INVESTIGATION OF THE TEMPERATURE FIELDS IN STRUCTURAL STEELS TAKING STRUCTURAL AND PHASE TRANSFORMATIONS INTO ACCOUNT

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The article presents the solution of the heat-transfer equation in a metal wall subjected to pulsed thermal effect, taking into account the dynamics of a number of structural and phase transformations, both in heating and cooling.

The numerous investigations dealing with the calculation of temperature fields in steels contained in the literature are based on the homogeneity of the materials and on the thermophysical characteristics of the material being independent of the current structure and phase state. On the other hand, in the practical operation of various products made of high-strength alloy steels, conditions may arise when structural and phase changes occur in the steel under the effect of high temperatures, and these are accompanied by a transformation of the structure according to the scheme initial α-phase of the steel (sorbite) — γ-phase (austenite), phase and thermal effects including the formation of a molten film entailing additional heat absorption. When the thermal load is removed and the material rapidly cooled, the high-temperature γ-phase is supercooled to temperatures of martensitic transformation (γ-phase — hardened α-phase). The process may be complicated by cyclic application (removal) of the thermal load, and consequently by cyclic phase and temperature strains; this is one of the causes why a network of fatigue cracks appears in the surface layers of the metal [1].

To provide a correct understanding of the processes occurring during heating and cooling of steel, and to devise a mathematical model of carrying out thermal calculations, we will deal with the characteristic of zones which may originate in steel exposed to cyclic heating and cooling.

In heating (Fig. 1) we can distinguish the following zones: of melt (ZM), of metal with austenitic structure (ZA), of austenitic transformation (ZAT), and of metal with the initial structure (IM). In cooling, the metal (Fig. 1) in zones containing austenite is subjected to martensitic transformation, and a quenched zone (ZQ) forms.

The zone of melt is characterized by the absence of crystalline bonds in the structure of the metal. In it, an amount of heat equivalent to the temperature of the intercrystalline bonds of the lattice of the metal is absorbed. Depending on the actual conditions of heating, the forming molten film may either be retained on the surface of the metal, it may run off freely under the effect of mass forces, or it may flow and disintegrate under the effect of external distorting forces.

The ZA is metal in which the processes of austenitic transformation have been brought to full completion. The thermophysical characteristics (TPC) of the steel in this layer depend only on the temperature.

The ZAT is characterized by processes of rearrangement of the structure of the steel throughout the thickness of the material. Here the TPC and the temperature of the phase transformation depend on the temperature and degree of transformation of the initial structure into austenitic structure, and they change from the values at the boundary of IM with ZAT to the values at the boundary of ZAT and ZA. The degree of transformation η is determined by the fraction of the elementary volume of the material in which transformation has occurred by the instant in question.

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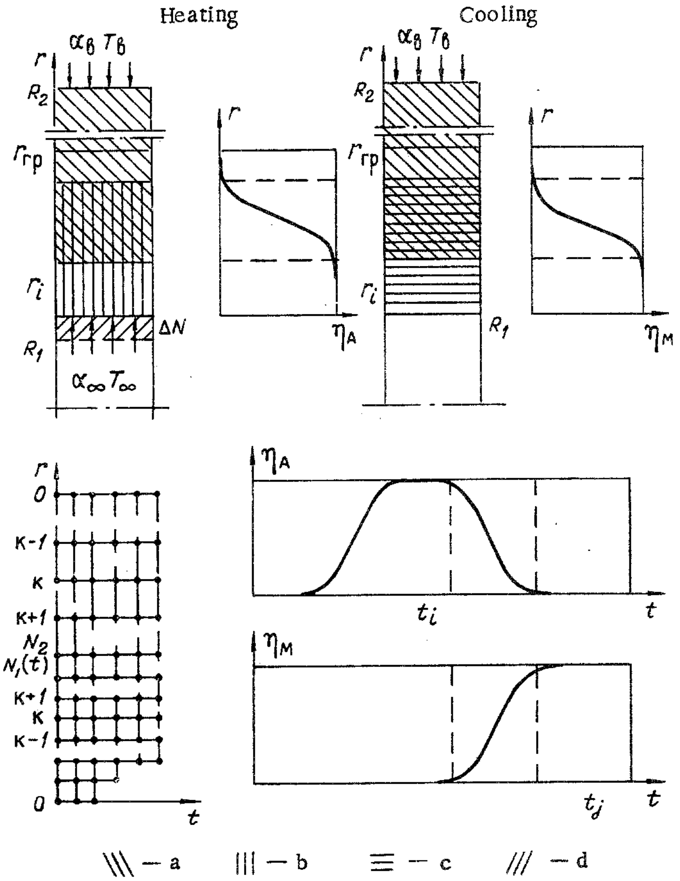

