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EFFECT OF RADIATION SCATTERING ON THE DYNAMICS OF THE TRANSITIONAL ZONE DURING SOLIDIFICATION OF A SEMITRANSPARENT MATERIAL

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The effect of isotropic scattering in a two-phase zone on the velocity of boundaries, thickness of the transitional zone, and distribution of the solid phase over the two-phase zone thickness in the course of solidification of a semitransparent material is considered. A generalized model of phase transition in a semitransparent medium is used. The results of numerical calculations show that radiation scattering can exert a significant effect on the structure and size of the two-phase zone and also on heat transfer (temperature gradient) in the crystal being formed.

Key words: *radiative–conductive heat transfer, semitransparent material, solidification, two-phase zone, generalized model, radiation scattering, isotropic scattering, numerical experiment.*

It was shown in [1–3] that the calculations of radiative–conductive heat transfer in the course of melting or crystallization of a semitransparent material with the use of the classical model of the phase transition of the first kind with radiative heat transfer playing the governing role revealed regimes with a nonmonotonic distribution of temperature ahead of the flat phase-transition front. It was noted that another model should be used here. A generalized model of phase transition was proposed in [4, 5]; the model takes into account the possible formation of a two-phase zone during melting or solidification of the semitransparent material. Based on this model, temperature and solid-phase distributions over the two-phase zone thickness and velocities of the transitional zone boundaries for absorbing and radiating media were obtained. It seems of interest to use this model to study the effect of radiation scattering in the two-phase zone, which was ignored previously and which can arise because of the inhomogeneous structure of this zone. If all the parameters of radiative heat transfer (radiation scattering, reflection of radiation from internal boundaries, and dependences of optical properties on the radiation wavelength) are taken into account, it is difficult to use the formal solutions of the radiation-transfer equation for a three-layer system [4, 5] because the expressions for radiation fluxes are rather cumbersome. In this situation, it seems possible to use the algorithm developed on the basis of the modified method of mean fluxes (MF method) to numerically solve the radiation-transfer equations. Application of this method to a two-layer system ensures high accuracy in studying radiative–conductive heat transfer with the use of the classical model of phase transition [1–3].

In the generalized model of phase transition, the medium where the phase transformation occurs is represented in the form of three layers with different optical properties; the layers are separated by flat boundaries (Fig. 1).

Neglecting diffusion and possible convective processes in the melt, we obtain a system of equations that describe the phase transformation, consisting of three equations of heat transfer for the liquid and solid phases and for the two-phase zone in thermodynamic equilibrium at the phase-transition temperature. The last equation takes into account release or absorption of latent heat of phase transition in the two-phase zone during partial solidification or melting. In the dimensionless form, with constant thermophysical parameters of the medium, the system has the following form [4, 5]:

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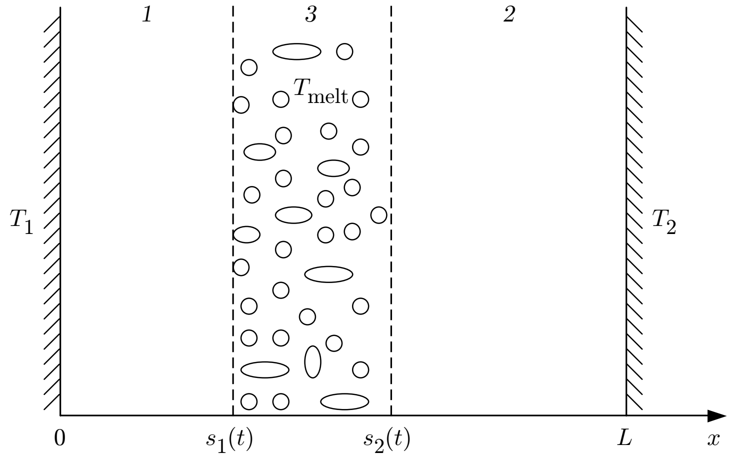

Fig. 1. Diagram of the generalized model of phase transition: 1) solid phase; 2) liquid phase; 3) two-phase zone.

