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THERMODYNAMICS OF DIFFUSE DAMAGE IN SOLIDS†

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A thermodynamic model of the accumulation of diffuse damage in deformed solids is proposed. A closed system of dynamic equations of thermo-fractomechanics is constructed. A solution of the non-linear equation of the “diffusion” of damage in the form of a plane stationary kink-shaped damage wave is obtained. It is shown that the velocity of the wave front is proportional to the invariants of the strain (stress) tensor and the “diffusion” coefficient, and inversely proportional to the force of resistance to damage accumulation.

ONE OF the most fruitful ideas when investigating the initiation and growth of microdamage in stressed structural components has been the introduction of the idea of scalar, vector and tensor measures of damage [1–5]. However, in the overwhelming majority of investigations devoted to studying the accumulation of microdamage in structures, the measures of damage are only considered as functions of time. The dependence on the spatial coordinates is ignored and the initiation and growth of damage is regarded either at a fixed, most stressed point, or uniformly over the whole volume of the structural component [1–10]. Here it is assumed that the process of damage accumulation is completed by the formation of a macrocrack due to the merging of microdefects or fracture of the specimen by loss of integrity. The occurrence and motion of the microfracture fronts usually escape the attention of researchers. In cases when the measures of damage depend on the coordinate vector via the nominal stresses, the form of the right-hand sides of the kinetic equations is established from empirical considerations, ignoring the spatial gradients of the field of the scattered microfractures [7, 11, 12].

The basis of the “point” models of the accumulation of damage is the ordinary differential equations $d\psi/dt = f(\psi, \sigma_{ab}, \xi, t)$, in which $\psi(\xi^a, t)$ is the scalar measure of damage, while the vector ξ is simply a parameter [2–12]. Continuum models, based on equations of the same type, take into account the dependence of the components of the stress tensor $\sigma_{ab} = \sigma_{ab}(\xi, t)$ on the vector ξ and the time t [2, 7, 10–12]. Here the equations of the accumulation of damage are considered together with the conditions of compatibility and the equations of equilibrium of the solid. A natural generalization of the evolution equations to distributed systems would be the introduction into the model of diffusion transfer processes, i.e. a change to partial differential equations of the parabolic type $\partial\psi/\partial t = f(\psi, \sigma_{ab}) + \nabla(D\nabla\psi)$. However, a drawback of this approach is the fact that there is no explicit connection with the equation of conservation of energy and the equation of entropy balance. To construct continuum models of fracture, which take into account the interaction of fields of different physical kinds, it is necessary to use fairly general principles based on fundamental variational equations.

One of the variational principles widely employed at the present time to construct the equations of motion of continuous media is the principle of stationary action. It turns out,

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however, that this principle does not hold for systems with non-holonomic constraints under non-potential external loads. In order to circumvent these difficulties, Sedov in 1964 proposed a variational principle which generalizes the principle of stationary action to irreversible processes and to the cases when there are non-conservative forces present [13, 14]. The basis of this principle was the generalized equation of the principle of virtual work which is closely connected with the equations of the first and second laws of thermodynamics.

In the present paper Sedov's variational principle is used to construct a thermodynamic mode of the irreversible growth of dispersed damage in deformed solids. A closed system of dynamic equations is derived within the framework of the continuum mechanism of the initiation and growth of diffuse damage. The general system of equations includes the equation of conservation of energy, the equation of balance of momentum, the equation of "diffusion" of irreversible damage, and also the defining equations of the thermomechanics of diffuse microfracture. To close the system of equations, Onsager's relations between the generalized thermodynamic forces and fluxes are employed.

1. Consider an inhomogeneous anisotropic non-linearly elastic solid in a field of thermomechanical forces. The action of these forces on the body is accompanied by the initiation and growth of microdamage, which may lead to defect cluster, the generation of a macrocrack, and fracture of the body as a whole. If the dimensions of the microdefects are small compared with the characteristic dimensions of the body, and the concentration of the defects is fairly high, one can introduce a scalar measure of damage $\psi(\xi^a, t)$ as a function of the Lagrange coordinates ξ^a and the time t to describe the microfracture on a continuum level.

To determine the thermodynamic state of a defect-free continuous medium using the mass internal energy density U it is necessary to specify seven scalar defining parameters: six components of the strain tensor $\varepsilon_{ab}(\xi^c, t)$ and the mass entropy density $s(\xi^a, t)$. In a damaged medium the parameters ε_{ab} and s are insufficient. To describe the irreversible destruction of a medium it is necessary for the internal energy density U to depend on the measure of damage $\psi(\xi^a, t)$ also. In other words, the scalar parameter ψ must reflect the change in the physical and mechanical properties of the material of the body due to irreversible processes of the initiation and growth of microdamage. Hence, the internal energy density of a strained solid in the damaged state must be represented in the form $U = U(\varepsilon_{ab}, s, \psi, \nabla_a \psi)$. The gradient term $\nabla_a \psi$ here takes into account the spatial inhomogeneity of the damage field; Latin subscripts from the first half of the alphabet a, b, c, \dots relate to the Lagrange system of coordinates and take on values of 1, 2, 3.