Fig. 1. Diagram of the structure and phase transformations in steel: a) initial structure (IM); b) austenitic (ZA); c) quenched (QM); d) melt (ZM).

The zone IM is characterized by regularities of heat propagation that are analogous to those in materials without structure and phase transformations. In this case, the TPC are functions of the temperature only.

As heating of the material proceeds, all the different kinds of zone form in the metal and gradually change from one into the other.

When steel is cooled to below the temperature of incipient martensitic transformation T_ξ^M, a zone of quenched structures forms in the zones ZA and ZAT. In the layer, which during heating was the zone ZA, there are austenitic and martensitic structures, and in the ZAT there is the initial structure, austenite, and martensite forming in the austenitic region. The processes of rearrangement of the zones occur continuously in time, and this leads to complex relationships of the TPC in them, and consequently also to the complex nature of the formation of the temperature field in a steel wall.

We will calculate the temperature fields in the zones with the aid of the following general equation of heat conduction:

$$c(T,\ \eta)\,\rho(T,\ \eta)\,\frac{\partial T}{\partial t} = \frac{1}{r^m}\,\frac{\partial}{\partial r}\left[\lambda(T,\ \eta)\,r^m\,\frac{\partial T}{\partial r}\right] + \sum_{i=1}^{2} Q_i(T,\ \eta)\,\delta(T - T^*), \tag{1}$$

where m = 0, 1, 2 is a flat wall, a hollow cylinder, and a hollow sphere, respectively; $T^* = T_\xi^{me}$ in melting; $T^* = T_\xi^A$ in austenitic transformation. The function

$$\delta(T - T^*) = \begin{cases} 1 & \text{for } T \geqslant T^*, \\ 0 & \text{for } T < T^*. \end{cases}$$

The boundary conditions for solving Eq. (1) on the assumption that the molten film is instantaneously removed ($\delta(T - T_\xi^{me}) = 0$) has the form

$$T(r, 0) = T_0(r), \qquad \eta(r, 0) = \eta_0(r), \tag{2}$$

where $R_1 \leqslant r \leqslant R_2$; $R_1 = R_1^0$ is a cylinder or sphere; $R_1 = 0$ is a flat wall; $R_2 = l^0$ is a flat wall;

the boundary conditions are

$$-\lambda(T, \eta)\frac{\partial T}{\partial r} = \alpha_\infty(t)\,[T_\infty(t) - T(R_1, t)] - Q_{me}; \tag{3}$$

$$\lambda(T)\frac{\partial T}{\partial r} = \alpha_B(t)\,[T(R_2, t) - T_B(t)].$$

The values Q and Q_{me}, characterizing heat sinks in the processes of bulk austenitic transformation and of frontal melting of the steel on the inner wall surface, respectively, are calculated by the dependences

$$Q = \sum_{i=1}^{n}\left[q_{fm}^{i}\frac{d(\rho\eta)}{dt}\right]; \quad Q_{me} = q_{me}\rho(T_{me})\,v_{me} \tag{4}$$

The melting rate v_{me} is determined from the speed with which the temperature T_ξ^{me} propagates into the bulk of the material. The assumption that the molten layer is instantly removed leads to the equations

$$v_{re} = v_{me}; \tag{5}$$

$$R_1 = R_1^0 + \int_0^t v_{re}(t)\,dt; \qquad l = l^0 - \int_0^t v_{re}(t)\,dt. \tag{6}$$

The thermophysical characteristics of the steel in different zones, necessary for solving the problem, are determined in the following way. When steel is impulse-heated and subsequently rapidly cooled, nonequilibrium phases form in it and exist for some time. For instance, the initial α-phase overheated by 100-300°C, and the high-temperature γ-phase supercooled by 800-900°C. The great difference in the thermophysical properties of the phases makes it impossible to use reference data because these refer to the equilibrium state of steel, and it would be necessary to establish the regularities of their change in each zone.

