THERMAL FIELDS IN CRYSTALLIZATION OF A PARTICLE OF A SPRAYED COATING

A. M. Dubasov

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An analytical solution of the problem of heat conduction in crystallization of a particle on a coating sprayed by an open jet onto a flat base (substrate) is given in a one-dimensional approximation. The initial temperature of the particle is equal to the melting temperature of its material. The coating is considered as a multilayer plate with a layer thickness of one crystallized scale particle; thermal resistance occurs between the layers and between the coating and the substrate. Examples of calculation of the temperatures in crystallization of the particle near the substrate and at a distance from it are given.

In spraying of a coating by an open jet, the processes in the coating and its properties are largely determined by the thermal fields in crystallization of the particles of the coating [1]. We give a solution of the problem of heat conduction in crystallization of a particle on a coating that is deposited onto a plane base (substrate). We take into account the thermophysical inhomogeneity of the coating caused by the fact that the cohesion of contacting scale particles occurs not over the entire area of their mutual contact; where the cohesion between the particles is absent, contact thermal resistance appears.

We will consider a coating as a laminar material with a thickness of the layers representing one scale particle; the planes of the bases of the layers are in parallel to the plane of the substrate (Fig. 1). The layers stick to each other and to the substrate discretely, in connection with which we will assume that we have the specific contact thermal resistance r_c (constant and the same everywhere) between the layers of the coating and between the coating and the substrate. Solving the problem of heat conduction, we assume that the thermophysical properties of materials are constant, the initial temperature of the particles is equal to the melting temperature T_m of the particle material, which is frequent in plasma spraying, and the particles have the same velocity of motion and the same diameter before collision with the coating. Upon collision with the coating, the particles become flattened, forming scales of constant thickness, in practice; the time t_{cr} of their crystallization on any layer of the coating is the same [2], and the free surface of crystallizing particles is heat-in-sulated.

In the central region of its base, the crystallizing particle sticks to the coating lying below, in connection with which the contact of the particle with the coating in this region is considered to be ideal. In the problem of heat conduction in question, we take into account only the part of the particle which lies above the region of ideal contact. We also assume that the initial temperature of the coating and the substrate T_{in} is constant and the heat fluxes in the crystallized layer of the particle, the coating, and the substrate are directed perpendicularly to the plane of the substrate. This assumption is substantiated by experimental data which demonstrate that the axes of columnar crystals growing in the crystallizing particle along the heat fluxes are located perpendicularly, in practice, to the surface of contact of the particle. We assume that the thickness of the coating layers, with the exception of, may be, a few layers adjacent to the substrate, is constant and equal to *h*. Taking into account that the specific thermal resistance of one layer of the coating r_{coat} is made up of

Joint Institute of High Temperatures, Russian Academy of Sciences, Moscow, Russia; email: aDubasov@uandex.ru. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 74, No. 6, pp. 162–166, November–December, 2001. Original article submitted December 8, 2000; revision submitted February 23, 2001.



Fig. 1. Scheme of a coating with a crystallizing particle on it: 1) coating; 2) liquid phase of the particle; 3) solid phase of the particle; 4) layers of the coating; 5) substrate.

the specific thermal resistance of the material of the coating layer r_{layer} and the contact resistance r_{cont} , $r_{\text{coat}} = r_{\text{cont}} + r_{\text{layer}}$, where $r_{\text{coat}} = h/\lambda_{\text{coat}}$ and $r_{\text{layer}} = h/\lambda_1$, from which we represent the quantity r_{cont} as

$$r_{\rm cont} = r_{\rm layer} \left(\frac{\lambda_1}{\lambda_{\rm coat}} - 1 \right). \tag{1}$$

Usually, the quantity λ_1 exceeds λ_{cont} by several times and in many cases by one or two orders of magnitude ([1], p. 135); consequently, according to (1), the quantity r_{cont} is approximately as many times larger than λ_{coat} . We will assume that λ_1 is approximately an order of magnitude larger than λ_{coat} . Then in crystallization of a particle on a coating surface, which is quite distant from the substrate base, the temperature increase in the coating at a distance larger than h from the particle base will be small, as will be confirmed below. In this case, in solution of the problem of heat conduction, the thickness of the layer lying under the layer with a particle on it can be considered to be infinite. This enables us to disregard the layers lying below and simplifies the solution of the problem.