The defining parameters $\varepsilon_{ab}(\xi^c, t)$, $s(\xi^a, t)$ and $\psi(\xi^a, t)$, however, do not form a system of independent functions. For example, the components of the strain tensor $\varepsilon_{ab}(\xi^c, t)$ are related to the equations of compatibility, while the entropy density $s(\xi^a, t)$, the entropy flux density $s^a(\xi^b, t)$ and the local rate of change of entropy $\sigma(\xi^a, t)$ satisfy the balance equation

$$\rho \frac{\partial s}{\partial t} + \nabla_a s^a = \sigma \quad (1.1)$$

where $\rho(\xi^a, t)$ is the natural density of the rest mass of the body, and ∇_a is the covariant derivative in a space with metric tensor $g_{ab}(\xi^c, t)$. Using the parametric representations for the quantities s , s^a and σ

$$s = -\frac{1}{\rho} \nabla_a \left(\frac{\eta^a}{\sqrt{g}} \right) + \frac{1}{\rho \sqrt{g}} \eta, \quad s^a = \frac{1}{\sqrt{g}} \frac{\partial \eta^a}{\partial t}, \quad \sigma = \frac{1}{\sqrt{g}} \frac{\partial \eta}{\partial t} \quad (1.2)$$

the entropy balance equation (1.1) is satisfied identically, while the parameters of the production and transfer of entropy $\eta(\xi^a, t)$, $\eta^a(\xi^b, t)$ are independent. Using the law of motion of a strained body in the form $x^k = x^k(\xi^a, t)$, where x^k are the spatial coordinates of an Euler system of coordinates, we can change from the dependent relations $\varepsilon_{ab}(\xi^c, t)$ to independent functions

$x^k(\xi^a, t)$. The fact that the system of defining parameters $x^k(\xi^a, t)$, $\eta(\xi^a, t)$, $\eta^a(\xi^b, t)$ and $\psi(\xi^a, t)$ are independent when deriving the dynamic laws from the variational principle is a conclusive fact.

2. We will construct a model of the diffuse fracture of a solid using the variational equation [13, 14]

$$\delta I + \delta W^* + \delta W = 0 \quad (2.1)$$

Here I is the action, defined for any possible processes and motions, δW^* is a non-holonomic functional, which takes into account irreversible thermodynamic processes and non-conservative forces, and δW is a scalar functional which takes into account the energy exchange at the boundary surfaces of the body, and also at the initial and final instants of time of the motion. The form of the functional δW is established from Eq. (2.1) after specifying the functionals I and δW^* which fix the thermodynamic model of the damaged solid.

We will represent the action I and the functional δW^* in a form similar to that proposed in [15]

$$I = \int_{t_0}^{t_1} \int_V \left\{ \frac{1}{2} v_a v^a - U(\varepsilon_{ab}, s, \psi, \nabla_a \psi) \right\} \rho \sqrt{g} d^3 \xi dt \quad (2.2)$$

$$\delta W^* = \int_{t_0}^{t_1} \int_V \left\{ (T \delta \eta + H_a \delta \eta^a) \frac{1}{\sqrt{g}} + Q^a \delta x_a + \Psi \delta \psi \right\} \sqrt{g} d^3 \xi dt \quad (2.3)$$

where $v_a(\xi^b, t)$ are the components of the velocity vector of points of the body, $g(\xi^a, t)$ is the determinant of the metric tensor, $T(\xi^a, t)$ is the thermodynamic temperature, $Q^a(\xi^b, t)$ are the components of the vector of the external volume forces, V is a region connected with the material particles of the damaged body, and $H_a(\xi^b, t)$ and $\Psi(\xi^a, t)$ are the generalized thermodynamic forces corresponding to the irreversible processes of heat conduction and microfracture.

We substitute (2.2) and (2.3) into the variational equation (2.1) and calculate the Lagrange variation of the action I . We finally obtain

$$\begin{aligned} & \int_{t_0}^{t_1} \int_V \left\{ \left(T - \frac{\partial U}{\partial s} \right) \frac{\delta \eta}{\sqrt{g}} + \left[H_a - \nabla_a \left(\frac{\partial U}{\partial s} \right) \right] \frac{\delta \eta^a}{\sqrt{g}} + \left(\Psi - \rho \frac{\delta U}{\delta \psi} \right) \delta \psi + \right. \\ & \quad \left. + \left[\nabla_b \left(\rho \frac{\partial U}{\partial \varepsilon_{ab}} \right) + Q^a - \rho \left(\frac{\partial v^a}{\partial t} + v^b \nabla_b v^a \right) \right] \delta x_a \right\} \sqrt{g} d^3 \xi dt + \\ & \quad + \int_{t_0}^{t_1} \int_V \left\{ \frac{\partial U}{\partial s} \frac{\delta \eta^b}{\sqrt{g}} - \rho \frac{\partial U}{\partial \nabla_b \psi} \delta \psi - \sigma^{ab} \delta x_a \right\} n_b dS dt + \\ & \quad + \left[\int_V \rho v^a \delta x_a \sqrt{g} d^3 \xi \right]_{t_0}^{t_1} + \delta W = 0 \end{aligned} \quad (2.4)$$

Here n_b are the components of the vector of the outward normal to the surface S , which bound the region V , occupied by the body, and $\delta U / \delta \psi = \partial U / \partial \psi - \rho^{-1} \nabla_a (\rho \partial U / \partial \nabla_a \psi)$ is the variational derivative.