The Zone IM. For steels with a not strain-hardened initial structure, the first point of phase equilibrium is the point of beginning austenitic transformation corresponding to the temperature $T_\xi^A = (0.5 - 0.7)\,T_\xi^{me}$. An analysis of the temperature dependences of the thermophysical characteristics in this region [2-5] shows that for the equilibrium phases applies

$$\rho_\alpha = a - bT; \quad c_\alpha = c_a + c_M; \quad \lambda_\alpha = \sum_{i=1}^{n} a_i T^{n-1}, \tag{7}$$

where $n = 3$; $c_a = a_1 + b_1 T$; $c_M = a_2 + \exp(-b_2/T)$.

The thermal conductivity of the α-phase is characterized by its decrease with increasing temperature.

When the α-phase is in a nonequilibrium state, the heat capacity c_α can be obtained by calculation by the mixing formulas, and density and thermal conductivity by the linear extrapolation of the dependences that apply to the equilibrium α-phase.

The Zone ZA. The equilibrium γ-phase exists from the temperatures T_ξ^A to T_ξ^{me}. An analysis of the data on the thermophysical characteristics of steels in this temperature range shows that density, heat capacity, and thermal conductivity are linear functions of the temperature. When the γ-phase is cooled to below the temperature of phase equilibrium

TABLE 1. Densities (kg/m³) of the Equilibrium Phases of Steel, $\rho_\alpha = a - bT$; $\rho_\gamma = A - BT$

Coefficients	Brand of steel								
	35-KhN3MF	30KhN3 [5]	30N3 [5]	30Kh [5]	steel 35 [5] hardened	steel 35 [5] annealed	steel 35 [1] hardened	steel 35 [1] annealed	steel 40 [5]
α-phase									
a, kg/m³	7936	7943	7954	7927	7895	7939	7884	7952	7966
$b \cdot 10^6$, kg/m³·°K	340	318	317	340	300	360	264	325	359
γ-phase									
A, kg/m³	8126	8141	8169	8089	8147		8283		8182
$B \cdot 10^6$, kg/m³·°K	476	460	480	450	510		527		506

at rates exceeding the critical hardening rate [6], it may occur in the steel up to the temperature of the end of martensitic transformation. In such a nonequilibrium γ-phase, density, heat capacity, and thermal conductivity of the material are determined analogously to the way it is done with the α-phase. A special feature of the nonequilibrium γ-phase is the absence of a magnetic peak of heat capacity and the decrease in thermal conductivity upon cooling.

The Zone ZAT. Density, heat capacity, and thermal conductivity in this zone depend on the temperature and degree of austenitic transformation of the metal η, i.e.,

$$\rho_{(\alpha+\gamma)}(T,\ \eta) = \left[\frac{\eta}{\rho_\gamma(T)} + \frac{1-\eta}{\rho_\alpha(T)}\right]^{-1}, \tag{8}$$
$$c_{(\alpha+\gamma)}(T,\ \eta) = c_\alpha(T)(1-\eta) + c_\gamma(T)\eta.$$

Proceeding from the peculiarities of the kinetics of austenite formation in steel, we can represent the metal in the form of a structure with closed inclusions of α-phase in the matrix of the forming γ-phase. Then we can calculate the thermal conductivity of the mixture by Odelevskii's formula [7]

$$\lambda_{(\alpha+\gamma)} = \lambda_\gamma\left[1 - (1-\eta)/\left(\frac{\lambda_\gamma}{\lambda_\gamma - \lambda_\alpha} - \frac{\eta}{3}\right)\right]. \tag{9}$$

The data on the thermophysical characteristics of the α-phase and γ-phase, necessary for the calculation, are presented in Table 1. This table also contains the experimental values of the characteristics for steel 35KhN3MF. The investigations were carried out at the A. V. Lykov Institute of Heat and Mass Exchange, Academy of Sciences of the BSSR, on a high-temperature installation which was described in detail by Shashkov and Tyukaev [8].

