INFLUENCE OF THE SURFACE LAYER ON THE PHASE TRANSITION
PROCESS IN AN INHOMOGENEOUS MEDIUM
WITH ACCOUNT OF HEAT FLUX RELAXATION

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When solving problems on heat conduction, the classical Fourier law given by $q = -KT_x$ is usually employed, and the thermal field differential equation based on it. Phase transition processes of the first kind in condensed media (the Stefan problem) have been thoroughly studied [1–3]. In the case of intensive nonstationary heat conduction processes the equation based on the classical Fourier law is generally inapplicable, since the relation between the heat flux and the temperature gradient is nonlinear. However, I. Prigogine and later A. Lykov showed that in most cases a linear approximation is sufficient, provided that the heat flux relaxation law is introduced as

$$\tau q_t + q = -KT_x. \tag{1}$$

This results in a hyperbolic heat-conduction equation [4–8].

In the present paper we study the influence of a thin surface layer on the melt solidification process within the framework of the nonstationary heat flux relaxation model given above (1). The geometry of the problem is shown in Fig. 1.

The materials comprising the given media have the following thermophysical characteristics: ρ_i, C_{pi}, K_i ($i = 1, 2$) which are the density, specific heat, and thermal conductivity of the first (refractory) and the second (fusible) material in the solid and liquid state, respectively.

In order to simplify the solution, we specify the initial and boundary conditions as follows. Let T_0 be the initial temperature of the system. It is required that $T_0 > T_f$ (T_f where is the phase transition temperature for the second material). On the left boundary (Fig. 1) constant temperature T_1 ($T_1 < T_f$) is maintained. As will be seen, this assumption is of no principal importance but allows us to simplify the analytical expressions significantly and make the analysis easier. Hence, for the period before a phase transition, the problem of the behavior of the system is set up as

$$\frac{\partial u_i}{\partial t} = \chi_i \frac{\partial^2 u_i}{\partial x^2}, \qquad i = 1, 2, \qquad \chi_i = \frac{K_i}{\rho_i C_{pi}}, \quad t > 0,$$

$$u_1(-l, t) = T_1 - T_0, \quad t > 0, \qquad u_1(0, t) = u_2(0, t), \quad t > 0, \tag{2}$$

$$K_1 \left.\frac{\partial u_1}{\partial x}\right|_{x=0-} = K_2 \left.\frac{\partial u_2}{\partial x}\right|_{x=0+}, \quad t > 0, \quad u_2(x \to \infty, t) = 0, \ t > 0 \ (u_i = T_i - T_0).$$

The solution of problem (2) of the thermal distribution before the beginning of a phase transition t_0 in the second material is readily derived employing the Laplace transformation [9]:

$$T_{(1)} = T_0 - (T_0 - T_1) \sum_{n=0}^{\infty} (\alpha_0)^n \left\{ \Phi^* \left[\frac{(2n+1)l + x}{2\sqrt{\chi_1 t}} \right] - \alpha_0 \Phi^* \left[\frac{(2n+1)l - x}{2\sqrt{\chi_1 t}} \right] \right\},$$

$$T_{(2)} = T_0 - \frac{2(T_0 - T_1)}{\sigma + 1} \sum_{n=0}^{\infty} (\alpha_0)^n \Phi^* \left[\frac{(2n+1)l + kx}{2\sqrt{\chi_1 t}} \right].$$
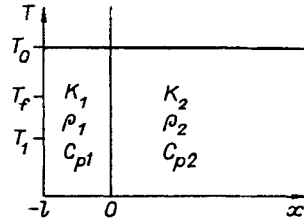
Fig. 1

Here $\Phi^*(x) = 1 - \Phi(x)$ is the adjoint integral of errors;

$$\chi_i = \frac{K_i}{\rho_i C_{pi}} \quad (i = 1, 2, 3); \qquad \sigma = \frac{K_2}{K_1} k; \qquad k = \sqrt{\frac{\chi_1}{\chi_2}}; \qquad \alpha_0 = \frac{\sigma - 1}{\sigma + 1}.$$