Let us consider first thermal processes in crystallization of a particle on a coating layer located at a large distance from the substrate base. We draw the X axis through the central point of the region of contact of the particle with the surface layer of the coating perpendicularly to its plane. We locate the origin of coordinates on the layer plane opposite to the plane of contact with the particle and guide the X axis toward the particle (Fig. 1). According to the above, the temperature distributions over any straight line that is in parallel to the X axis differ not only in the zero time reference which corresponds to the instant at which the region of contact of the particle with the coating crosses the straight line in question. For the X axis the zero time reference corresponds to the instant of contact of the particle with the surface, and the system of equations for calculation of the thermal fields on the X axis in crystallization of particles will be written as

$$\chi_1 \frac{\partial^2 T_1}{\partial x^2} = \frac{\partial T_1}{\partial t}, \quad 0 \le x \le X(t);$$
(2)

$$T_1 = T_{\rm in} \text{ for } 0 \le x \le h, \ t = 0;$$
 (3)

$$T_1 = T_{\rm m}; \quad \lambda_1 \frac{\partial T_1}{\partial x} = L \rho_1 \frac{\partial X(t)}{\partial t} \quad \text{for} \quad x = X(t); \tag{4}$$

$$X(0) = h; X(t_{cr}) = 2h;$$
 (5)

$$\chi_0 \frac{\partial^2 T_0}{\partial x^2} = \frac{\partial T_0}{\partial t} \quad \text{for} \quad x < 0 ;$$
(6)

$$\lambda_1 \frac{\partial T_1}{\partial x} = \lambda_0 \frac{\partial T_0}{\partial x}; \quad \lambda_1 \frac{\partial T_1}{\partial x} = \frac{T_1 - T_0}{r_{\text{cont}}} \quad \text{for} \quad x = 0;$$
(7)

$$T_0 = T_{\rm in} \quad \text{for} \quad t = 0, \ x < 0.$$
 (8)

So as to decrease the number of parameters and represent the solution of the problem in general form, we employ the reduced quantities

$$\tau = \frac{t}{t_{\rm cr}}; \quad \tau_{\rm cr} = 1; \quad x_0 = \sqrt{\chi_1 t_{\rm cr}}; \quad y = \frac{x}{x_0};$$

$$H = \frac{h}{x_0}; \quad Y(\tau) = \frac{X(t_{\rm cr}\tau)}{x_0}; \quad \theta_i = \frac{T_i - T_{\rm in}}{T_{\rm m} - T_{\rm in}}; \quad R_{\rm cont} = \frac{r_{\rm cont}}{x_0} = \frac{H}{\lambda_1} \left(\frac{\lambda_1}{\lambda_{\rm coat}} - 1\right), \tag{9}$$

where $x_0 = \sqrt{\chi_1 t_{\rm cr}}$.

In reduced variables, the basic equations with the initial and boundary conditions will have the form

$$\frac{\partial^2 \theta_1}{\partial y^2} = \frac{\partial \theta_1}{\partial \tau}, \quad 0 \le y \le Y(\tau);$$
(10)

$$\theta_1 = 0 \text{ for } 0 \le y \le H, \ \tau = 0;$$
(11)

$$\theta_1 = 1; \quad \frac{\partial \theta_1}{\partial y} = \frac{1}{\sqrt{\pi} B} \frac{dY}{d\tau} \quad \text{for} \quad y = Y(t);$$
(12)

$$Y(0) = H; Y(1) = 2H;$$
 (13)

$$\frac{\chi_0}{\chi_1} \frac{\partial^2 \theta_0}{\partial y^2} = \frac{\partial \theta_0}{\partial \tau} \quad \text{for} \quad y < 0 ;$$
(14)

$$\frac{\partial \theta_1}{\partial y} = \frac{\lambda_0}{\lambda_1} \frac{\partial \theta_0}{\partial y}; \quad \lambda_1 \frac{\partial \theta_1}{\partial y} = \frac{\theta_1 - \theta_0}{R_{\text{cont}}} \quad \text{for} \quad y = 0;$$
(15)

$$\theta_0 = 0 \text{ for } \tau = 0, \ y < 0,$$
 (16)

where $B = c_1((T_m - T_{in})/(\sqrt{\pi}L))$

The solution to the nonlinear problem of heat conduction (10)–(16) will be sought by solution of the linear boundary-value problem for an unbounded composite solid body:

$$\frac{\partial^2 \theta_1}{\partial y^2} = \frac{\partial \theta_1}{\partial t}, \quad 0 \le y < \infty ; \tag{17}$$

$$\frac{\chi_0}{\chi_1} \frac{\partial^2 \theta_0}{\partial y^2} = \frac{\partial \theta_0}{\partial \tau}, \quad -\infty \le y < 0 ;$$
(18)

$$\frac{\partial \theta_1}{\partial y} = \frac{\lambda_0}{\lambda_1} \frac{\partial \theta_0}{\partial y}; \quad \lambda_1 \frac{\partial \theta_1}{\partial y} = \frac{\theta_1 - \theta_0}{r_{\text{cont}}} \quad \text{for} \quad y = 0;$$
(19)

$$\theta_0 = 0; \quad \theta_1 = \psi(y) \quad \text{for} \quad \tau = 0,$$
 (20)

here, $\psi(y) = 0$ for $0 \le y \le H$.

The function $\psi(y)$ is selected such that for the solution obtained the function $Y(\tau)$ satisfies the relations

$$\Theta_1 \Big|_{y=Y(\tau)} = 1, \quad 0 \le \tau \le 1;$$
(21)

$$Y(0) = H, \quad Y(1) = 2H;$$
 (22)

$$\left. \frac{\partial \theta_1}{\partial y} \right|_{y=Y(\tau)} = \frac{1}{\sqrt{\pi} B} \frac{dY}{d\tau}, \quad 0 \le \tau \le 1 .$$
(23)

Then the solution of the boundary problem (17)–(20) in the case where conditions (21)–(23) are fulfilled will be the solution of the boundary-value problem (10)–(16) as well. We note that the Green function $G_i(y, y', \tau)$ for the boundary-value problem (17)–(20) is known ([3], p. 368), and the solution of this problem will be written as

$$\theta_i = \int_{H}^{\infty} G_i(y, y', \tau) \psi(y') dy', \quad i = 0; 1.$$
(24)

The function $\psi(y)$ can be represented as follows:

$$\Psi = \sum_{j=0}^{\infty} c_j \varphi_j (y, b_j) , \qquad (25)$$

where

$$\varphi_j(y, b_j) = \begin{cases} 0 & \text{for } y \le b_j, \\ 1 & \text{for } y > b_j, \end{cases}$$
(26)

the constants $b_0 = H$, $b_{j+1} > b_j$, c_j , j = 0, 1, ..., and b_j , j = 1, 2, ..., are selected such that the function $\Psi(y)$ ensures the fulfillment of conditions (21)–(23).

Having substituted (25) into (24), we find

$$\theta_i = \sum_{j=0}^{\infty} c_j \theta_i^{(j)}, \quad i = 0, 1, \qquad (27)$$

here

$$\theta_{i}^{(j)} = \int_{b_{j}}^{\infty} G_{i}(y, y', \tau) \, dy' \,.$$
⁽²⁸⁾

Having employed the known expressions for G_i and having taken integrals (28), we obtain

$$\theta_{1}^{(j)} = \frac{1}{2} \left[1 + \Phi\left(\frac{y - b_{j}}{2\sqrt{\tau}}\right) + p_{1}\Phi^{*}\left(\frac{y + b_{j}}{2\sqrt{\tau}}\right) \right] + p_{2} \exp\left[K\left(y + b_{j}\right) + K^{2}\tau\right] \Phi^{*}\left(\frac{y + b_{j}}{2\sqrt{\tau}} + K\sqrt{\tau}\right),$$

$$\theta_{0}^{(j)} = (p_{1} + p_{2}) \left\{ \Phi^{*}\left(\frac{b_{j} + |y| \sqrt{\frac{\chi_{1}}{\chi_{0}}}}{2\sqrt{\tau}}\right) - \exp\left[K^{2}\tau + K\left(b_{j} + |y| \sqrt{\frac{\chi_{1}}{\chi_{0}}}\right)\right] \Phi^{*}\left(\frac{b_{j} + |y| \sqrt{\frac{\chi_{1}}{\chi_{0}}}}{2\sqrt{\tau}} + K\sqrt{\tau}\right) \right\},$$
(29)

where

$$p_{1} = \frac{1 - A}{1 + A}; \quad p_{2} = \frac{A}{1 + A}; \quad A = \frac{\lambda_{0}}{\lambda_{1}} \sqrt{\frac{\chi_{1}}{\chi_{0}}} = \sqrt{\frac{\lambda_{0}c_{0}\rho_{0}}{\lambda_{1}c_{1}\rho_{1}}};$$

$$K = \frac{1 + A^{-1}}{\lambda_{1}^{-1}R_{\text{cont}}} = \frac{1 + A^{-1}}{H\left(\frac{\lambda_{1}}{\lambda_{\text{coat}}} - 1\right)}; \quad \Phi^{*}(x) = 1 - \Phi(x),$$
(30)

 $\Phi(x)$ is the error function ([3], p. 470).