$$c_1 \frac{\partial \theta}{\partial \eta} = \Lambda_1 N \frac{\partial^2 \theta}{\partial \xi^2} - \frac{1}{4} \frac{\partial \Phi_1}{\partial \xi}, \qquad 0 < \xi < s_1(\eta),$$

$$c_2 \frac{\partial \theta}{\partial \eta} = \Lambda_2 N \frac{\partial^2 \theta}{\partial \xi^2} - \frac{1}{4} \frac{\partial \Phi_2}{\partial \xi}, \qquad s_2(\eta) < \xi < 1, \tag{1}$$

$$Y \frac{\partial \alpha}{\partial \eta} = \frac{1}{4} \frac{\partial \Phi_2}{\partial \xi}, \qquad \theta = \theta^*, \quad s_2(\eta) < \xi < s_1(\eta).$$

From the heat-balance conditions at the discontinuity, we obtain the following conditions at the boundaries of the transitional zone s_1, s_2:

— during melting,

$$\alpha\Big|_{s_1^+} Y \frac{ds_1}{d\eta} = -\Lambda_1 N \frac{\partial \theta}{\partial \xi}\Big|_{s_1^-}, \qquad \alpha\Big|_{s_2^-} = 1, \qquad \frac{\partial \theta}{\partial \xi}\Big|_{s_2^+} = 0; \tag{2}$$

— during solidification,

$$\Big(1 - \alpha\Big|_{s_1^+}\Big) Y \frac{ds_1}{d\eta} = \Lambda_1 N \frac{\partial \theta}{\partial \xi}\Big|_{s_1^-}, \qquad \alpha\Big|_{s_2^-} = 0, \qquad \frac{\partial \theta}{\partial \xi}\Big|_{s_2^+} = 0. \tag{3}$$

In (1)–(3), $\theta = T/T_r$ is the dimensionless temperature, $c_i = C_i\rho_i/(C_r\rho_r)$ is the dimensionless heat capacity, $\Lambda_i = \lambda_i/\lambda_r$ is the dimensionless thermal conductivity, $\xi = x/L$ is the dimensionless coordinate, $s_i = S_i/L$ are the dimensionless coordinates of the two-phase zone boundaries, $\Phi_i = E_i/(\sigma T_r^4)$ is the dimensionless density of the resultant radiation flux, $\theta^* = T_{\text{ph}}/T_r$ is the dimensionless temperature of phase transition, $Y = \gamma\rho_{\text{ph}}/(\rho_r C_r T_r)$ is the dimensionless latent heat of phase transition, $\eta = 4\sigma T_r^3 t/(\rho_r C_r L)$ is the dimensionless time, $N = \lambda_r/(4\sigma T_r^3 L)$ is the radiative–conductive parameter, C [J/(kg · K)] is the specific heat capacity, ρ [kg/m^3] is the density, λ [W/(m · K)] is the thermal conductivity, L [m] is the total thickness of the layer, E [W/m^2] is the density of the resultant radiation flux, γ [J/kg] is the latent heat of phase transition, and σ [W/(m^2 · K^4)] is the Stefan–Boltzmann constant; the subscript r refers to scale parameters; subscript i (i = 1, 2, 3) indicates the numbers of the layers; $\alpha(\xi, \eta)$ is the fraction of the solid phase in the transitional zone, whose value varies from 0 to 1.

The solution of the problem consists of determining the dimensionless distributions of the temperature $\theta(\xi, \eta)$, the density of the resultant radiation flux $\Phi(\xi, \eta)$, and the fraction of the solid phase over the thickness of the two-phase zone $\alpha(\xi, \eta)$, and also the positions of internal boundaries $s_1(\eta)$, $s_2(\eta)$ at each time instant in the region $0 \leqslant \xi \leqslant 1$.

The boundary-value problem (1)–(3) with initial and boundary conditions was solved numerically by the finite-difference method. The implicit difference scheme was constructed by the integrointerpolation method. The Newton method was used to determine the unknown s_1 and s_2.

