DIFFUSION THEORY OF THE ANELASTICITY OF METALS

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The notion of the redistribution of atoms during deformation of metals was first put forward by V. S. Gorskii, who laid the foundation of the diffusion aftereffect theory. This notion was developed in S. T. Konobeevskii's studies of the effect of nonuniformity of the stress state on diffusion in isothermal processes. A further development of the theory of the effect of the stress state on the diffusion process in solid solutions may be found in [1, 2]. The principles of the diffusion theory of creep of metals were developed in a number of investigations of B. Ya. Pines [3]. General linear differential equations taking into account the interaction between the processes of diffusion, heat conduction, and deformation are derived from principles of the thermodynamics of irreversible processes in [4].

It is necessary to point out, however, that in all the investigations known to us the diffusion processes are related only to the gradient of the first invariant of the stress tensor (average pressure), owing to which in the described solids all the laws governed by the irreversibility of the physical processes are virtually the same as those pertaining to fluids. In particular, the diffusion processes only condition the relaxation of the average pressure, whereas the stress deviator remains thermodynamically stable.

This may be attributed, in particular, to the fact that the physical state of a solid, like that of a liquid, is characterized by a scalar – the mass density. At the same time, the resistance of solids to shear stresses in the state of mechanical equilibrium clearly distinguishes them from liquids, in which shear stresses, in conformity with existing models, can arise only as a result of mechanical motion. Therefore, in the general case of deformation of solids the distribution of mass may be nonisotropic. Hence it follows that the physical state of a solid should be characterized not by the scalar density ρ but by a certain tensor quantity ρ.

On the basis of these considerations a system of differential equations and boundary conditions for determining the state of a certain theoretical model of metal bodies (treated as solid isotropic solutions) is derived below by the methods of the mechanics of continua and the thermodynamics of irreversible processes [5, 6]. It is shown that the known rheological relationships between stress and strain tensors and their velocities, derived from the general principles of the thermodynamics of irreversible processes without introducing any model concepts, follow from the proposed diffusion theory as a particular case, provided that the irreversibility of the processes is determined only by the presence of fluxes through the surface of the body and the irreversibility associated with fluxes inside the body is disregarded.

1. Density tensor. Starting equations

Henceforth we will treat a solid as a continuum filling a part or the whole of the space in which the rectangular Cartesian coordinate system $x_1x_2x_3$ is established.

Let us examine in the initial state two infinitely close small particles of a medium whose centers of mass are located at points M and M_1. Assuming in the initial state $MM_1 = dl_0$, we construct with this segment as edge a substantive cube with volume $dV_0 = (dl_0)^3$ containing mass dm, and define the density ρ_0 and specific volume v_0 at point M, as usual by the relations

$$\rho_0 = dm \,/\, dV_0, \qquad v_0 = dV_0 \,/\, dm\,. \tag{1.1}$$

Designating by **1** the unit vector in direction MM_1, we will call the quantity $dV_l = (dl)^3/3$, where dl is the distance between the considered two particles of the medium in any state, the elementary volume at point M in direction **1**.

The density ρ_l and specific volume v_l of the body at point M in direction **1** we define as

$$\rho_l = dm \,/\, dV_l, \qquad v_l = dV_l \,/\, dm\,. \tag{1.2}$$

By virtue of these definitions we obtain

$$\begin{aligned} \rho_l &= \rho_0 \left({}^1/_3\delta_{ij} - e_{ij}\right) \cos\,(l,\, x_i) \cos\,(l,\, x_j) \\ v_l &= \rho_0^{-1} \left({}^1/_3\delta_{ij} + e_{ij}\right) \cos\,(l,\, x_i) \cos\,(l,\, x_j) \end{aligned} \tag{1.3}$$

Here the components e_{ij} of the small strain tensor are related to the components u_i of the displacement vector by

$$e_{ij} = {}^1/_2\,(\nabla_i u_j + \nabla_j u_i)\,. \qquad (1.\,4)$$

It follows from (1. 2)-(1. 4) that in the case under consideration the density and the specific volume of the body at a point are characterized by symmetric tensors of the second rank $\boldsymbol{\rho}$ and $\mathbf{v}$, whose components are

$$\rho_{ij} = \rho_0\,({}^1/_3\delta_{ij} - e_{ij}), \qquad v_{ij} = \rho_0^{-1}V_{ij} \qquad (V_{ij} = {}^1/_3\,\delta_{ij} + e_{ij})\,, \qquad (1.\,5)$$

where δ_{ij} is the Kronecker delta.