In the interest of obtaining a simpler solution, we confine ourselves to the "thin layer" approximation. This implies that $(l/\sqrt{\chi_1 t_0} \simeq 1)$ or, in other words, that the thermal distribution in the first layer is almost linear. In reality, this assumption is not necessary. However, had it been omitted, t_0 would be a solution to the transcendental equation $T_{(2)}(0, t_0) = T_f$. Within this approximation, summing up the expansions of $\Phi^*(x)$ truncated at the linear terms yields

$$t_0 \cong \left[\frac{\sigma - 1}{\sigma + 1} \frac{l}{\sqrt{\pi \chi_1}} \frac{T_0 - T_1}{T_f - T_1} \right]^2.$$

Note that the "thin layer" approximation allows us to find the moment of the beginning of the phase transition in the second material in the explicit form. Due to the fact that t_0 is much greater that the relaxation time of the layer and the liquid, the classical statement (and, therefore, the solution) of the problem of cooling is justified.

When $t > t_0$, the problem of the phase transition front arises. Let us solve it, employing the energy-integral method [10–14] within the framework of the nonstationary heat flux relaxation model. Here the system of equations has the form

$$\alpha T_{xx} = \tau T_{tt} + T_t, \qquad 0 < x < s(t), \qquad t > t_0, \qquad T \equiv T_3; \tag{3}$$

$$T(x, t_0) = T_{(2)}(x, t_0), \qquad 0 < x < +\infty,$$

$$\chi_2 T_{2xx} = T_{2t}, \qquad s(t) < x < +\infty, \qquad t > t_0,$$

$$T(0, t) = T^*(t), \qquad t > t_0, \tag{4}$$

$$T^*(t) = T_f - \frac{2(T_f - T_1)}{\sigma^* + 1} \sum_{n=0}^{\infty} (\alpha_0^*)^n \Phi^* \left[\frac{(2n + 1)l}{2\sqrt{\chi_1 t - t_0}} \right],$$

$$\sigma^* = \frac{K_2}{K_1} k^*, \qquad k^* = \sqrt{\frac{\chi_1}{\chi_2}}, \qquad \alpha^* = \frac{\sigma^* - 1}{\sigma^* + 1};$$

$$T(s(t), t) = T_f, \qquad t > t_0; \tag{5}$$

$$[q(s(t), t)] = -\beta s_t(t), \qquad t > t_0, \qquad s(t_0) = 0, \qquad \beta = \rho_3 L, \tag{6}$$

where L is the latent heat of phase transition and τ is the heat flux relaxation time.

To reduce the number of expressions and to avoid excessive rewriting of the problem statement, we use the designation $t' = t - t_0$, and drop the prime everywhere below. Following the method of [13], we rewrite (6) in a more convenient form

$$T(s(t), t)[\gamma^2 - (s_t)^2] = A(s_{tt} + (1/\tau)s_t) + (\eta)^2 T_{2x}(s(t), t). \tag{7}$$

Here

$$(\eta)^2 = \gamma_1 \sigma^*; \quad \gamma_1 = \frac{K_2}{\tau \rho_2 C_{p2}}; \quad \sigma^* = \frac{\rho_2 C_{p2}}{\rho_3 C_{p3}}; \quad A = L/C_{p3}; \quad \gamma^2 = \alpha/\tau = \frac{K_3}{\tau \rho_3 C_{p3}}.$$

Now, introducing the notation

$$u_1(x,t) = T_f - T(x,t) \qquad \text{and} \qquad u_2(x,t) = T_f - T_2(x,t),$$

we arrive at the final statement of the phase transition front problem:

$$\alpha u_{xx} = \tau u_{1tt} + u_{1t}, \qquad 0 < t < s(t), \qquad t > 0; \tag{8}$$

$$u_1(0,t) = T_f - T^*(t) = u_0(t), \qquad t > 0; \tag{9}$$

$$u_1(s(t),t) = u_2(s(t),t); \tag{10}$$

$$\chi_2 u_{2x} = u_{2t}; \tag{11}$$

$$T(s(t),t)[\gamma^2 - (s_t)^2] = A(s_{tt} + (1/\tau)s_t) + (\eta)^2 T_{2x}(s(t),t); \tag{12}$$

$$u_2(x,0) = T_f - T_b(x). \tag{13}$$

Integrating the governing differential equation (8) with respect to x from 0 to $s(t)$ and employing (10) and (12), we obtain

$$L_\tau[\Theta(t) + As(t)] - (\eta)^2 u_{2x}(s(t),t) = -\alpha u_{1x}(0,t), \tag{14}$$

where

$$L_\tau = \left(\tau \frac{d^2}{dt^2} + \frac{d}{dt}\right); \qquad \Theta(t) = \int_0^{s(t)} u_1(x,t)\, dt.$$

Here $\Theta(t)$ stands for the so-called energy integral. Expression (14) is the energy-integral equation.

