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Physical and Mathematical Model of Heat Transfer in Porous Systems

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Abstract

A mathematical model of heat transfer in porous media with phase transitions is formulated to describe the processes of high-speed melting of a powder layer of binary metal alloys with peritectic transformation. The modeling of nonstationary thermal fields was carried out using a two-phase zone model [2], extended to the case of high rates of medium heating and heat transfer by the mechanisms of thermal conductivity and radiation. The following physical assumptions were used in the formulation of the system of equations

Key words: a temperature, physical assumptions, the thermal conductivity equation, the absolute temperature, the laser radiation, the COMSOL MultiPhysics.

A mathematical model of heat transfer in porous media with phase transitions is formulated to describe the processes of high-speed melting of a powder layer of binary metal alloys with peritectic transformation. The modeling of nonstationary thermal fields was carried out using a two-phase zone model [2], extended to the case of high rates of medium heating and heat transfer by the mechanisms of thermal conductivity and radiation. The following physical assumptions were used in the formulation of the system of equations:

• the cooling rates of the alloy $V_c > 103$ K/s, therefore, when describing the kinetics of solidification on a macroscopic scale, the zonal liquation of the components is neglected. Therefore, the use of the thermal equation of the quasi-equilibrium zone is justified;

• at the observed cooling rates, the peritectic reaction is suppressed, therefore, at $T < T_P$, where T_P is the temperature of peritectic crystallization, the peritectic phase is formed directly from the liquid;

• heat transfer mechanisms take into account: (a) heat transfer by diffusion mechanism, (b) penetration of laser radiation into the porous medium at the heating stage, (c) evaporation of metal from the sample surface, (d) radiation cooling of the surface, (e) release of latent heat of the phase transition.

Taking into account the accepted assumptions, the thermal conductivity equation can be reduced to the thermal equation of the two-phase zone model [2]:

$$\Psi(T)\frac{\delta T}{\delta t} = a(\varepsilon_V, \varepsilon_\sigma)\nabla^2 T + F(q_L), \qquad (1)$$

where Ψ is the dimensionless effective heat capacity, taking into account the release of latent heat of the phase transition; T is the absolute temperature; t is the time; a is the thermal conductivity coefficient; e_v and ε_σ are the porosity characteristics of the powder layer, defined as the volume fraction of pores and the proportion of pores in a flat section, respectively; ; $F = \alpha q_L$ is the intensity of the volumetric heat source associated with with the power of laser exposure at different depths y of the powder layer. Here q_L and α are the energy flux density of laser radiation and the absorption coefficient of light radiation in the local volume of the powder layer, respectively. The coefficient α depends on both the temperature and the phase composition of the local volume, determining in the model the change in the depth of penetration of laser radiation during the melting of particles and the change in the morphology of the porous body. Since it was not possible to measure this dependence experimentally, an estimated value of α = const was chosen based on data on the depth of the sintered layer under various processing modes. The geometry of the computational domain Ω is shown in Figure 4.1, where the powder layer and the substrate are represented by the subdomains Ω_P and Ω_S. Absorption upon penetration of laser radiation into a substance is characterized by a law functionally close to Booger's law for optically homogeneous media, written for the selected coordinate system (Fig. 4.1) in the form:

$$q_L(t, x, y) = q_{L0}(t, x)|_{y=0}\, exp(-\alpha y), \qquad (2)$$

where $q_{L0}(t, x)|_{y=0}$ is the density of the irradiation energy flux on the sample surface. The dependence of thermal conductivity on porosity was calculated by an equation similar to the approach [3]:

$$a = a_0\frac{1-\varepsilon_\sigma}{1-\varepsilon_V}, \qquad (3)$$

where a_0 is the thermal conductivity of a continuous medium.