We will call tensors $\boldsymbol{\rho}$ and $\mathbf{v}$, respectively, the density tensor and the specific volume tensor of the body at point M. The quantities

$$\rho = \rho_{\alpha\alpha}, \qquad v = v_{\alpha\alpha} = \rho_0^{-1}V_{\alpha\alpha} \qquad (1.\,6)$$

are the average volume density and average specific volume of the body at point M. Note that the tensor V_{ij} was introduced in [2] from other considerations.

We will define the mass flux J as a tensor of the third rank obtained by dyadic multiplication of the velocity vector w and the density tensor

$$\mathbf{J} = \mathbf{w}\boldsymbol{\rho} \qquad (J_{ijk} = w_i\rho_{jk})\,.$$

In this case we have the following equation of conservation of mass

$$d\boldsymbol{\rho}\,/\,d\tau + \boldsymbol{\rho}\,\operatorname{div}\mathbf{w} = 0 \qquad (\tau - \text{time})\,. \qquad (1.\,7)$$

As a result of contraction of (1. 7), in conformity with (1. 6), we obtain

$$d\rho\,/\,d\tau + \rho\,\operatorname{div}\mathbf{w} = 0. \qquad (1.\,8)$$

For solutions, from the equations of conservation for each of the components we can easily obtain

$$d\mathbf{c}_k\,/\,d\tau + \operatorname{div}\mathbf{J}_k = 0 \quad (k = 1, \ldots n) \qquad (\mathbf{c}_k = \boldsymbol{\rho}_k\,/\,\rho,\ \mathbf{J}_k = (\mathbf{w}_k - \mathbf{w})\,\boldsymbol{\rho}_k)\,. \qquad (1.\,9)$$

Here ρ_k is the density tensor, w the center-of-mass velocity, and w_k the velocity of component k. Along with (1. 9), we will also use two other equations of the mechanics of continua, namely, the equation of motion and the equation of conservation of energy

$$\operatorname{div}\boldsymbol{\sigma} = \rho\,\frac{d\mathbf{w}}{d\tau}\,, \qquad \rho\,\frac{du}{d\tau} = -\operatorname{div}\mathbf{J} + \sigma_{ij}\,\frac{de_{ij}}{d\tau}\,. \qquad (1.\,10)$$

Here u is the internal energy of unit mass, J the heat flux vector, $\boldsymbol{\sigma}$ the stress tensor with components σ_{ij}.

2. Internal energy. Equations of state

The change in the internal energy of unit mass of a fluid mixture is given by the Gibbs equation [6]:

$$du = Tds - p\,dv + \mu_k\,dc_k\,. \qquad (2.\,1)$$

Here T is the temperature, s the entropy of unit mass, p the pressure, v the average specific volume, μ_k the chemical potential, and c_k the concentration of component k.

If we are dealing with a solid, then in place of (2. 1) we must write

$$du = Tds + \sigma_{ij}dv_{ij} + \mu_{ij}^{(k)}dc_{ij}^{(k)}\,. \qquad (2.\,2)$$

In particular, for a two-component solution, taking into consideration (1. 5), (1. 6), we obtain

$$du = Tds + \rho_0^{-1}\sigma_{ij}de_{ij} + \mu_{ij}dc_{ij}\,. \qquad (2.\,3)$$

Here μ_{ij} are the components of the chemical potential tensor, and c_{ij} the components of the solute concentration tensor.

With Eqs. (1. 9), (1. 10), and (2. 3) it is no longer difficult, using the theory developed in [7, 8], to obtain all the necessary relationships for determining the state of the body at any instant of time and at any point for small deviations from the state of equilibrium.