Following the method developed in [9], we seek a solution $u_1(x,t)$ in the form of a second-degree polynomial

$$u_1(x,t) = a(t)(x-s) - b(t)(x-s)^2, \qquad s \equiv s(t).$$

The unknown coefficients $a(t)$ and $b(t)$ are determined from Eqs. (9) and (12). As (12) is awkward to handle, we bring it into the form

$$Au_{1xx}(s(t),t) = (u_{1x}(s(t),t))^2 + \alpha u_{1x}(\eta)^2 \frac{u_{2x}(s(t),t)}{\gamma^2 - (s_t)^2}.$$

As a result, $a(t)$ and $b(t)$ are expressed as

$$a(t) = A\lambda, \qquad b(t) = -\frac{A}{2}\left(\lambda^2 - \frac{g(s(t),t)}{sA}\beta\right).$$

Here

$$\beta = \left[1 - s\frac{g(s(t),t)}{2A}\right]; \qquad \lambda = \frac{\beta - [\beta^2 + 2u_0/A]^{1/2}}{s};$$

$$u_0 \equiv u_0(t) = T_f - T^*(t); \qquad g(s(t),t) = (\eta)^2 \frac{u_{2x}(s(t),t)}{\gamma^2 - (s_t)^2}.$$

The thermal distribution has the form

$$T_3(x,t) = T_f - A\left[\lambda(x-s) + \frac{\lambda^2}{2}(x-s)^2 - \frac{g(s(t),t)}{2sA}\beta(x-s)^2\right]. \tag{15}$$

Substituting the expression for the thermal field (15) into the energy-integral equation results in a nonlinear

equation

$$L_\tau\left(s\left[5+\mu+[\beta^2+\mu]^{1/2}+s\frac{g(s(t),t)}{A}\left(s\frac{g(s(t),t)}{A}-\frac{3}{4}+[\beta^2+\mu]^{1/2}\right)\right]\right)$$

$$=(\eta)^2g(s,t)+\frac{6\alpha}{s}\left[1+\mu-[\beta^2+\mu]^{1/2}+s\frac{g(s(t),t)}{A}\left(s\frac{g(s(t),t)}{A}-\frac{5}{2}-[\beta^2+\mu]^{1/2}\right)\right]$$

$$\left(\mu\equiv\mu(t)=\frac{2(T_f-T^*(t))}{A},\quad s(0)=0,\quad s_t(0)=b\right).$$

We seek its solution in the form of a series in τ

$$s=s^{(0)}+s^{(1)}+\dots,\quad s^{(1)}/s^{(0)}\simeq\tau,\quad s^{(1)}\simeq\tau^2,\quad s^{(0)}\simeq\tau^0+\tau^1.$$

Under the assumption $\gamma\gg s_t$, which is justified by the fact that γ is the heat disturbance propagation speed and s_t is the relaxation speed of the medium at a phase transition, we obtain

$$s^{(0)}L_\tau\left[s^{(0)}[5+\mu+\sqrt{1+\mu}]\right]=6\alpha[1+\mu-\sqrt{1+\mu}];\tag{16}$$

$$s^{(0)}L_\tau\left[s^{(0)}\left[-\frac{1}{2}s^{(0)}\frac{g^*(s,t)}{A\sqrt{1+\mu}}-\frac{3}{4}s^{(0)}\frac{g^*(s,t)}{A}+s^{(0)}\frac{g^*(s,t)}{A}\sqrt{1+\mu}\right]+s^{(1)}[5+\mu+\sqrt{1+\mu}]\right]$$