The function Ψ of the dimensionless heat capacity is generally defined by the expression $\Psi(T) = 1 + \theta\,(dS/dT)$, where θ is the adiabatic temperature, S is the volume fraction of the liquid phase in the local volume, the heat capacity of which is calculated. The expression for Ψ, obtained by the authors [2] in the approximation of a small zonal liquation of impurity components, was used in the work:

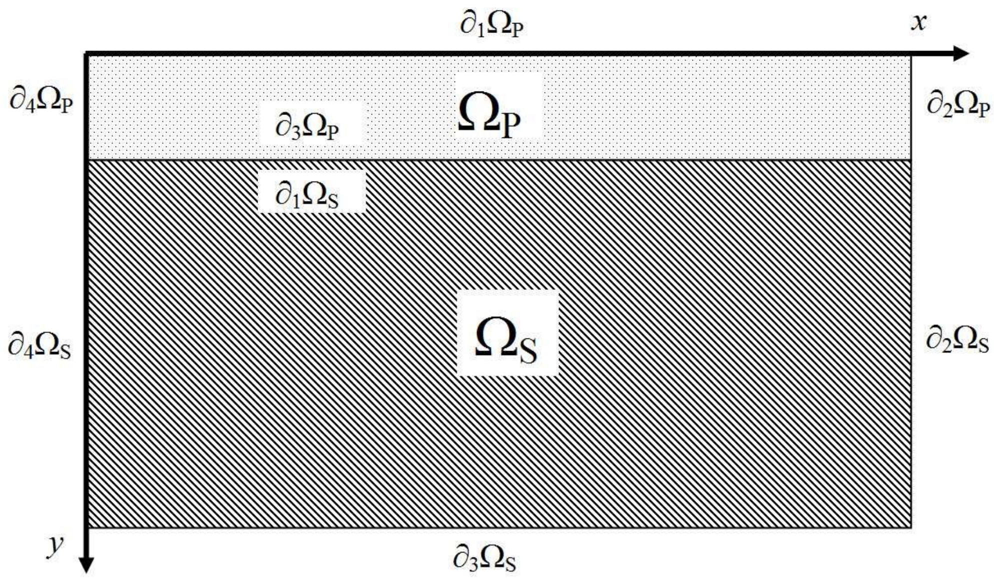


Figure 1. The calculated area Ω is divided into two subdomains Ω_P and Ω_S corresponding to the powder layer and the substrate. The boundary conditions are determined by equations (5)–(12).

$$\Psi = 1 - \frac{\theta}{(1-k)C\varphi'(C)} exp\left\{-\int_{C_0}^{C}\frac{dC}{(1-k)C}\right\} \tag{4}$$

where C is the concentration of the impurity (non–basic) component, $k = C_S/C_L$ is the distribution coefficient obtained from the phase diagram and equal to the ratio of C_S and C_L concentrations at the solid–melt interface, $T_L = \varphi(C)$ is the equation describing the dependence of the liquidus temperature T_L (the phase equilibrium line determined by the alloy state diagram) from the concentration. For a linear phase diagram, the liquidus temperature is given by $T_L = T_A + mC$, где T_A, where T_A is the crystallization temperature of the main component, m is the tangent of the slope of the liquidus line. At high speeds of the solidification front movement observed in laser reflow experiments, it is necessary to take into account relaxation processes in the diffusion transfer of impurities and the dependences of k and m on the degree of deviation from thermodynamic equilibrium both at the interface and in the melt volume [4]. In this work, the equilibrium values of the parameters k and m obtained from the equilibrium phase diagrams were used [1]. The expansion of the model taking into account locally nonequilibrium diffusion is the subject of further research.

The thermal effect of laser radiation in equation (1) is taken into account by a volumetric source F, depending on the flow $q_L(t,x,y)$, determined, in turn, by the flow $q_{L0}(t,x)$ of heat on the sample surface in equation (2). The function $q_{L0}(t,x)|y=0$ is defined by a function periodic in time and dependent on spatial coordinates, reflecting both the pulsed nature of the laser radiation and the distribution of the radiation density inside the laser beam:

$$q_{L0}(t,x)|_{y=0} = \frac{P_{act}}{R_b} g(x)\xi(t),\ \ g(x) = g_u(x) \text{ или } g_n(x), \tag{5}$$

$$g_u(x) = \left(\frac{1}{2}\right) H(|x - X_b| - R_b), \tag{6}$$

$$g_n(x) = \frac{R_b^2}{(2\pi\sigma_b^2)^{1/2}} \exp\left(-\frac{(x-X_b)^2}{2\sigma_b^2}\right), \tag{7}$$