By equating the coefficients of independent variations of the defining parameters in (2.4) to zero, we obtain the following system of dynamic equations of the thermomechanics of diffuse fracture

$$\rho(\partial v^a / \partial t + v^b \nabla_b v^a) = \nabla_b \sigma^{ab} + Q^a, \quad \rho \delta U / \delta \psi = \Psi \quad (2.5)$$

$$T = \partial U / \partial s, \quad \sigma^{ab} = \rho \partial U / \partial \varepsilon_{ab}, \quad H_a = \nabla_a T \quad (2.6)$$

The first equation in (2.5) is the equation of the balance of momentum. The second equation in (2.5) controls the processes of damage accumulation in the stressed body. Equations (2.6) are the defining equations of the thermomechanics of the damaged body: the first equation defines the absolute temperature, the second equation defines the Piola–Kirchhoff stress tensor, and the third is Fourier's law of heat conduction.

By specifying the functional δW on the boundary of the four-dimensional region $V \times [t_0, t_1]$ by the equation

$$\begin{aligned} \delta W = & - \int_{t_0}^{t_1} \int_S \left\{ T_0 \frac{\delta \eta^a}{\sqrt{g}} n_a + \rho J_0 \delta \psi - p^a \delta x_a \right\} dS - \\ & - \left[\int_V \rho v_0^a \delta x_a \sqrt{g} d^3 \xi \right]_{t_0}^{t_1} \end{aligned} \quad (2.7)$$

we can also obtain from the variational equation (2.4) alternative boundary conditions for $\xi^a \in S$

$$(T - T_0) n_a \frac{\delta \eta^a}{\sqrt{g}} = 0, \quad \rho \left(\frac{\partial U}{\partial \nabla_a \psi} n_a + J_0 \right) \delta \psi = 0, \quad (\sigma^{ab} n_b - p^a) \delta x_a = 0 \quad (2.8)$$

and the limiting (or initial) condition for $t = t_0$ and $t = t_1$

$$\rho(v^a - v_0^a) \delta x_a = 0 \quad (2.9)$$

The dynamic condition $T = T_0$ in the first equation of (2.8) gives the temperature on the boundary of the body, while the kinematic condition $n_a \delta \eta^a / \sqrt{g} = 0$, using (1.2), gives the entropy flux s^a or the heat flux $q^a = T s^a$ through the boundary surface with normal n_a . In the case of convective heat exchange with the external medium the kinematic boundary condition can be represented in the form $q^a n_a = k(T - T_0)$, where k is the heat-transfer coefficient.

The kinematic condition $\delta W = 0$ gives the boundary value of the measure of damage $\psi = \psi_0$; the dynamic condition, defined by the second equation of (2.8), means the continuity of the damage flux through the contact surface of the solids. If $J_0 = 0$, the condition $J^a n_a = -(\partial U / \partial \nabla_a \psi) n_a = 0$ means that there is no damage flux through the boundary surface S .

The dynamic conditions $\sigma^{ab} n_b = p^a$ and the kinematic conditions δx_a , corresponding to the last equation in (2.8), express the usual boundary conditions in stresses and displacements used in the mechanics of a strained solid [8]. Conditions (2.9) specify the spatial distributions of the coordinates and momenta of the material particles of the body at the initial instant of time.

3. In a Lagrangian system of coordinates in projections on to the axis of the basis, the general system of unknowns contains the components of the vector of the displacements of points of the body $u^a(\xi^b, t)$, the components of the velocity vector $v^a(\xi^b, t)$, connected with the displacements u^a by the relations

$$v^a = \partial u^a / \partial t + v^b \nabla_b u^a \quad (3.1)$$

the natural density of the body $\rho(\xi^a, t)$, the mass entropy density $s(\xi^a, t)$, and the scalar measure of damage $\psi(\xi^a, t)$, i.e. nine scalar quantities in all. However, the system of dynamic equations

(1.1), (2.5), (2.6) and (3.1) is not closed and must be supplemented by the equation of local mass balance

$$\rho\sqrt{g} = \rho_0\sqrt{g_0} = f(\xi^a) \quad (3.2)$$

by the Cauchy–Almansi relations

$$\varepsilon_{ab} = \frac{1}{2}(\nabla_a u_b + \nabla_b u_a - \nabla_a u_c \nabla_b u^c) \quad (3.3)$$

and also by the equations defining the thermodynamic forces $H_a(\xi^b, t)$ and $\Psi(\xi^a, t)$.