The degree of austenitic transformation η is determined by the kinetic Arrhenius-type equation

$$d\eta/dt = K_0(1-\eta)^n \exp(-E/RT). \tag{10}$$

The constants K_0, n, and E are individual characteristics of the steels, they depend on the composition of the steels and are determined experimentally. To calculate these constants, the Leningrad Mechanical Institute used a dilatometer type "tube in a tube" with electronic displacement sensor to heat and cool steel specimens, to record the change in length of the specimens, and to plot the dependences η = f(T, t). From these curves, the kinetic constants were determined on the basis of the condition of minimization of the discrepancy function type

$$\min\left\{F^i = \sum_{j=1}^{N}\left[\ln K_{fj}^i - \left(-\frac{E^i}{RT_j} + \ln K_{0j}^i\right)\right]^2\right\},$$

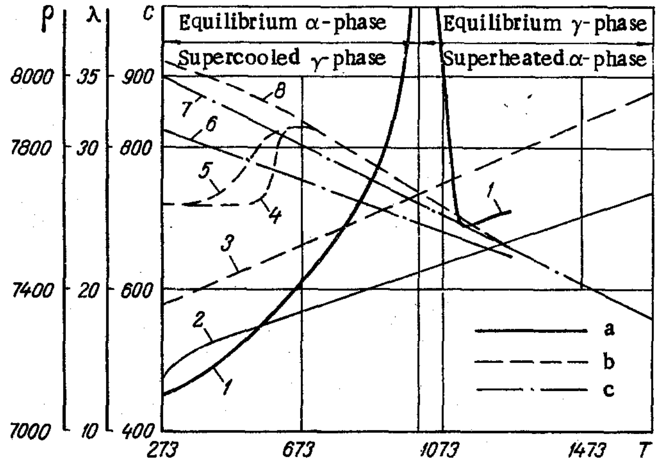

Fig. 2. Change in the thermophysical characteristics of steel 35KhN3MF in dependence on the temperature: 1, 6) α-phase; 2, 3, 7) γ-phase; 4, 5) hardening α-phase (4) rapid heating; 5) slow heating); 8) initial α-phase; a) heat capacity; b) thermal conductivity; c) density. T, °K; c, J/kg · °K; λ, W/m² · °K; ρ, kg/m³.

where j is the number of experimental points ($1 \leqslant j \leqslant N$). For steel 35Kh3MF the following constants were obtained: n = 1.68; E/R = 805,000; ln K_0 = 72.

The temperatures of the phase transformations were taken from [9], the melting points are experimental results. For steel 35Kh3MF of average chemical composition, this value, obtained on the installation of the Institute of Heat and Mass Transfer, is close to the melting point of pure iron and amounted to q_{me} = 271500 J/kg. The experiments were carried out at normal pressure in an argon atmosphere. Melting of the steel occurred in the temperature interval 1720-1840°K.

The Zone of Hardening. In continuous cooling, the martensitic transformation below the temperature T_E^M occurs both in the zone of austenitic transformation (ZAT) and in the zone of steel with the structure of the γ-phase (ZA). The available data [5, 6, 9] as well as dilatometric investigations show that in the temperature range of martensitic transformation, the density and heat capacity of the initial structure and of the forming hardened α-phase are similar, and that they therefore can be determined by formulas (7). The thermal conductivity of the hardened structures of steel is substantially lower than the initial structures of high tempering. For carbon steels it may be accepted according to the data of [5, 9, 10] (Fig. 2). In the formation of martensite in steel in the zone ZA, the metal may be regarded as a two-phase structure with interpenetrating components since the martensite forms in the form of needles or platelets. For such structures, the following relationships [11] may be used:

$$\lambda_{(\gamma+M)} = \lambda_M [c^2 + \nu (1-c)^2 + 2\nu c (1-c)/(\gamma c + 1 - c)];$$

$$\nu = \lambda_\gamma / \lambda_M; \quad c = 0.5 + a \cos(\varphi/3); \tag{11}$$

$$a = -1, \quad \varphi = \frac{3}{2}\pi + \arcsin(1 - 2m) \quad \text{for } m \in \{0;\ 0.5\};$$

$$a = 1, \quad \varphi = \frac{3}{2}\pi + \arcsin(2m - 1) \quad \text{for } m \in \{0.5;\ 1.0\};\ m = 1 - \eta.$$

When the martensitic transformation occurs in the zone of incomplete austenitic transformation, i.e., there is a mixture of three components in which martensite and austenite are the matrix with interpenetrating components, and the initial α-phase is a closed inclusion, the principle of successive reduction of the structures to the binary structure [11] is applied. For instance, the thermal conductivity of such a mixture is determined by the formula

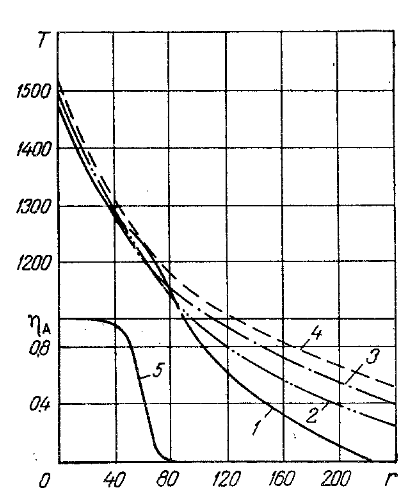

Fig. 3

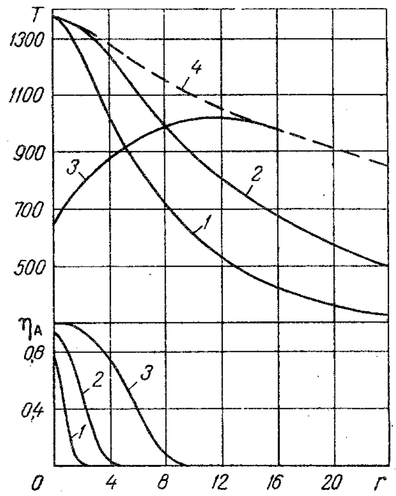

Fig. 4

Fig. 3. Effect of impulse friction on the formation of the temperature field and the degree of transformation of the initial structure of the steel (pair Cu—Fe, $t_B = 10^{-4}$ sec, $T_0 = 293°K$, $T_\infty = 1370°K$): 1) $\bar{t} = 2.02$; 2) 0.5; 3) 1; 4) envelope of the maximum temperatures; 5) degree of transformation.

Fig. 4. Effect of nonlinear (1) and partially linear (2-4) statements in solving the system of equations (1)-(12) on the maximum temperatures and depth of transformation: 2) without taking the structure-phase transformations into account; 3) TPC = TPC of the γ-phase; TPC = const.

$$\lambda_{(\alpha+M+\gamma)} = \lambda_{(M+\gamma)}\left[1-(1-\eta)/\left(\frac{1}{1-\nu_2}+\frac{\eta}{3}\right)\right], \tag{12}$$

where $\nu_2 = \lambda_\alpha/\lambda_{(M+\gamma)}$, and the thermal conductivity of the component $\lambda_{(M+\gamma)}$ is determined by relationships (11) in which we have to put $m = (\eta-\eta_M)/\eta$.

The kinetics of martensitic transformation is diffusionless and is characterized by zero activation energy [6-10], therefore the relationship $\eta_M = f(T)$ can be obtained directly from dilatometric investigations. For steel 35KhN3MF at temperatures of 220, 380, 470, 500, 520, 530, 540, 560, 570°K, the degree of transformation η_M is equal to 1.00, 0.93, 0.79, 0.68, 0.58, 0.49, 0.35, 0.06, 0, respectively.