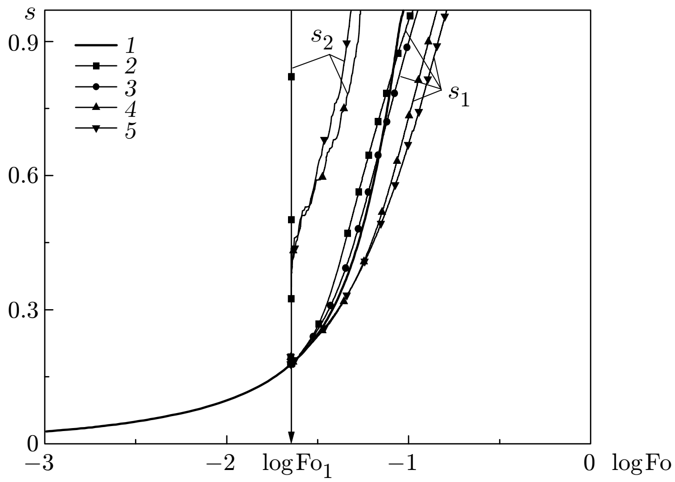

Fig. 2

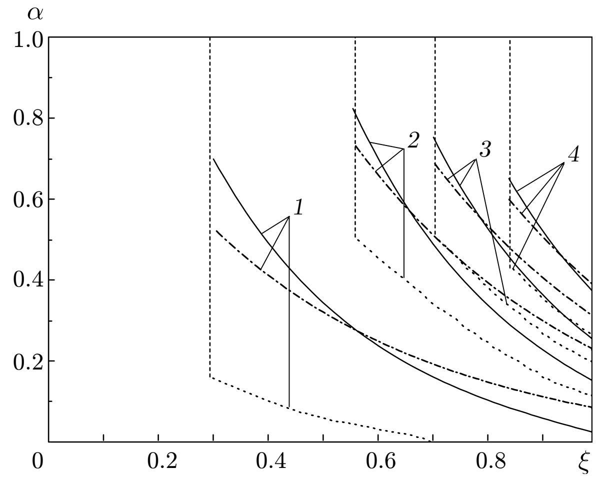

Fig. 3

Fig. 2. Motion of the transitional zone boundaries in the course of solidification of a semitransparent material with isotropic scattering in the two-phase zone: calculation by the classical model of phase transition (1) and for $\omega_3 = 0$ (2), 0.5 (3), 0.7 (4), and 0.9 (5).

Fig. 3. Distribution of the solid phase over the thickness of the two-phase zone at different times: the solid curves refer to $\omega_3 = 0$ and $\eta = 3.45$ (1), 5.25 (2), 6.57 (3), and 8.233 (4); the dot-and-dashed curves refer to $\omega_3 = 0.5$ and $\eta = 3.69$ (1), 5.97 (2), 7.34 (3), and 9.08 (4); the dotted curves refer to $\omega_3 = 0.7$ and $\eta = 4.11$ (1), 7.72 (2), 9.69 (3), and 11.85 (4).

The calculations were first performed in the classical Stefan formulation, and the generalized model was used from the moment monotonicity was violated. In calculations by the classical model with certain values of parameters, the monotonicity of the temperature distribution is not violated. In this case, the classical model of phase transition is valid, which becomes inapplicable if the two-phase zone is formed, which is taken into account in the generalized model. After the transitional zone disappears, the generalized model again reduces to the classical one.