We will use the variational equation (2.1) to construct the equations of conservation of internal energy $U(\xi^a, t)$ and the dissipative function $\sigma(\xi^a, t)$. We replace the arbitrary Lagrange variation $\delta\mu^a$ of the defining parameters μ^a in (2.1) by the variation $\delta^0\mu^a = (\partial\mu^a/\partial t)\delta\tau$, which is the analogue of the Lie differential in Newtonian space with absolute time. Equation (2.1) can then be rewritten in the form

$$\begin{aligned} & \int_{t_0}^t \int_V \frac{\partial L}{\partial t} \delta\tau \rho \sqrt{g} d^3\xi dt + \int_{t_0}^t \int_V \left\{ T \frac{\partial\eta}{\partial t} + H_a \frac{\partial\eta^a}{\partial t} \right\} \frac{1}{\sqrt{g}} + \\ & + Q^a v_a + \Psi \frac{\partial\Psi}{\partial t} \delta\tau \sqrt{g} d^3\xi dt - \int_{t_0}^t \int_V \nabla_b \left[\frac{\partial U}{\partial s} \frac{\partial\eta^b}{\partial t} \frac{1}{\sqrt{g}} - \right. \\ & \left. - \rho \frac{\partial U}{\partial \nabla_b \Psi} \frac{\partial\Psi}{\partial t} - \sigma^{ab} v_a + \rho \frac{\partial}{\partial t} (v_a v^a) \right] \delta\tau \sqrt{g} d^3\xi dt = 0 \end{aligned} \quad (3.4)$$

Further, using relations (1.2), (2.5) and (2.6) and taking into account the fact that Eq. (3.4) must be satisfied for any values of the region $V[t_0, t_1]$ and an arbitrary constant $\delta\tau$, we obtain the following energy equation in local form

$$\begin{aligned} & -\rho \frac{\partial U}{\partial t} + \sigma^{ab} \nabla_b v_a - \nabla_a q^a + \nabla_a \left(\rho \frac{\partial U}{\partial \nabla_a \Psi} \frac{\partial\Psi}{\partial t} \right) + \\ & + T\sigma + T^{-1} H_a q^a + \Psi \frac{\partial\Psi}{\partial t} = 0 \end{aligned} \quad (3.5)$$

Then eliminating σ from Eqs (1.1) and (3.5) we obtain

$$\begin{aligned} & \rho \frac{\partial U}{\partial t} - \sigma^{ab} \nabla_b v_a + \nabla_a q^a - \nabla_a \left(\rho \frac{\partial U}{\partial \nabla_a \Psi} \frac{\partial\Psi}{\partial t} \right) - \\ & - T \left(\rho \frac{\partial s}{\partial t} + \nabla_a s^a + T^{-2} H_a q^a + T^{-1} \Psi \frac{\partial\Psi}{\partial t} \right) = 0 \end{aligned} \quad (3.6)$$

Equation (3.6) is a logical consequence of the basic variational equation (2.1) and contains, in synthesized form, the first and second laws of thermodynamics. The first row of this equation, in reduced form, contains the equation of internal energy balance, while the second contains the equation of entropy balance. It can be shown that one equation follows from the other. Consequently, it will be necessary for what follows to postulate an additional condition: either the internal energy balance equation or the entropy balance equation is an identity by virtue of Eqs (2.5) and (2.6). It is natural to take as being identically satisfied the internal energy balance equation

$$\rho \frac{\partial U}{\partial t} - \sigma^{ab} \nabla_b v_a + \nabla_a q^a - \nabla_a \left(\rho \frac{\partial U}{\partial \nabla_a \psi} \frac{\partial \psi}{\partial t} \right) = 0 \tag{3.7}$$

We then obtain the entropy balance equation from (3.6)

$$\rho \frac{\partial s}{\partial t} + \nabla_a s^a = \sigma, \quad \sigma \equiv -T^{-2} q^a \nabla_a T - T^{-1} \Psi \frac{\partial \psi}{\partial t} \geq 0 \tag{3.8}$$

in which the dissipative function $\sigma(\xi^a, t)$ defines the value of the irreversible increase in entropy due to heat conduction and microfracture.

When there are relations between the thermodynamic forces $H_a = \nabla_a T$, Ψ and the fluxes q^a and $\partial \psi / \partial t$, the quantity σ , by Onsager's theory, can be regarded as a quadratic form in the thermodynamic fluxes or forces. Then, in accordance with the local formulation of non-equilibrium thermodynamics, we can represent the relation between the thermodynamic fluxes and the forces in the following simplified form

$$q^a = -\lambda^{ab} \nabla_b T, \quad \Psi = -\Gamma \partial \psi / \partial t \tag{3.9}$$

The phenomenological coefficients λ^{ab} and Γ are, generally speaking, non-linear tensor functions of the defining parameters and their derivatives. The components of λ^{ab} here form a thermal-conductivity tensor in the undamaged solid, while the first equation of (3.9) expresses Fourier's heat-conduction law. We will call the parameter Γ the resistance coefficient of the accumulation of damage; it has the dimensions of the volume density of action [J s/m³]. The generalized thermodynamic force Ψ is equal to the work which must be expended to move the microfracture front in the deformed solid. Relations (3.9) close the general system of equations of thermodynamics of microfracture in the nine unknown quantities u^a, v^a, ρ, s, ψ .