The associated system of equations (1)-(2) was solved by the digital method of matching by regions [12]. The approximation of the equation of thermal conductivity and of the boundary conditions by the method of the implicit triangle was used. The approximating equations and the matching relationships have the form:

$$T_{\kappa-1}^{l+1} = x_\kappa T_\kappa^{l+1} + y_\kappa \quad (\kappa = 0,\ 1,\ 2,\ \ldots,\ N);$$

$$x_0 = (2\lambda_{\kappa-1/2}^{l+1} - \alpha^{l+1}h)(2\lambda_{\kappa-1/2}^{l+1} + \alpha^{l+1}h)^{-1};$$

$$y_0 = 2\alpha^{l+1}T_1^{l+1}h(2\lambda_{\kappa-1/2}^{l+1} + \alpha^{l+1}h) - Q_{me}\rho^{l+1}(T_\xi^{me})\frac{h_1^2}{\tau_i\lambda_{\kappa-1/2}^{l+1}}\Delta N\delta(T_1^{l+1} - T_\xi^{me});$$

$$x_{\kappa+1} = -\frac{C_{\kappa+1}}{B_{\kappa+1} + A_{\kappa+1}x_\kappa}; \qquad y_{\kappa+1} = \frac{D_{\kappa+1} - A_{\kappa+1}y_\kappa}{B_{\kappa+1} + A_{\kappa+1}x_\kappa};$$

$$A_{\kappa+1} = \frac{1}{(c\rho)_\kappa^{l+1}}\left(\frac{\lambda_{\kappa-1/2}^{l+1}}{h^2} - \frac{m\lambda_\kappa^{l+1}}{2hr_\kappa}\right);$$

$$B_{\kappa+1} = -\left(\frac{1}{\tau_i} + \frac{2}{h^2}\frac{\lambda_\kappa^{l+1}}{(c\rho)_\kappa^{l+1}}\right);$$

$$C_{\kappa+1} = \frac{1}{(c\rho)_\kappa^{l+1}}\left(\frac{\lambda_{\kappa+1/2}^{l+1}}{h^2} + \frac{m\lambda_\kappa^{l+1}}{2hr_\kappa}\right);$$

$$D_{\kappa+1} = -\frac{T_\kappa^l}{\tau_i} - q_{fm}\frac{\rho_\kappa^{l+1}}{(c\rho)_\kappa^{l+1}}K_{fk}^{l+1}(1-\eta_\kappa^{l+1})^n\,\delta(T_\kappa^{l+1} - T_\xi^A);$$

$$K_f = K_0\exp(-E/RT);\quad \eta(t) = 1 - \left[1 + (n-1)\int_0^t K_f\,dt\right]^{\frac{1}{1-n}};$$

$$\int_0^t K_f\,dt = \frac{\tau_i}{2}K_0[\exp(-E/RT_\kappa^{l+1}) + \exp(-E/RT_\kappa^l)].$$

For the subregion 1, $\alpha = \alpha_\infty$; $h = h_1$; $T_1 = T_\infty$; $N = N_1$. For the subregion 2, $\alpha = \alpha_B$; $h = h_2$; $T_1 = T_H$; $N = N_2$. The condition of conjugation of the subregions is the following:

$$T_{N_1}^{l+1} = T_{N_2}^{l+2} = \left(\frac{\lambda_{N_1-1/2}^{l+1}}{h_1}y_{N_1} + \frac{\lambda_{N_2-1/2}^{l+1}}{h_2}y_{N_2}\right)\left[\frac{\lambda_{N_2-1/2}^{l+1}}{h_2}(1-x_{N_2}) + \frac{\lambda_{N_1-1/2}^{l+1}}{h_1}(1-x_{N_1})\right]^{-1}.$$

The problem was realized in the form of an ALGOL program for a BÉSM-6 computer. The step along the coordinate h and time τ was selected by the method of successive approximations. The specified convergence of the solution (ε = 0.001) was attained in dependence on the conditions of heating with $h = (0.1\text{-}5)\cdot 10^{-6}$ m and $\tau = (0.001\text{-}0.01)t_B$, where t_B is the total heating time. As an example, Figs. 3 and 4 show the results of the calculation of a metallic cylindrical wall with boundary conditions corresponding to the third and first kind, respectively. Figure 4 shows the maximum temperatures in the surface layer for a number of theoretical cases. The obtained theoretical data on the depths of the zones of phase transformations agree with the experimental values determined on microsections [13].

