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A GEOMETRICAL MODEL OF THE DEFECT STRUCTURE OF AN ELASTOPLASTIC CONTINUOUS MEDIUM

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We consider a new class of elastoplastic models which are based on the assumption that internal interaction between the continuum particles has affine-metric geometrical structure. From the physical viewpoint, the affine-metric objects are intrinsic thermodynamic variables which describe the evolution of various defect structures in a deformable material and also interaction between themselves and with the field of reversible strains. The analysis performed allows one to establish a relation between the classical mechanical characteristics of elastoplastic materials and the field of dislocation density and other types of defects.

Introduction. It is shown that the mechanical model of the classical theory of elasticity contains latent thermodynamic parameters which characterize the geometrical structure of internal interactions between the particles. In the classical theory, these parameters vanish, which is attributed to the hypothesis that the intrinsic geometry of a material coincides with the geometry of the observer's Euclidean space. If this hypothesis is rejected, the latent parameters become nonzero and admit a natural interpretation as geometrical objects of affine-metric spaces. The use of affine-metric objects to describe internal interactions between the continuum particles allows one to extend the classical theory to the broad class of elastoplastic mechanical behavior of models of materials and relate these objects to the characteristics of the defect structure of the continuum. The interaction between the defects and the field of reversible elastic strains is determined by the character of dissipative processes in the continuum according to the principles of nonequilibrium thermodynamics.

1. Elastic Continuous Medium with Defects. The experimental investigations show that the test specimens that have not been treated preliminarily possess internal stresses, which affect the behavior of the structures under external loads. The initial stresses can be reduced by various technological techniques (for example, by annealing). For hardening, the useful properties of internal stresses (cold-work hardening, quenching, etc.) can also be used. From the physical viewpoint, the internal stresses are due to various defect structures in the material: dislocations, disclinations, and point defects. Although the problem of occurrence and existence of internal stresses has been known for a long time, there is no consistent theory for modeling the properties of real elastic materials. The main difficulty is the necessity to take into account the interaction between all defect structures and reversible elastic strains in the material.

The idea of an approach to solution of this problem arises from analysis of the classical elastic-continuum model. It is known [1, 2] that the general equations of motion for an elastic body are written in the form

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho v_k}{\partial x_k}=0,\quad \rho\frac{dv_i}{dt}=\frac{\partial\sigma_i^j}{\partial x^j}+\rho f_i,\quad \rho T\frac{ds}{dt}=\frac{\partial}{\partial x_i}\left(\lambda\frac{\partial T}{\partial x^i}\right),$$

$$U=U(s,\varepsilon_{ij}),\quad T=\frac{\partial U}{\partial s},\quad \sigma_i^j=(\delta_{ik}-2\varepsilon_{ik})\rho\frac{\partial U}{\partial\varepsilon_{kj}}, \tag{1.1}$$

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$$\frac{\mathcal{D}\varepsilon_{ij}}{\mathcal{D}t} \equiv \frac{d\varepsilon_{ij}}{dt} + \varepsilon_{ik}\frac{\partial v^k}{\partial x^j} + \varepsilon_{jk}\frac{\partial v^k}{\partial x^i} = e_{ij} = \frac{1}{2}\left(\frac{\partial v_i}{\partial x^j} + \frac{\partial v_j}{\partial x^i}\right).$$

Here $U = U(s, \varepsilon_{ij})$ is the internal energy, s is the entropy, ε_{ij} is the elastic strain tensor characterizing the internal geometrical structure of the material, σ_i^j are the components of the stress tensor, f_i are the components of the acceleration of the external mass forces, and ρ is the density. In the classical theory of elasticity, the elastic strain tensor ε_{ij} coincides with the complete strain tensor A_{ij} (the Almansi tensor). In the observer's system of reference connected with three-dimensional Euclidean space, the complete strain tensor A_{ij} [1, 2] is determined via the Lagrangian characteristics $\xi^k = \xi^k(\boldsymbol{x}, t)$ of the continuum particles from the relation

$$A_{ij} = \frac{1}{2}\Big(\delta_{ij} - \frac{\partial \xi^\alpha}{\partial x^i}\frac{\partial \xi^\alpha}{\partial x^j}\Big). \tag{1.2}$$

For the Almansi tensor, the representation (1.2) in terms of the vector field $\xi^k(\boldsymbol{x}, t)$ is always valid and it does not depend on the physical mechanism of the deformation process; here A_{ij} characterizes the shape of the deformable specimen.