4. The specific model of the damaged solid can be fixed to an equal degree using the internal energy $U(\epsilon_{ab}, s, \psi, \nabla_a \psi)$, the free Helmholtz energy $F(\epsilon_{ab}, T, \psi, \nabla_a \psi)$, or the Gibbs thermodynamic potential $\Phi(\sigma^{ab}, T, \psi, \nabla_a \psi)$. If, for example, we need to solve the dynamic coupled thermofractomechanics problem, then, in the position of thermodynamic equilibrium, the Helmholtz free energy is a minimum. If the body is situated in a quasi-static thermal force field, thermodynamic equilibrium begins when the Gibbs thermodynamic potential reaches a minimum. The relation between these potentials is established by Legendre transformations

$$F = U - Ts, \quad \Phi = F - \sigma^{ab} \epsilon_{ab} \tag{4.1}$$

and the defining equations of thermomechanics can be written as follows:

$$\begin{aligned} \sigma^{ab} &= \rho (\partial U / \partial \epsilon_{ab})_{s, \psi} = \rho (\partial F / \partial \epsilon_{ab})_{T, \psi}, \quad \epsilon_{ab} = -(\partial \Phi / \partial \sigma^{ab})_{T, \psi} \\ T &= (\partial U / \partial s)_{e, \psi}, \quad s = -(\partial F / \partial T)_{e, \psi} = -(\partial \Phi / \partial T)_{\sigma, \psi} \end{aligned} \tag{4.2}$$

To fix our ideas we will consider the Helmholtz free energy. We will represent the mass density F in the form of the sum $F = F_n + F_s$, where $F_n(\epsilon_{ab}, T)$ is the free energy density of the solid without damage, and $F_s(\epsilon_{ab}, T, \psi, \nabla_a \psi)$ is the difference between the free energies of the body in the damaged and undamaged states. From (2.5) and (3.9) we have $\rho \delta F / \delta \psi = -\Gamma \partial \psi / \partial t \geq 0$. Hence we see that microfractures lead to a reduction in the free energy of the body, i.e. $F_s \leq 0$. Assuming that F_n and F_s are holomorphic functions of the scalar arguments (T, ψ) and tensor arguments $(\epsilon_{ab}, \nabla_a \psi)$ we can expand them in Taylor series in the neighbourhood of the initial state

$$\rho_0 F_n(\epsilon_{ab}, T) = \rho_0 F_0 - \rho_0 s_0 \theta + \sigma_0^{ab} e_{ab} -$$

$$-\frac{1}{2}\rho_0 c_0 \theta^2 T_0^{-1} + \frac{1}{2} E_0^{abcd} e_{ab} (e_{cd} - 2\alpha_{cd}\theta) + \dots \quad (4.3)$$

$$\rho_0 F_* = -A(\epsilon_{ab}, T)(m+1)^{-1} \psi^{m+1} + B(m+n+1)^{-1} \psi^{m+n+1} + D^{ab} \nabla_a \psi \nabla_b \psi + \dots \quad (4.4)$$

Here ρ_0 is the density at the initial instant of time, F_0 , s_0 and σ_0^{ab} are unimportant constants, $e_{ab} = \epsilon_{ab} - \epsilon_{ab}^0$, $\theta = T - T_0$, ϵ_{ab}^0 and T_0 are the strain tensor and the absolute temperature of the body in the initial state, c_0 is the heat capacity of the continuous medium for constant strain E_0^{abcd} and α_{ab} are the elastic-constant tensor and the tensor of the coefficients of linear thermal expansion, and D^{ab} are the components of the tensor of the damage "diffusion" coefficients.

We will discuss the strain dependence of the coefficients in (4.4) in more detail. If the process of initiation and growth of the damage is connected with the local microstress tensor, the fracture surface can be made to correspond to this tensor in six-dimensional strain space. In the case of an active load the limiting surface in strain space will be shifted and deformed, following the anisotropic strengthening processes. Hence, the relations between the stresses and the strains should differ considerably from linear-elastic. In this connection, the term proportional to $A(\epsilon_{ab}, T)$ in (4.4) should contain, as a minimum, linear invariants of the strain tensor, while the coefficients B and D^{ab} can be assumed to be constants of the material, to a first approximation.

We will show that this is so. Consider a body with a uniform distribution of defects in a field of constant thermo-elastic stresses. The function F_* should then not depend on the spatial coordinates ξ^a , and the expansion of the free energy can be represented in the form

$$\rho_0 F = \rho_0 F_n - A(\epsilon_{ab}, T)(m+1)^{-1} \psi^{m+1} + B(m+n+1)^{-1} \psi^{m+n+1} \quad (4.5)$$

Differentiating this expression with respect to ψ we obtain the values of the measure of damage for which the free energy of the body has an extremum

$$\psi_0 = 0, \quad \psi_* = (A/B)^{1/n} \in [0, 1) \quad (4.6)$$

Since the process of the accumulation of damage is irreversible, the rate of growth of the damage density is a non-negative quantity. The value $\psi = 0$ corresponds to an undamaged material, and when $\psi = 1$ either a macrocrack is formed or the material is fractured by a loss of integrity. Consequently, for any n the coefficients A and B will have the same signs. At the point $\psi = \psi_0$ the free energy has a maximum $F(\psi_0) = F_n$; when $\psi = \psi$, the free energy reaches a minimum

$$\rho_0 F(\psi_*) = \rho_0 F_n - nA[(m+1)(m+n+1)]^{-1} (A/B)^{(m+1)/n} \quad (4.7)$$

Hence we see that in the damaged state of the material the coefficients A and B must be positive, and the coefficient A when $\epsilon_{ab} = \epsilon_{ab}^0$, $T = T_0$ must be equated to zero, while the coefficient B can be assumed constant.