$$\xi = H(\tau_2 - tmod\tau_1). \tag{8}$$

where P_{act} is the actual irradiation power of the surface, $g(x)$ is the distribution function of the flux density in the laser beam, ξ is the function of the U-shaped modulation of laser radiation, R_b, V_b, X_0 and $X_b = X_0 + V_b t$ is the radius, velocity, initial position and current coordinate of the center of the laser beam, respectively, σ_b is the standard deviation, τ_1 and τ_2 are the time (period) between pulses and the duration of one pulse, H is the Heaviside function. The function g is given as a homogeneous or Gaussian distribution by choosing the functions g_u or g_n, respectively, depending on the characteristics of the focusing system. The normalization of the function g is carried out from the condition that 90% of the laser radiation power falls on the surface element limited by the effective radius R_b of the laser beam. Figure 2 shows graphs of the functions ξ, g_u and g_n that modulate the heat flow relative to the temporal and spatial coordinates.

Convective and radiative cooling occurs on the surface of $\partial_1\Omega_P$ of the sample in accordance with [5]

$$\vec{n}\cdot\vec{q}|_{\partial_1\Omega_P} = h_{эфф}(\mathrm{T}-T_{окр}) + \epsilon\epsilon_{SB}(T^4 - T_{окр}^4), \qquad (9)$$

where ϵ is the surface emission coefficient, $\epsilon_{SB} = 5.67\times10^{-8}$ Вт м$^{-2}$К$^{-4}$ is the Stefan-Boltzmann constant, Current $T_{окр}$ is the ambient temperature, and the normal vector $\vec{n}$ is directed from the powder layer into the gas medium. The evaporation of metal from the surface is taken into account in the model by means of the effective heat transfer coefficient heff:

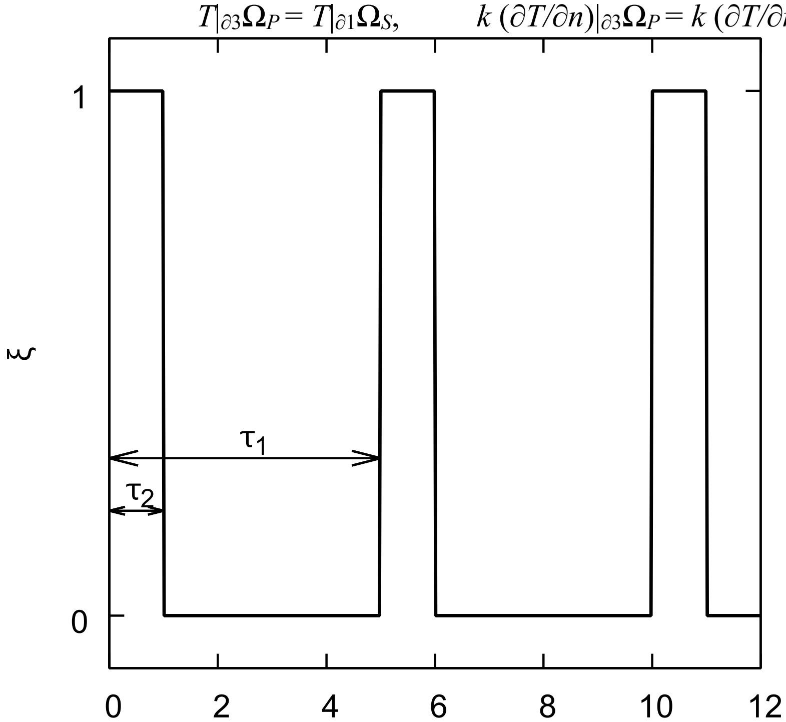
$$h_{эфф}(T) = h_{конв} + \left(\frac{1}{2}\right)(h_{кип} - h_{конв})tanh\left(\frac{T - T_{кип}}{\Delta Th}\right), \qquad (10)$$

where the transition from convective cooling of the surface, determined by the coefficient $h_{конв}$ of heat exchange due to convection in a gaseous medium, to cooling due to evaporation, determined by $h_{кип}$, occurs near the boiling point of $T_{кип}$ in the temperature range ΔT_h. Taking into account the $h_{конв}$ of the chamber purge rate, heat transfer during laser treatment in an inert medium can be further refined. The boundary conditions on the lower surface of the substrate are given by