By virtue of (2. 3), for the free energy f of unit mass of an isotropic solution we can write

$$\rho_0 (f - f_0) = -{}^1/_2 c T^{-1} t^2 - \alpha K e_{\alpha\alpha} t + {}^1/_3 ({}^1/_2 \beta c_{\alpha\alpha}^2 + \\ + \gamma c_{\alpha\beta}{}^2 - b c_{\alpha\alpha} t) + {}^1/_2 \lambda e_{\alpha\alpha}{}^2 + G e_{\alpha\beta}{}^2 - \lambda' e_{\alpha\alpha} c_{\alpha\alpha} - 2G' e_{\alpha\beta} c_{\alpha\beta} . \tag{2. 4}$$

Here f_0 is the value of the free energy in the initial state; t, c_{ij} the changes in temperature and the components of the concentration tensor relative to the initial state; c the heat capacity; α the coefficient of temperature deformation; λ', G' quantities associated with the coefficients of concentration deformation; λ', G the elastic Lamé constants; and K the bulk modulus; β, γ, b are defined as the first derivatives of the components of the chemical potential tensor with respect to the components of the concentration tensor and the temperature for constant deformation. Of course, the values of the material characteristics introduced depend on the nature of the thermodynamic process.

The following equations of state may be derived from (2. 4):

$$\rho_0 s = c T^{-1} t + {}^1/_3 b c_{\alpha\alpha} + \alpha K e_{\alpha\alpha} , \tag{2. 5}$$

$$\sigma_{ij} = \lambda e_{\alpha\alpha} \delta_{ij} + 2G e_{ij} - (\lambda' c_{\alpha\alpha} \delta_{ij} + 2G' c_{ij}) - \alpha K t \delta_{ij} , \tag{2. 6}$$

$$\rho_0 \mu_{ij} = {}^1/_3 (\beta c_{\alpha\alpha} \delta_{ij} + 2\gamma c_{ij} - b t \delta_{ij}) - (\lambda' e_{\alpha\alpha} \delta_{ij} + 2G' e_{ij}) . \tag{2. 7}$$

3. Entropy. Phenomenological relations

To set up the entropy balance equation we will use equations (1. 9), (1. 11), and (2. 3). Eliminating u and c_{ij}, after some obvious transformations, we obtain

$$\rho \frac{ds}{d\tau} + \operatorname{div} \mathbf{J}_s = \sigma_s \\ \left(T \sigma_s = J_\alpha X_\alpha + J_{\alpha\beta\gamma} X_{\alpha\beta\gamma} , \quad X_i = -\frac{1}{T^2} \nabla_i T , \quad X_{ijk} = -T \nabla_i \frac{\mu_{jk}}{T} \right) . \tag{3. 1}$$

Here J_s is the entropy flux vector, X_i, X_{ijk} the components of the thermodynamic forces, and ∇_i the operator of differentiation with respect to x_i.

In the case of small thermodynamic fluxes, disregarding heat of transfer, for an isotropic body we can write

$$\sigma_s = {}^1/_2 L_q X_\alpha{}^2 + L_1 X_{\beta\alpha\alpha} X_{\beta\gamma\gamma} + L_2 X^2{}_{\alpha\beta\gamma} . \tag{3. 2}$$

Here the phenomenological relations are of the form

$$J_i = L_q X_i , \qquad J_{ijk} = L_1 X_{i\alpha\alpha} \delta_{jk} + 2L_2 X_{ijk} . \tag{3. 3}$$

Substituting into (3. 3) the expressions for the thermodynamic forces from (3. 1) and taking into account (2. 7), we easily obtain relations expressing thermodynamic fluxes in terms of the variables t, e_{ij}, c_{ij}. After linerization these relations have the form

$$J_i = -\lambda^* \nabla_i t , \qquad J_{ijk} = -\frac{\rho_0 D}{3k} (k \nabla_i c_{\alpha\alpha} - b \nabla_i t - 3K' \nabla_i e_{\alpha\alpha}) \delta_{jk} + \\ + \frac{\rho_0 D^*}{3\gamma} [(\gamma \nabla_i c_{\alpha\alpha} - 3G' \nabla_i e_{\alpha\alpha}) \delta_{jk} - 3\gamma \nabla_i c_{jk} + 9G' \nabla_i e_{jk}] \\ (K' = \lambda' + {}^2/_3 G' , \quad k = \beta + {}^2/_3 \gamma) . \tag{3. 4}$$

Here D, D* are diffusion coefficients.