Taking the above observations into account we can write the function $\rho_0 F_*$ in the form

$$\begin{aligned} \rho_0 F_* = & -[A^{ab}(e_{ab} - \alpha_{ab}\theta) + \frac{1}{2} A^{abcd}(e_{ab} - \alpha_{ab}\theta)(e_{cd} - \alpha_{cd}\theta)] \times \\ & \times (m+1)^{-1} \psi^{m+1} + B(m+n+1)^{-1} \psi^{m+n+1} + D^{ab} \nabla_a \psi \nabla_b \psi + \dots \end{aligned} \quad (4.8)$$

where A^{ab} , A^{abcd} are the components of the fracture-surface tensors in strain space [16]. Substituting the mass free-energy density into the first equation of (4.2) we obtain the following expression for the components of the stress tensor

$$\sigma^{ab} = \frac{\rho}{\rho_0} \left\{ \sigma_0^{ab} + [E_0^{abcd} - (m+1)^{-1} \psi^{m+1} A^{abcd}] (e_{cd} - \alpha_{cd}\theta) - (m+1)^{-1} \psi^{m+1} A^{ab} \right\} \quad (4.9)$$

By virtue of the principle of the existence of the fundamental state when $\epsilon_{ab} = \epsilon_{ab}^0$, $T = T_0$, the

components of the tensor σ_0^{ab} are zero. The density ρ for small strains can be replaced by the quantity ρ_0 .

We will represent the components of the tensor A^{ab} as follows:

$$A^{ab} = (m+1) \left[E_0^{abcd} - (m+1)^{-1} \psi^{m+1} A^{abcd} \right] C_{cd}$$

and we will introduce the following notation

$$\varepsilon_{ab}^* = C_{ab} \psi^{m+1} \quad (4.10)$$

We can then rewrite (4.9) in the form

$$\sigma^{ab} = \left[E_0^{abcd} - (m+1)^{-1} \psi^{m+1} A^{abcd} \right] (\varepsilon_{cd} - \varepsilon_{cd}^0 - \alpha_{cd} \theta - \varepsilon_{cd}^*) \quad (4.11)$$

In the equilibrium state we have $\psi = [A(\varepsilon_{ab}, T)/B]^{1/n}$. Hence, the defining equations (4.11) reflect not only the thermo-elastic properties of the material but also the inelastic properties due to the initiation and growth of microfractures. The tensor with components (4.10) can serve as a measure of inelastic strains due to the formation of volume pores.

We will define the free-energy density in an isotropic solid by the expression

$$\begin{aligned} \rho_0 F = & \rho_0 F_0 - 9K_0 \alpha \theta e - \frac{1}{2} \rho_0 c_0 \theta^2 T_0^{-1} + \frac{1}{2} K_0 e^2 + \\ & + \frac{3}{2} G_0 e_i^2 - \left[9K_0 A_0 (e - \alpha \theta) + \frac{3}{2} G_0 A_1 e_i^2 \right] (m+1)^{-1} \psi^{m+1} + \\ & + B(m+n+1)^{-1} \psi^{m+n+1} + D(\nabla \psi)^2 \end{aligned} \quad (4.12)$$

Using formulae of the type (4.2) we obtain

$$\begin{aligned} \sigma &= (\rho_0 / 3) \partial F / \partial e = 3K_0 [e - \alpha \theta - A_0 (m+1)^{-1} \psi^{m+1}] \\ \sigma_i &= \rho_0 \partial F / \partial e_i = 3G_0 [1 - A_1 (m+1)^{-1} \psi^{m+1}] e_i \end{aligned} \quad (4.13)$$

Here K_0 and G_0 are the isothermal volume modulus and the shear modulus in an undamaged solid, $e = \frac{1}{3} g_{ab} e^{ab}$ is the mean volume strain, $e'_{ab} = e_{ab} - e g_{ab}$ is the strain tensor deviator, $e_i = (\frac{3}{2} e'_{ab} e^{ab'})^{1/2}$ is the intensity of the shear strain, $\sigma = \frac{1}{3} g_{ab} \sigma^{ab}$ is the mean hydrostatic stress, $\sigma'_{ab} = \sigma_{ab} - \sigma g_{ab}$ is the stress-tensor deviator, and $\sigma_i = (\frac{3}{2} \sigma'_{ab} \sigma^{ab'})^{1/2}$ is the shear stress intensity. The term $A_0 (m+1)^{-1} \psi^{m+1}$ in the first of the equations in (4.13) defines the measure of inelastic volume strain for a uniform tension due to the formation of micropores. The strain ε is then made up of the elastic component $\varepsilon_e = \sigma / (3K_0)$, the initial component $\varepsilon_0 = \frac{1}{3} g_{ab} \varepsilon_0^{ab}$, the temperature component $\varepsilon_t = \alpha \theta$ and the inelastic component $\varepsilon_* = A_0 (m+1)^{-1} \psi^{m+1}$. The term $A_1 (m+1)^{-1} \psi^{m+1}$ in the second of the equations in (4.13) takes into account the effect of damage on the value of the tangential shear modulus $G = G_0 [1 - A_1 (m+1)^{-1} \psi^{m+1}]$.