Satisfaction of conditions (21)-(23) using the solution (27) will be considered with the example of the characteristic case

$$T_{\rm in} = 290 \ K; \ \frac{\lambda_1}{\lambda_{\rm coat}} - 1 = 10.$$
 (31)

With the aim of satisfying approximately conditions (21) and (23), we confine ourselves to the employment of just the first term of series (27); we take θ_i in the form

$$\boldsymbol{\theta}_i = c_0 \boldsymbol{\theta}_i^{(0)} \,, \tag{32}$$

and c_0 and $Y(\tau)$ in the form

$$c_0 = \frac{2}{1 + \Phi(\alpha_0)}; \quad Y(\tau) = 2 (\alpha_0 + \alpha_1 \tau) \sqrt{\tau} + H.$$
(33)

1579



Fig. 2. Dependence of θ_0 and θ_1 on y in crystallization of a particle on a coating layer which is quite distant from the substrate and the dependence of θ'_0 and θ'_1 on y in the case of a thermophysically homogeneous coating; β is the plane of contact of the particle with the coating.

Here $\alpha_1 = -0.013$, while α_0 is the root of the equation

$$\alpha \left(1 + \Phi \left(\alpha\right)\right) \exp \alpha^{2} = B . \tag{34}$$

The quantity *B* for metals and high-temperature ceramics at $T_{in} = 290$ K is very close to unity ([3], p. 280); therefore, when B = 1 from (34) we obtain $\alpha_0 = 0.5$. Substituting the values of $Y(\tau)$ from formulas (33) into (22), we will have

$$H = 2 (\alpha_0 + \alpha_1) = 0.97 . \tag{35}$$

Thus, the function $Y(\tau)$ exactly satisfies relations (22). Having substituted expressions (32) and (33) into relations (21) and (23), we find that the latter are fulfilled in the crystallization interval approximately; the left-hand side differs from the right-hand side by less than 2% in (21) and by less than 4% in (23). Furthermore, when y = -H, according to (29) we have

$$\theta_0 < 0.012$$
 . (36)

Thus, expression (32) is an approximate solution of the boundary-value problem (10)–(16), and with account for (36) it is an approximate solution of the problem of crystallization of a particle on a multilayer coating. The dependence of θ_0 and θ_1 on y for $\tau = 1$ is presented in Fig. 2. According to (32) and (29), the reduced temperature $\theta_{1\text{cont}}$ of contact of a particle is expressed as follows:

$$\theta_{1\text{cont}} = \theta_1 \Big|_{y=H} = \frac{1}{1 + \Phi(\alpha_0)} \left[1 + \exp(2KH + K^2 \tau) \Phi^* \left(\frac{H}{\sqrt{\tau}} + K\tau \right) \right].$$
(37)

It follows from (37) that, as τ increases from 0 to 1, $\theta_{1\text{cont}}$ increases slowly from the initial value $1/(1 + \Phi(\alpha_0))$ to a magnitude 14% higher than this value (Fig. 3). The quantity $1/(1 + \Phi(\alpha_0))$ is a reduced temperature of contact of the particle with the coating in the case $\lambda_{\text{coat}} = \lambda_1$.

The temperature distributions according to the above solution differ significantly from the temperature distribution according to the solution of [2], where the coating was considered as a homogeneous semibounded body with a thermal-conductivity coefficient λ_{coat} . For comparison, Fig. 2 presents the reduced temperatures θ_0 and θ_1 and θ'_0 and θ'_1 as functions of y at the instant of completion of crystallization ($\tau = 1$). The function θ'_0 , i.e., the distribution of the reduced temperature in the coating, and the function θ'_1 , i.e., the distribution of the reduced temperature in the particle, are calculated from the solution mentioned [2] of the problem where the coating is considered as a homogeneous material and the reduced height which corresponds to this solution is denoted as H'.