Clearly, the diffusion flux is related not only with the gradient of volume expansion (average pressure) but also with the gradients of each of the components of the strain tensor (stress tensor) individually, as was also pointed out in monograph [3].

Contracting the second equality of (3. 4) with respect to the indices j, k, we find

$$J_{i\alpha\alpha} = -\frac{\rho_0 D}{k} (k \nabla_i c_{\alpha\alpha} - b \nabla_i t - 3K' \nabla_i e_{\alpha\alpha}) . \tag{3. 5}$$

4. System of differential equations. Boundary conditions

We will write the required system of differential equations in displacements.

Substituting into the equation of motion (1. 10) the expressions for the stresses from (2. 6) and using (1. 4), after linearization we obtain

$$\begin{gathered} G\Delta \mathbf{u} + (\lambda + G)\,\mathbf{grad\ div\ u} = \\ = \rho_0 \frac{\partial^2 \mathbf{u}}{\partial \tau^2} + \lambda'\,\mathbf{grad}\ c_{\alpha\alpha} + 2G'\ \mathbf{div\ c} + \alpha K\,\mathbf{grad}\,t\,. \end{gathered} \tag{4. 1}$$

The equation of conservation (1. 9) and relations (1. 7), (3. 4) give

$$\begin{gathered} \frac{D}{3k}(k\Delta c_{\alpha\alpha} - b\Delta t - 3K'\ \mathbf{div}\ \Delta\mathbf{u})\,\delta_{ij} - \frac{D^*}{3\gamma}\,[(\gamma\Delta c_{\alpha\alpha} - 3G'\ \mathbf{div}\ \Delta\mathbf{u})\,\delta_{ij} - \\ - 3\gamma\Delta c_{ij} + \frac{9}{2}G'\Delta\,(\nabla_i u_j + \nabla_j u_i)] = \frac{\partial c_{ij}}{\partial \tau}\,. \end{gathered} \tag{4. 2}$$

Finally, from the equation of conservation of energy, relations (2. 3), (2. 5), and the first equality of (3. 3), we have

$$\varkappa \Delta t = \frac{\partial t}{\partial \tau} + \frac{b}{3c}\frac{\partial c_{\alpha\alpha}}{\partial \tau} + \frac{\alpha K}{c}\frac{\partial}{\partial \tau}\mathbf{div\ u}\,, \tag{4. 3}$$

where $\varkappa$ is the thermal diffusivity.

Thus, for determining ten functions of u_i, $c_{ij} = c_{ji}$, t we have the system of linear differential equations (4. 1)-(4. 3).

To ensure the uniqueness of the solution of this system, additional (initial and boundary) conditions are needed.

In the theory of heat conduction the heat flux through the boundary of a body is frequently subjected to Newton's condition

$$J_\alpha \cos(n, x_\alpha) - h\,(t - t_c) = 0\,. \tag{4. 4}$$

Here n is the exterior normal to the boundary surface, h the heat transfer coefficient, and t_c the temperature of the external medium.

In a number of cases an analogous condition can be assumed with respect to the mass flux

$$J_{\alpha ij}\cos(n, x_\alpha) - {}^1/_3\rho^2 / k\,[H_1(\mu_{\alpha\alpha} - \mu_{\alpha\alpha}{}^c)\,\delta_{ij} + 2H_2(\mu_{ij} - \mu_{ij}{}^c)] = 0\,. \tag{4. 5}$$

Here H_1, H_2 are mass transfer coefficients, μ_c the chemical potential tensor of the solute in the ambient medium.

The boundary conditions applying to the mechanical variables and the initial conditions can be formulated as usual in the linear mechanics of continua and the theory of diffusion and heat conduction.

5. Diffusion theory of deformation and rheology

Some of the equations of the diffusion theory of deformation derived above follow from the basic principles of the thermodynamics of irreversible processes. On the other hand, many rheological relations linking the components of stress tensors and strain tensors and their velocities also follow, as has now been established, from the same principles of thermodynamics. It is natural, therefore, to consider the question of the relation between the differential equations of the diffusion theory of anelasticity and the aforementioned rheological relations.