The mass entropy density s in the case of an anisotropic damaged solid in a non-equilibrium state is given by relations (4.2), (4.3) and (4.8) as follows:

$$\begin{aligned} s = & -(\partial F / \partial T)_{\varepsilon, \psi} = s_0 + c_0 \theta T_0^{-1} + E_0^{abcd} e_{ab} \alpha_{cd} \rho_0^{-1} - \\ & - [A^{ab} \alpha_{ab} + A^{abcd} (e_{ab} - \alpha_{ab} \theta) \alpha_{cd}] (m+1)^{-1} \psi^{m+1} \rho_0^{-1} \geq s_0 \end{aligned} \quad (4.14)$$

The specific heat capacity for constant strain in a non-equilibrium microfracture process in the approximation $|\theta/T_0| \ll 1$ can be calculated from the equation

$$c = T(\partial s / \partial T)_{\varepsilon, \psi} = c_0 + A^{abcd} \alpha_{ab} \alpha_{cd} (m+1)^{-1} \psi^{m+1} T_0 \rho_0^{-1} \geq c_0 \quad (4.15)$$

In the initial state, when $\epsilon_{ab} = \epsilon_{ab}^0$, $T = T_0$, we have $\psi = 0$ and, consequently $c = c_0$. When thermodynamic equilibrium is reached in a uniform solid $\partial\psi/\partial t = 0$, $\nabla_a\psi = 0$, $\Psi = 0$ and $\psi = \psi_*$. The measure of damage then loses its independence of a number of defining parameters and becomes a function of the strain and the temperature: $\psi = \psi_*(\epsilon_{ab}, T)$. The equilibrium value of the heat capacity in this case is determined by the total derivative

$$\begin{aligned} c_* &= T(\partial s / \partial T)_{\epsilon, \psi} = T(\partial s / \partial T)_{\epsilon, \psi} + T(\partial s / \partial \psi)_{\epsilon, T}(\partial \psi / \partial T)_{\epsilon, \psi} = \\ &= c_0 + T_0 \rho_0^{-1} \psi_*^{m+1} \left\{ (m+1)^{-1} A^{abcd} \alpha_{ab} \alpha_{cd} + (nB)^{-1} [A^{ab} \alpha_{ab} + \right. \\ &\left. + A^{abcd} (\epsilon_{ab} - \epsilon_{ab}^0 - \alpha_{ab} \theta) \alpha_{cd} \right]^2 \psi_*^{-n} \} \geq c \end{aligned} \tag{4.16}$$

In a similar way we can calculate the other equilibrium thermodynamic coefficients

$$E_*^{abcd} = (\partial \sigma^{ab} / \partial \epsilon_{cd})_{T, \psi}, \quad \alpha_{ab}^* = -S_{abcd}^* (\partial \sigma^{cd} / \partial T)_{\epsilon, \psi}$$

where S_{abcd}^* are the components of the isothermal compliance tensor of the solid in the equilibrium state.

5. To construct the microfracture “diffusion” equation we will assume that the coefficient of resistance to the accumulation of damage in the second of the equations in (3.9) is a non-linear function of the measure of damage: $\Gamma = \Gamma_0(1 - C\psi^l)$, where Γ_0 , C and l are phenomenological constants. When $C > 0$, $l > 0$ the parameter $\Gamma(\psi)$ takes into account the effect of the density of accumulated microfractures on the rate of damage of the remaining structural components of the solid [6–9]. Substituting the free energy density $F(\epsilon_{ab}, T, \psi, \nabla_a\psi)$ and the generalized thermodynamic force of resistance to damage $\Psi = -\Gamma \partial\psi / \partial t$ into the second equation of (2.5) we obtain a non-linear parabolic equation of the propagation of microfractures in the strained solid

$$\Gamma_0(1 - C\psi^l) \partial\psi / \partial t = A(\epsilon_{ab}, T) \psi^m - B\psi^{m+n} + \nabla_a(D^{ab} \nabla_b \psi) \tag{5.1}$$

If the components of the “diffusion” tensor D^{ab} are equal to zero, Eq. (5.1) describes the accumulation of damage uniformly within the volume of the solid. With the additional condition $B = 0$ we have a self-similar model process of accumulation of damage taking into account the redistribution of the strains in the undamaged structural components. If, in addition, we also have $C = 0$, we obtain a model in which the strains in the structural components are independent of the level of accumulated damage. The additional proposition that $m = 0$ leads to a linear rule for the summation of the damages [1–12].

In general, the accumulation of damage simultaneously at all points of the strained body is somewhat improbable. The following mechanism of the accumulation of damage is more realistic: the occurrence of microfractures at the most stressed points, an increase in the damage density up to the thermodynamically equilibrium value, the relay-propagation of the damage in the medium, the fusion of spatial regions of microfractures, and the formation of a continuous damage zone over the whole volume of the strained solid. Obviously, the rate of propagation of the damage front, like the equilibrium value of the measure of damage, must be proportional to the invariants of the strain or stress tensor.

