initial stage of melting.

NOTATION

T_i, temperature (the subscript i = 1 refers to the fluid and i = 2 to the solid state of the material); T_k, melting point; T_c, temperature on the crystallization front; x, coordinate measured from the surface deep into the material; t, time from the beginning of action of the impulse; τ, pulse duration; q, flux density; a_i, thermal diffusivity; λ_i, heat conductivity; c_i, specific heat; $a = a_2$; $\lambda = \lambda_2$; $c = c_2$; ρ, material density; Q_0, heat of fusion per unit mass; y, position of the phase interface; $t_0 = (T_\text{к}\lambda/2q)^2\pi/a$, time of the beginning of melting; ν_0, mean frequency of the thermal vibrations; d, characteristic dimension per atom; U, activation energy of atom displacement in the fluid; k, Boltzmann constant; $\Delta G = L(1 - T_c/T_\text{к})$, change in thermodynamic potential during passage of the atom from the liquid into the solid phase; L, heat of fusion per atom; $h = L/kT_\text{к}$; $\Phi = T_c/T_\text{к}$; F_i, f, Φ, $\varkappa$, r, p, ξ, θ, ψ, η, ζ, z, s, δ, dimensionless parameters that describe F_i, temperature distribution; f and Φ, surface temperature and the phase interface; $\varkappa$, r, p, spatial coordinate; ξ, θ, ψ, η, time; z, ζ, position of the interphasal boundary;

s, depth of heat penetration measured from the phase interfacial surface; δ, liquid overheating on the surface above the boiling point; φ_i, components of the expansion of z in powers of Q^{-1}; $Q=Q_0/cT_{\text{к}}$; $H(1-\xi)$, Heaviside function; $\zeta_j=\zeta(\xi_j)$; $s_j=s(\xi_j)$; $f_j=f(\xi_j)$; ξ_j, instants of time; beginning of melting j = 0, pulse termination j = 1, melting j = 2, crystallization j = c, temperature equilibration in the liquid phase j = 3, $\varepsilon=\varepsilon_m\tau/T_{\text{к}}$; $\gamma=\gamma_m\tau/T_{\text{к}}$; ε_m and γ_m are mean cooling rates of the interphasal and external surfaces.

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A PHYSICAL MODEL FOR SUBLIMATION OF A CONTINUOUS MATERIAL IN AN UNSTABLE DOMAIN

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A physical method is developed for the sublimation process during conductive energy delivery, which permits determination of the configuration and velocity advancement of the phase separation boundaries.

Known methods of analyzing processes associated with the solid—vapor phase transition are based on models in which the position of all points of the interphasal boundary is determined by one coordinate, i.e., the boundary is considered a plane cylindrical of spherical "one-dimensional boundary." However, such an approach often yields results that diverge substantially from the data of practice. An attempt is made in this paper to analyze the sublimation dehydration process during conductive energy supply under conditions when the stability of the one-dimensional sublimation front is spoiled. The instability of a one-dimensional interphasal boundary is understood to be that development of the process for which any fluctuations causing deviation from a one-dimensional surface (lunes, cracks, etc.) that are inevitable under real conditions, increase monotonically. The advancement of the different interphasal surface sections here occurs at a dissimilar velocity because the surface itself acquires a complex configuration. Therefore, necessary for a correct analysis of the process is the determination of the local rate of phase transformation front advancement.

Underlying the physical model is the assumption that the single reason causing a change in phase transition boundary configuration is entrainment of the substance because of its sublimation. Any random distortion of the plane front resulting in diminution of the distance to the heating surface, is accompanied by an increase in the heat flux in the fluctuation zone because of growth of the temperature gradient. In turn, this effect increases the local velocity of the process, which causes a further development of fluctuations. Consequently,

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