The elastic strain tensor ε_{ij} determines the intrinsic metric tensor

$$g_{ij} = \delta_{ij} - 2\varepsilon_{ij}. \tag{1.3}$$

The transfer equation for this tensor

$$\frac{\mathcal{D}g_{ij}}{\mathcal{D}t} \equiv \frac{dg_{ij}}{dt} + g_{il}\frac{\partial v^l}{\partial x^j} + g_{jl}\frac{\partial v^l}{\partial x^i} = 0 \tag{1.4}$$

follows from (1.1) and (1.3). If $A_{ij} = \varepsilon_{ij}$, the solution of this equation is represented in the form

$$g_{ij} = \frac{\partial \xi^\alpha}{\partial x^i}\frac{\partial \xi^\alpha}{\partial x^j}. \tag{1.5}$$

However, it is known [1, 2] that the validity of relation (1.5) results from the vanishing of the Riemann R^l_{ijq}, twisting C^k_{ij}, and nonmetricity K_{kij} tensors:

$$R^l_{ijq} \equiv \frac{\partial \Gamma^l_{ij}}{\partial x^q} - \frac{\partial \Gamma^l_{iq}}{\partial x^j} + \Gamma^l_{\alpha q}\Gamma^\alpha_{ij} - \Gamma^l_{\alpha j}\Gamma^\alpha_{iq} = 0; \tag{1.6}$$

$$C^k_{ij} \equiv \frac{1}{2}(\Gamma^k_{ij} - \Gamma^k_{ji}) = 0; \tag{1.7}$$

$$K_{kij} = \nabla_k g_{ij} \equiv \frac{\partial g_{ij}}{\partial x^k} - \Gamma^s_{ik}g_{sj} - \Gamma^s_{jk}g_{si} = 0. \tag{1.8}$$

Since the coupling coefficients Γ^k_{ij} are symmetric relative to the lower indices and match the metrics [conditions (1.7) and (1.8), respectively], they are expressed in terms of the components of the metric tensor by the Christoffel formulas [1–3]:

$$\Gamma^k_{ij} = \frac{1}{2}g^{ks}\Big[\frac{\partial g_{sj}}{\partial x^i} + \frac{\partial g_{si}}{\partial x^j} - \frac{\partial g_{ij}}{\partial x^s}\Big], \qquad g^{is}g_{sj} = \delta^i_j. \tag{1.9}$$

The tensors R^l_{ijq}, C^k_{ij}, and K_{ijk} (see, e.g., [4]) characterize the non-Euclidean properties of a variety for which they are calculated. These tensors vanish in the classical continuum model [conditions (1.6)–(1.8)]. This means that the simplest geometrical model (the Euclidean model) is used to describe the intrinsic elastic properties of the material. The condition that the Euclidean properties of the intrinsic geometry of elastic continuum do not change during motion can be formulated in differential form. Combining (1.4) and (1.6)–(1.9), we obtain the transfer equation along the trajectories for the Riemann, twisting, and metricity tensors in the form

$$\frac{\mathcal{D}R^l_{ijq}}{\mathcal{D}t} = \frac{d}{dt}R^l_{ijq} + \frac{\partial v^p}{\partial x^i}R^l_{pjq} + \frac{\partial v^p}{\partial x^j}R^l_{ipq} + \frac{\partial v^p}{\partial x^q}R^l_{ijp} - \frac{\partial v^l}{\partial x^p}R^p_{ijq} = 0,$$

$$\frac{\mathcal{D}C_{ij}^k}{\mathcal{D}t} = \frac{d}{dt}C_{ij}^k + \frac{\partial v^l}{\partial x^i}C_{lj}^k + \frac{\partial v^l}{\partial x^j}C_{il}^k - \frac{\partial v^k}{\partial x^l}C_{ij}^l = 0, \tag{1.10}$$
$$\frac{\mathcal{D}K_{kij}}{\mathcal{D}t} = \frac{d}{dt}K_{kij} + K_{sij}\frac{\partial v^s}{\partial x^k} + \frac{\partial v^s}{\partial x^i}K_{ksj} + K_{kis}\frac{\partial v^s}{\partial x^j} = 0.$$

Since these equations are linear, the zero initial conditions give a zero solution at any moment of time. From the geometrical viewpoint, this result means that the elastic-continuum model is closed. Strains that occur during the motion of elastic continuum can be considered as a one-parameter mapping family which do not alter the intrinsic Euclidean structure of the material. Moreover, the coupling Γ_{ij}^k is nonzero. Using (1.4) and (1.9), we obtain

$$\frac{\mathcal{D}\Gamma_{ij}^k}{\mathcal{D}t} = \frac{d}{dt}\Gamma_{ij}^k + \Gamma_{is}^k\frac{\partial v^s}{\partial x^j} + \Gamma_{sj}^k\frac{\partial v^s}{\partial x^i} - \Gamma_{ij}^s\frac{\partial v^k}{\partial x^s} = -\frac{\partial^2 v^k}{\partial x^i \partial x^j}. \tag{1.11}$$

The nonzero source on the right-hand side of (1.11) gives a nonzero solution even for the zero initial condition for Γ_{ij}^k. The mechanical meaning of this change in Γ_{ij}^k is attributed to the transformation of the coordinate system which is "frozen" into the medium from the Cartesian system at the initial moment of time to a curvilinear system during deformation.