$$\vec{n}\cdot\vec{q}|\partial_3\Omega_s = h_{конв}(T - T_{окр}) \qquad (11)$$

The interface between the powder layer and the substrate is characterized by the continuity of temperature and heat flow:

$$T|_{\partial3}\Omega_P = T|_{\partial1}\Omega_S, \qquad k\,(\partial T/\partial n)|_{\partial3}\Omega_P = k\,(\partial T/\partial n)|_{\partial1}\Omega_S. \qquad (12)$$



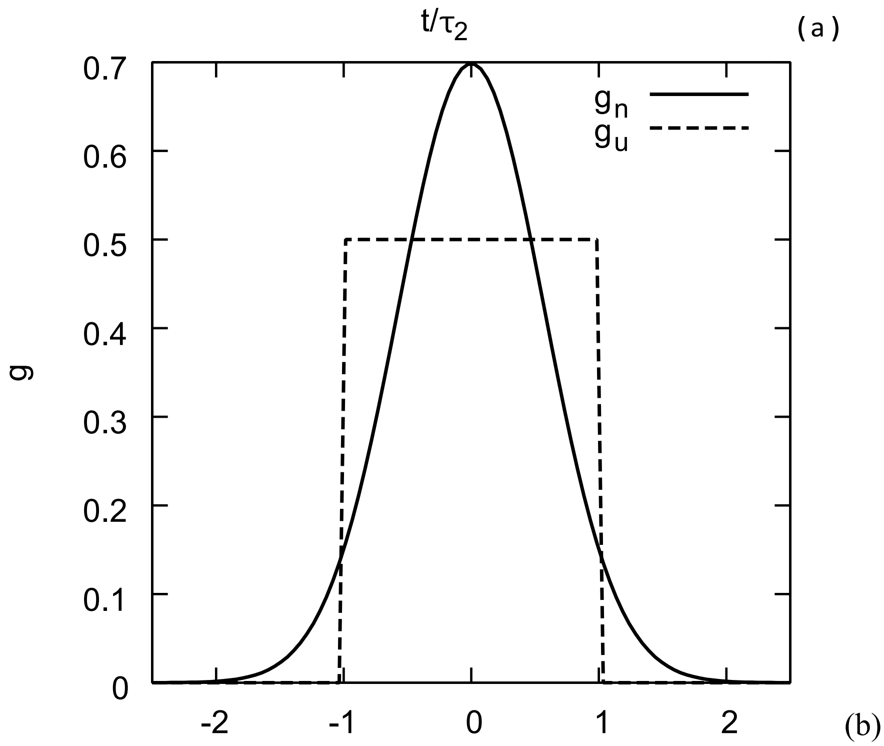


Figure 2. (a) Modulation of the laser beam flux during pulse processing by a function ξ, depending on the dimensionless time t/τ_2, where τ_1 and τ_2 are the time (period) between pulses and the duration of one pulse, respectively. (b) The distribution g of the heat flux density as a function of the dimensionless distance $(x - X_b)/R_b$ from the center of the laser beam. The function g can be given in the form of a homogeneous g_u or normal g_n distribution.

At the vertical boundaries $\partial_2\mathbf{\Omega}_P$ and $\partial_4\mathbf{\Omega}_P$ of the powder layer and the boundaries $\partial_2\mathbf{\Omega}_S$ and $\partial_4\mathbf{\Omega}_S$ of the substrate, periodic boundary conditions are set, similar to equations (12), when the temperature and fluxes at opposite boundaries are equated to reduce the estimated time. The initial conditions are accepted in the form of

$$T|_{\Omega_P \Omega_S}/= T_{\text{нач}} \quad (13)$$

where $T_{\text{нач}}$ is the temperature to which the sample is preheated.

Thus, the system of equations (1)–(13) describes the process of pulsed laser treatment of the powder layer and is closed. The numerical model was implemented in the COMSOL MultiPhysics commercial computing package designed to solve physical and engineering problems. The unsteady heat equation for the boundary value problem was calculated by the finite element method.

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