We will show that Eq. (5.1) has a solution in the form of a stationary kink-shaped solitary wave. Suppose the parameters $A(\epsilon_{ab}, T)$, B , C , $D^{ab} = Dg^{ab}$ and Γ_0 are constants of the material. Then the stationary solution of Eq. (5.1) with boundary conditions $\psi = \psi_*$ when $\xi \rightarrow -\infty$ and $\psi = 0$ when $\xi \rightarrow +\infty$ will be sought in the form of a plane wave $\psi(\xi, t) = \psi(\xi - Vt) \equiv \psi(x)$, where V is the velocity of propagation of the damage front. Substituting the required solution into (5.1) we obtain the ordinary differential equation

$$-V\Gamma_0(1 - C\psi^l) d\psi / dx = A\psi^m - B\psi^{m+n} + Dd^2\psi / dx^2 \tag{5.2}$$

By introducing the new variable $\varphi = d\psi/dx$ we can reduce the order of this equation and represent its solution in the form $\varphi = \varphi_0\psi(A - B\psi^n)$, where φ_0 is an unknown constant. As a result we have

$$V\Gamma_0 + D\varphi_0A - V\Gamma_0C\psi^l + \varphi_0^{-1}\psi^{m-1} - D\varphi_0B(n+1)\psi^n = 0 \quad (5.3)$$

Equation (5.3) will be satisfied for any values of $\psi \in [0, \psi_*]$, if we require that the conditions $l = m - 1 = n > 0$ and

$$V\Gamma_0 = -D\varphi_0A, \quad mD\varphi_0^2B + V\Gamma_0C\varphi_0 = 1 \quad (5.4)$$

are satisfied. Hence we obtain the parameters of the problem V and φ_0

$$V = \frac{A}{\Gamma_0} \sqrt{\frac{D}{N}} > 0, \quad \varphi_0 = -\frac{1}{\sqrt{DN}} < 0, \quad N = (n+1)B - AC > 0 \quad (5.5)$$

Obviously, as the thermomechanical strains increase the coefficient $A(\epsilon_{ab}, T)$ and, consequently, the velocity of the damage front V , will also increase. Naturally, the velocity of the damage front is also proportional to the "diffusion" coefficient ($V \sim \sqrt{D}$) and inversely proportional to the force of resistance to the accumulation of damage ($V \sim 1/\Gamma_0$).

The relation $\varphi = d\psi/dx = \varphi_0\psi(A - B\psi^n)$ is an equation with separable variables and can easily be integrated

$$\int_{\psi_1}^{\psi} \frac{d\psi}{\psi(A - B\psi^n)} = \frac{1}{nA} \ln \left| \frac{\psi^n(\psi_*^n - \psi_1^n)}{\psi_1^n(\psi_*^n - \psi^n)} \right| = \int_0^x \varphi_0 dx = \varphi_0 x \quad (5.6)$$

After reduction we obtain the solution of the non-linear equation (5.1) in the form of a plane stationary kink-shaped solitary wave

$$\psi(\xi, t) = \psi_* \left\{ 1 + \left[(\psi_* / \psi_1)^n - 1 \right] \exp[-nA\varphi_0(\xi - Vt)] \right\}^{-1} \quad (5.7)$$

Since $\varphi_0 < 0$, this solution satisfies the given boundary conditions as $\xi \rightarrow \pm\infty$. The damage wave moves in the positive direction of the ξ axis, changing the state of the medium $\psi = 0$ to the state $\psi = \psi_*$. The propagation of the solitary wave is ensured by the dynamic equilibrium between the non-linear process of the accumulation of damage and the "diffusion" of damage in the strained body. The free energy is stored at each point of the volume of the medium and the travelling damage wave serves as a signal for it to be released. The value of the released energy here is exactly equal to the energy required to maintain the motion of the wave.

It can be seen from (5.5) and (5.7) that the velocity and slope of the wavefront increase for large nominal values of the strains. In the limit $A(\epsilon_{ab}, T) \rightarrow B$, $\psi_* \rightarrow 1$ the formation of a shock wave propagating with velocity

$$V_* = [DB / (n+1 - C)]^{1/2} / \Gamma_0 < V_0 \quad (5.8)$$

occurs, where V_0 is the minimum velocity of the shear wave in the solid. Hence it follows that the phenomenological constant C must be bounded by the inequalities

$$0 \leq C < n+1 - DB(V_0\Gamma_0)^{-2} \quad (5.9)$$

Note also that when the above-mentioned limitations on the coefficients of Eq. (5.1) are satisfied, the solution (5.7) is unique and stable in the class of monotone functions [17].

Hence, a thermodynamic analysis of the accumulation of diffuse damage in solids enables us

to draw the following conclusions. The initiation and growth of microdamage under any loading conditions reduce the free energy of the strained solid. The kinetic equations of the damage accumulation, obtained using the variational principle, can only contain integral powers of the measure of damage, the absolute temperature, and the invariants of the strain (stress) tensor. By taking into account the dependence of the free energy on the measure of diffuse damage, one can determine the value of the inelastic strain due to the formation of micropores and microcracks, and estimate the effect of the damage on the change in the shear moduli, the entropy and the heat capacity. We have shown that the propagation of damage in strained solids can take the form of a wave, and the velocity of motion of the damage front depends on the nominal strains, the viscosity of the microfractures, and the "diffusion" coefficient of the damage.

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