In the present work, we numerically study the effect of radiation scattering in the two-phase zone on the dynamics of the transitional zone in the course of crystallization of a flat layer of a semitransparent medium whose optical properties correspond to a gray body. The problem conditions are the same as in [4, 5]. For the solidification process, we have $c_1 = c_2 = 1$, $\Lambda_1 = \Lambda_2 = 1$, $Y = 0.1$, $\theta^* = 0.5$, $N = 0.01$, $\theta(\xi, 0) = 0.7$, $\theta(0, \eta) = 0.3$, and $\partial\theta(1, \eta)/\partial\xi = 0$. The refractive indices are assumed to be identical for all phases ($n_1 = n_2 = n_3 = 1.5$); therefore, there is no reflection from internal boundaries. The algorithm for solving the radiation-transfer equations was developed on the basis of the MF method [1–3] modified for the conditions of a three-layer system. The differential equations are solved for three layers ($i = 3$), and the spectral range of absorption corresponds to $i = 1$ in the gray body approximation. Divergence of the radiation flux is determined in the finite-difference form from the values of radiation fluxes, in contrast to the previous works where formal solutions were used. In determining the radiation fluxes on the basis of the MF algorithm, the dimensionless thickness of each layer is assumed to equal unity; in solving the energy equations, the total thickness of the initial layer is set equal to unity. The positions of internal boundaries vary from zero to unity. The scale correspondence of the regions is obtained by interpolation of temperature and radiation distributions.

It is assumed that only the two-phase zone being formed is a scattering medium. The two-phase zone is a radiating, absorbing, and scattering medium. The scattering coefficient, scattering albedo, and the type of radiation scattering in the two-phase zone depend on a particular structure of the two-phase zone and, strictly speaking, can be determined only experimentally. Such experiments, however, were never performed. Therefore, it seems important to numerically simulate the dynamics of the transitional zone, depending on the prescribed values of the optical thickness (attenuation factors) and albedo of single scattering. Radiation scattering anisotropy, as is shown in [2], does not introduce any principal changes in the character of temperature fields but alters the velocity of the interface. In the present work, we consider isotropic scattering.

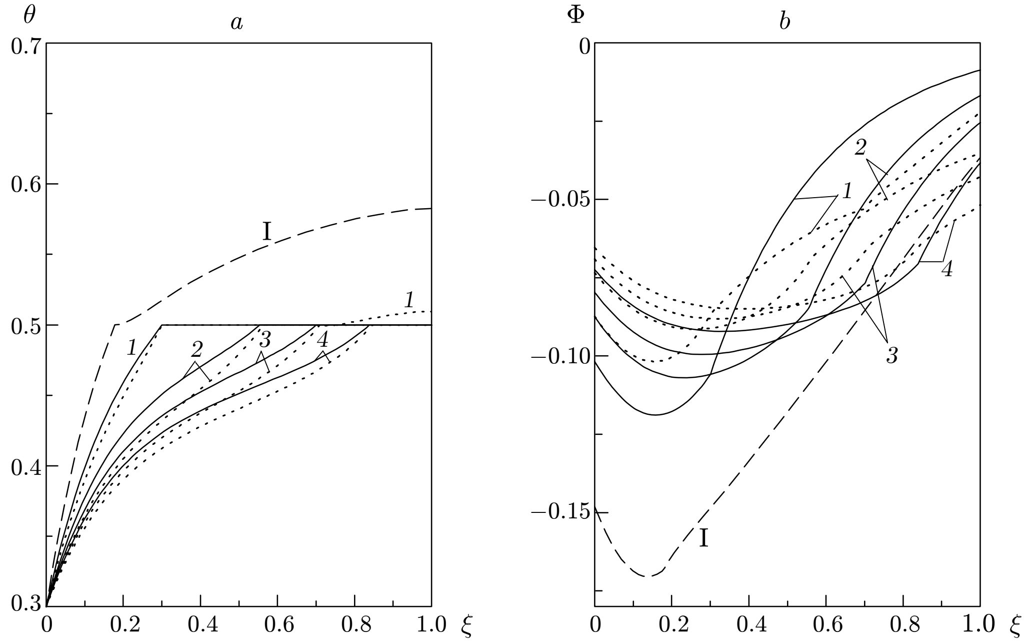

Fig. 4. Distributions of temperature (a) and radiation fluxes (b) in the course of solidification of the layer of a semitransparent material with formation of a two-phase zone: the solid curves refer to $\omega_3 = 0$ and $\eta = 3.45$ (1), 5.25 (2), 6.57 (3), and 8.233 (4); the dotted curves refer to $\omega_3 = 0.7$ and $\eta = 4.11$ (1), 7.72 (2), 9.69 (3), and 11.85 (4); curve I is the initial temperature distribution.