NOTATION

t, $\bar{t} = t/t_B$, time; τ, time step; h, step along the coordinate; T*, critical temperature; T, current temperature; η, degree of transformation; r, longitudinal coordinate; R_1, R_2, inner and outer radius, respectively, of a hollow cylinder (sphere); l, thickness of the platelet; λ, thermal conductivity; α, heat-transfer coefficient; Q, internal heat sources (sinks); ρ, density of steel; v_{me}, melting rate; c, heat capacity; K_0, preexponent; n, order of the reaction; K_{fm}, coefficient of the transformation rate; E, activation energy; R, universal gas constant; x, y, matching coefficients. Subscripts: M, martensite; A, austenite; ξ, critical value; α, α-phase; γ, γ-phase; 0, initial value; ∞, B, inner or outer parameters; K, coordinate index; l, time index; i, number of iterations; me, melting.

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VARIATIONAL METHOD OF CRACK-CONTOUR LOCATION FOR THREE-DIMENSIONAL PROBLEM WITH UNILATERAL CONSTRAINTS

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Extremal properties are established for the solution of the problem of cohesionless normal-rupture crack formation: namely, that the true contour of a Christianovich crack corresponds to the maximum volume of the cavity. Examples of the application of this principle are considered.

Mathematical Model of Christianovich Crack in an Elastic Body

In an elastic space compressed at infinity by a uniform stress σ, acting perpendicularly to the plane $S : z = 0$, forces symmetric with respect to S but in the opposite direction are applied, leading to the formation of normal rupture over a certain part of this plane of maximum tensile stress (breakdown). If the effect of the cohesive forces of the material over the S plane may be neglected in comparison with the applied forces, the resulting check (slit) may be described using the Christianovich model [1-4], developed in the context of the mechanics problems of hot rocks (for an evaluation of the limits of applicability of this cohesionless approximation to applied problems, see [5]).

In formulating the problem, the scheme of [4] is followed. Suppose that two half spaces with identical elastic properties (which may vary over the depth) are pressed together by a uniformly distributed stress $\sigma_{zz} = -\sigma$ (Fig. 1). Identical but opposite loads $q(\mathbf{r})$ tend to break the contact between these half spaces (such loads acting on the contour of the developing slit also result, as is known, from the above-mentioned volume forces disrupting the material [6, 7]). The displacements $\pm w(\mathbf{r}, \sigma)$ of the contours of the plane slit developing in the body, of unknown shape G_σ in plan, and the normal pressure on the half spaces composing the body $p(\mathbf{r}, \sigma) = -\sigma_z|_S$ must satisfy on S conditions in the form of alternating equalities and inequalities

$$\begin{gathered} p(\mathbf{r}, \sigma) = q(\mathbf{r}) - \sigma, \quad w(\mathbf{r}, \sigma) > 0, \ \mathbf{r} \in G_\sigma, \\ p(\mathbf{r}, \sigma) \geqslant q(\mathbf{r}) - \sigma, \quad w(\mathbf{r}, \sigma) = 0, \ \mathbf{r} \in S \setminus G_\sigma. \end{gathered} \tag{1}$$

Here and below, in view of the symmetry, the conditions are written only for the upper half space; $\mathbf{r} = (x, y)$ is a point of S. There are no tangential stresses nor cohesive forces at S. The inequalities in the conditions of Eq. (1) (unilateral constraints) reflect the physically clear requirement of "nonoverlapping" of the slit edges and the absence of a resulting tensile stress on the continuation of the slit — in the region of overlap of the half spaces (see also [8]). In the given formulation, this problem of the breakdown of an

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