$$+s^{(1)}L_\tau\left[s^{(0)}[5+\mu+\sqrt{1+\mu}]\right]=(\eta)^2g^*(s,t)+6\alpha\left[\frac{1}{2}s^{(0)}\frac{g^*(s,t)}{A\sqrt{1+\mu}}\right]\tag{17}$$

$$(g^*(s,t)=u_{2x}(s(t),t)/\gamma^2).$$

Equation (16) is solved in [10]. The solution has the form

$$s^{(0)}(t)=\frac{1}{h(t)}\left[\sqrt{2F(t)+b^2\tau^2h(0)^2}-b\tau h(0)\,e^{-t/\tau}\right],\tag{18}$$

where

$$F(t)=\int_0^t f(\xi)\,d\xi;\qquad f(t)=r(t)h(t);\qquad h(t)=5+\mu+\sqrt{1+\mu};$$

$$r(t)=6\alpha[1+\mu-\sqrt{1+\mu}];\qquad\mu\equiv\mu(t)=\frac{2(T_f-T)}{A}.$$

Let us solve (17), employing solution (18) of Eq. (16). Substituting (16) and (18) into (17) yields a second-order nonhomogeneous ordinary differential equation. Making simple transformations, we bring it to the standard form and find the solution

$$s^{(1)}=\frac{\exp\left(-t/2\tau\right)}{h(t)}\left\{\sin\left(\int_0^t\omega(\xi)^{-1/2}d\xi\right)\int_0^t\mathrm{ctg}\left(\int_0^\xi\omega(\eta)^{-1/2}d\eta\right)\ae(\xi)\,d\xi\right.$$

$$\left.-\cos\left(\int_0^t\omega(\xi)^{-1/2}d\xi\right)\int_0^t\ae(\eta)\,d\eta\right\}.\tag{19}$$

Here

$$\omega(\xi)=1/4\tau^2-1/2\tau+r(t)/(s^{(0)}h(t)\tau);$$

$$\ae(t)=\frac{\exp(t/2\tau)}{\tau}\left[g^*(t)\left((\eta)^2/s^{(0)}+\frac{3\alpha}{A\sqrt{1+\mu}}\right)+L_\tau\left\{(s^{(0)})^2\frac{g^*(t)}{A}\left(\frac{5}{4}-\sqrt{1+\mu}\right)\right\}\right];$$
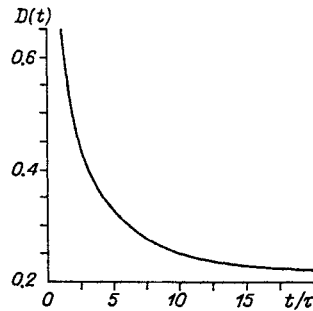
Fig. 2

$$g^*(t) = \frac{\left.\dfrac{\partial}{\partial x} u_2\right|_{x=s(t)}}{\gamma^2}.$$

The qualitative behavior of the differences between the solidification front penetration depths is shown in Fig. 2,

$$D(T) \equiv \text{hyperbolic}\,(s^{(0)}(t/\tau)/N) - \text{parabolic}\,(s(t/\tau)/N),$$

from which it is seen that when the time is small, the hyperbolic solidification front is significantly ahead of the classical solution, but as the time becomes large $(T \gg \tau)$, the front has pure root asymptotics, i.e., the classical parabolic solution.

Unfortunately, a detailed asymptotic analysis of the correction term $s^{(1)}$ (19) is rather complicated, since the solution is irrelevant in the case $t \ll \tau$. However, formally extending the expansion of $s^{(1)}$ for $t \ll \tau$ to $t < \tau$ we may conclude that the correction term $s^{(1)}$ is of aperiodic nature. The correction accelerates and slows down the front until the oscillations are damped by the exponential factor. Such behavior of $s^{(1)}$ may be attributed to the existence of a time-dependent isotherm phase transition zone.

The approach to the problems of phase transition-intensive processes presented here can also be applied to the problems of vapor explosion. In the latter, positive acceleration of phase transition front propagation has a crucial effect on the development of Rayleigh–Taylor instability of the vapor–liquid interface, which finally leads to fine-scale dispersion caused by physical detonation [15, 16].

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