Figure 2 shows the numerical results on motion of the transitional zone boundaries during solidification versus the albedo of single isotropic scattering ω_3 in the two-phase zone ($\mathrm{Fo} = \eta N$ is the Fourier number). The attenuation factor of the two-phase zone $æ_3$ is determined from the condition $\tau_3 = æ_3 L = 2$, and the coefficients of absorption of the solid phase (α_1) and liquid phase (α_2), as in [1–5], are determined from the conditions $\tau_1 = æ_1 L = 1$ and $\tau_2 = æ_2 L = 2$ ($L = 0.1$ m). Curve 1 corresponds to the calculation by the classical model of phase transition. As was indicated above, when monotonicity of the temperature field is violated, which corresponds to $\log \mathrm{Fo}_1$ in Fig. 2, the calculation is performed in the generalized formulation of the Stefan problem. Curves 2 and 3 in Fig. 2 refer to calculations for a non-scattering two-phase zone. As in [5], the boundary of the two-phase zone s_2 is almost immediately shifted to the right boundary, and the boundary s_1 moves monotonically until it reaches the right boundary of the three-layer system. A comparison with the results of [5] shows that the difference in the methods of calculating radiative heat transfer is manifested at the end of the process: the motion of the left boundary of the two-phase zone $s_1(\eta)$ becomes slower. The distribution of the solid phase over the thickness of the two-phase zone $\alpha(\xi)$ at different times η in the absence of radiation scattering (solid curves in Fig. 3) is in good agreement with the distribution obtained in [5] for a non-scattering medium. It follows from Fig. 2 that isotropic scattering of radiation in the two-phase zone attenuates the motion of the left boundary of the two-phase zone. In the case of strong scattering (curves 4 and 5 in Fig. 2), a finite-thickness two-phase zone is initially formed, and then the second boundary of the two-phase zone reaches the right (opaque) boundary of the three-layer system. The role of radiation absorption and also the role of radiative cooling (own radiation) in the two-phase zone become less important because of the strong scattering (with increasing albedo ω_3). This is also evidenced by the distribution of the solid phase over the two-phase zone thickness (dotted curves in Fig. 3). The fraction of the solidified phase in the two-phase zone is considerably smaller than for $\omega_3 = 0$ and $\omega_3 = 0.5$. It follows from Fig. 3 that the contributions of scattering and absorption to radiative cooling of the melt in the two-phase zone are identical for $\omega_3 = 0.5$ (dot-and dashed curves in Fig. 3). Thus, radiation scattering in the two-phase zone and the two-phase zone structure are interrelated.

Figure 4 shows the calculated distributions of temperature and radiation fluxes in the course of solidification of a flat layer of a semitransparent medium with formation of a two-phase zone. Curve I corresponds to the initial temperature distribution. The temperature in the two-phase zone is maintained equal to the phase-transition temperature. With allowance for radiation scattering, the absolute values of the resultant radiation fluxes are lower than in the case of an only absorbing layer. The temperature in the solid layer also decreases, which alters the temperature gradients. The calculation results for radiation fluxes and temperature distributions are in good agreement with the calculations of [5], which confirms the validity of using the algorithm developed on the basis of the MF method for numerical determination of radiation fluxes and divergence of the radiation flux in a multilayer semitransparent system.

The existence of the two-phase zone in the case of rapid crystallization of refractory oxides semitransparent for thermal radiation was experimentally confirmed in [6]. The necessity of using the mathematical model of melting and solidification of semitransparent materials with allowance for formation of an extended two-phase zone caused by radiative heat transfer is also noted in [6]. This model of phase transition in a semitransparent medium requires further improvement: it is necessary to take into account all physical phenomena accompanying the crystallization or melting process with formation of a two-phase zone and to use experimental data on the properties and structure of the two-phase zone.

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