To simplify the calculations, let us take the case of isothermal processes, since taking finite heat conductivity into account does not introduce any additional effects.

Let us examine Eq. (1. 9), from which Eq. (4. 2) was obtained by means of phenomenological relations (3. 4). Integrating (1. 9) over the volume V occupied by the body and bounded by surface Σ, we find

$$-\int_V \mathbf{div J}\ dV = \int_V \rho \mathbf{c}^{\cdot}\,dV, \tag{5. 1}$$

where the dot means a substantive derivative.

Transforming the volume integral on the left side of (5. 1) into a surface integral and taking into consideration boundary conditions (4. 5), we have

$$-\int_\Sigma \rho^2\ [H_1\,(\mu_{\alpha\alpha} - \mu_{\alpha\alpha}{}^c)\,\delta_{ij} + 2H_2\,(\mu_{ij} - \mu_{ij}{}^c)]\,d\Sigma = 3k\int_V \rho c_{ij}{}^{\cdot}\,dV. \tag{5. 2}$$

We now assume that the thermodynamic states of the body and of the ambient medium are each individually homogeneous. Then, in place of (5. 2) we obtain

$$H_1\mu_{\alpha\alpha}\delta_{ij} + 2H_2\mu_{ij} + 3\frac{kd}{\rho}c_{ij}^{\cdot} = H_1\mu_{\alpha\alpha}{}^c\delta_{ij} + 2H_2\mu_{ij}{}^c \qquad \left(d = \frac{V}{\Sigma}\right), \tag{5. 3}$$

where d is the average dimension of the region accupied by the body.

Eliminating the quantity c_{ij} from (2. 6), (2. 7), and (5. 3) and using the general thermodynamic relations, for the spherical part of the corresponding tensors we find

$$\sigma_{\alpha\alpha} + n\sigma_{\alpha\alpha}^{\cdot} = 3K_\mu e_{\alpha\alpha} + 3nK_c e_{\alpha\alpha}^{\cdot} - 3\frac{\rho K_c K_\sigma'}{k_e}\mu_{\alpha\alpha}{}^c. \tag{5. 4}$$

Here K_μ and K_c are values of the bulk modulus for constant $\mu_{\alpha\alpha}$ and $c_{\alpha\alpha}$,

$$K_\mu = K_c\frac{k_\sigma}{k_e}, \qquad n = \frac{d}{H}\frac{k_\sigma}{k_e}, \qquad H = H_1 + \frac{2}{3}H_2, \tag{5. 5}$$

k_σ, k_e are values of the coefficient k for constant $\sigma_{\alpha\alpha}$ and $e_{\alpha\alpha}$, and, finally, λ_σ', G_σ' are values of the coefficients λ' and G' for constant $\sigma_{\alpha\alpha}$.

Analogous dependences are also obtained between the components of the deviatoric parts of the stress and strain tensors and their derivatives:

$$\sigma_{ij}{}^d + m(\sigma_{ij}{}^d)^{\cdot} = 2G_\mu e_{ij}{}^d + 2mG_c(e_{ij}{}^d)^{\cdot} - 2\rho G_c G_\sigma' / \gamma_e, \tag{5. 6}$$

where G_μ and G_c are values of the shear modulus for constant μ_{ij} and c_{ij} $(i \neq j)$,

$$G_\mu = G_c\frac{\gamma_\sigma}{\gamma_e}, \qquad m = \frac{9}{4}\frac{d}{H_2}\frac{k_\sigma}{\gamma_e}. \tag{5. 7}$$

Relations (5. 4), (5. 6) are the most general for a rheological model characterized by a linear dependence between the stresses and strains and their first derivatives. Here the physical sense of the long-time and instantaneous moduli of elasticity and the relaxation time is established by formulas (5. 5), (5. 7).

Hence rheological relations (5. 4), (5. 6) follow from the equations of the diffusion theory as a particular case provided that the thermodynamic states of the body and the ambient medium are individually homogeneous and the irreversibility of the process is attributable only to a discontinuous change in the state of the system upon transition through the body-medium interface. Evidently, this is theoretically possible only for infinitely large conductivity of the media and a certain finite resistance at the interface.

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