Fig. 3. Dependence of θ_{1cont} on τ in crystallization of a particle on the first layer of the coating (1) and on the second and subsequent layers of the coating (2).

The solution (27) obtained for description of the thermal fields in crystallization of a particle on the coating layers located at a distance from the substrate can be employed with the corresponding replacement of the quantities for the remaining layers as well (in particular, for the layers located near the substrate), as will be done below. The reduced thickness H_1 of the first layer of the coating can be determined based on the known solution [2] for thermal processes in crystallization of a particle on the substrate. Let us consider the case where the thermal-conductivity coefficient of the substrate is substantially higher than the thermal-conductivity coefficient λ_1 of the coating layer and $T_{in} = 290$ K. Setting $A^2 = 10$ and B = 1, according to [2] we obtain $H_1 = 1.34$.

Let us turn to a description of the thermal fields in crystallization of a particle in the first layer in the case indicated. The difference of this problem from the previous one is that the thickness of the layer in which the particle is crystallizing is known, as is the contact resistance determined in the first problem. In this case, the boundary-value problem in dimensionless quantities will be described by relations (10)–(16) with the replacement of H by H_1 in condition (11); in condition (13), it is only the first equality that is left with replacement of H by H_1 . The quantity R_{cont} is determined in the previous problem and is described by the formula reduced in (9) for H which is given in (35). Accordingly in the auxiliary problem for an unbounded composite solid body, H in condition (20) is replaced by H_1 , while in condition (22) only the first relation is left with replacement of H by H_1 . The approximate solutions are sought in the form (32) with the value of c_0 determined from formula (33) and with the following expression for $Y(\tau)$:

$$Y(\tau) = 2 (\alpha_0 + \alpha_1 \tau) \sqrt{\tau} + H_1; \quad \alpha_1 = -0.004.$$
(38)

According to (38), the reduced thickness H_2 of the second layer of the coating is as follows:

$$H_2 = 2\alpha_0 + 2\alpha_1 = 0.992$$
.

The solution obtained approximately satisfies conditions (21) and (23); the left-hand side differs from the right-hand side by less than 1% in (21) and by less than 2% in (23). The reduced temperature $\theta_{1\text{cont}}$ of contact of the particle is described by formula (37) with replacement of *H* by *H*₁. The quantity $\theta_{1\text{cont}}$ in this case is close to the constant $1/(1 + \Phi(\alpha_0))$, differing from it by less than 5% only at the end of crystallization (Fig. 3). In a similar way, solving the problems of crystallization on the second and subsequent layers, we arrive at the conclusion that these solutions coincide, in practice, with the solution obtained earlier for layers which are at a distance from the base. The contact temperature in crystallization of the particle on the first layer is lower than on the other layers of the coating, which is explained by its larger thickness produced by a thermal conductivity of the base substantially higher than that of the layer. The found decrease in the temperature substantiates the assumption of a number of researchers that the decrease in the strength of the coating near the substrate is related to a possible decrease in the contact temperature of the particles at this site; the cohesive strength of the particles strongly depends on the contact temperature ([1], p. 134). Within the framework of the investigations performed it is shown that despite the possibility of $\lambda_{\text{coat}} \ll \lambda_1$, the contact temperature of a particle is comparatively close to the contact temperature for $\lambda_{\text{coat}} = \lambda_1$.

NOTATION

 T_i , temperature, λ_i , thermal-conductivity coefficient; χ_i , thermal-diffusivity coefficient; ρ_i , specific weight; c_i , specific heat (i = 1 refers to the values of the temperatures and to the thermophysical properties in the region $x \ge 0$, while i = 0 refers to these values and properties in the region x < 0); L, specific heat of hardening of the particle material; X(t), coordinate of the crystallization front; h_1 , thickness of the first layer of the coating; x, coordinate; t, time; λ_1 , thermal-conductivity coefficient of the solid phase of the particle; λ_{coat} , thermal-conductivity coefficient of the coating of the material of one layer of the coating of thickness h. Reduced quantities: τ , time; τ_{cr} , crystallization time of the particle, $\tau_{\text{cr}} = 1$; y, coordinate; y', integration variable; H, thickness of the coating layer at a distance from the substrate; Y(t), coordinate of the crystallization front; θ_i , temperature; r_{cont} , specific contact thermal resistance.

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