It should be noted that the Riemann R_{ijq}^l, twisting C_{ij}^k, and nonmetricity K_{kij} tensors are the "latent" parameters in the theory of elasticity. Equations (1.10) have nontrivial solutions for the nonzero initial condition. Therefore, the functions R_{ijq}^l, C_{ij}^k, and K_{kij} should be treated as the determining parameters of the theory of elasticity. This enhancement of the Euclidean structure of the classical theory of elasticity corresponds to a transition to the geometry of affine-metric spaces [4, 5]. The defect structures, such as disclinations, dislocations, and point defects, can be taken into account by using the tensors R_{ijq}^l, C_{ij}^k, and K_{kij} [6, 7]. The internal energy of the material with these defects is of the form $U = U(s, \varepsilon_{ij}, R_{ijq}^l, C_{ij}^k, K_{ijk})$. Using the same assumption that dissipation is ignored in Eqs. (1.1), one can obtain the following equations of state for these materials using the formalism of nonequilibrium thermodynamics [8]:

$$\sigma_i^j = (\delta_{ik} - 2\varepsilon_{ik})\rho\frac{\partial U}{\partial \varepsilon_{kj}} + \rho\Big(\frac{\partial U}{\partial C_{kl}^i}C_{kl}^j + 2\frac{\partial U}{\partial C_{lj}^k}C_{il}^k\Big) - \rho\Big(\frac{\partial U}{\partial K_{jkl}}K_{ikl} + 2\frac{\partial U}{\partial K_{kjl}}K_{kil}\Big)$$
$$+\rho\Big(\frac{\partial U}{\partial R_{kpq}^i}R_{kpq}^j - \frac{\partial U}{\partial R_{jpq}^k}R_{ipq}^k - 2\frac{\partial U}{\partial R_{pjq}^k}R_{piq}^k\Big). \tag{1.12}$$

From (1.12) and (1.1), it follows that, if various types of defects are taken into account, the stress-tensor components contain additional terms which have the meaning of internal stresses which depend on the defect structure of the material. The state of equilibrium of the material is described by the equations

$$\frac{\partial \sigma_i^j}{\partial x^j} = 0, \qquad \sigma_i^j n_j\Big|_{\partial V} = 0. \tag{1.13}$$

For a distribution of defects (the tensors R_{ijq}^l, C_{ij}^k, and K_{kij}) specified at the initial moment of time, the elastic strain tensor ε_{ij} is determined from (1.12) and (1.13) with a certain arbitrariness. The fact that the functions R_{ijq}^l, C_{ij}^k, and K_{ijk} are nonzero, i.e., the transition to the affine-metric model of the intrinsic geometrical structure of the material, means that a representation for the tensor ε_{ij} cannot be constructed in terms of the displacement vector $\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{\xi}(\boldsymbol{x}, t)$. As mentioned above, for the Almansi tensor A_{ij}, the representation (1.2) always exists. We assume the following relation between the tensors A_{ij} and ε_{ij}:

$$A_{ij} = \varepsilon_{ij} + \pi_{ij}. \tag{1.14}$$

Here π_{ij} is a tensor that characterizes the irreversible deformation of the material. For the classical elastic-continuum model, we have $\pi_{ij} = 0$. Since for the state of equilibrium, the Lagrangian characteristics can be found from the condition $A_{ij} = 0$, then $\varepsilon_{ij} = -\pi_{ij}$. Thus, the plastic strain, together with defects, allows the specimen to preserve its shape in the state of equilibrium. The occurrence of π_{ij} and the defects is due to the manufacturing of a specimen of specified shape. Obviously, this process is not unique and each of similar processes will result in a specific set of the fields of ε_{ij}, R^l_{ijq}, C^k_{ij}, and K_{ijk}, which are fit by the equilibrium conditions (1.13) with stress tensor (1.12).

2. Affine-Metric Model of Elastoplastic Materials. The use of the affine-metric space geometry is natural when the intrinsic geometrical structure of the elastic continuum model is enhanced to describe the occurrence of defect structures. The total number of independent functions is 33: six components of the metric tensor g_{ij} and 27 coefficients of the affine coupling ${}^*\Gamma^k_{ij}$. Generally, in contrast to the metric coupling ${}^*\Gamma^k_{ij}$ calculated by the Christoffel formulas (1.9), the affine coupling Γ^k_{ij} is not symmetric relative to the lower indices. Moreover, since the functions ${}^*\Gamma^k_{ij}$ are independent of the metric tensor g_{ij}, the affine coupling does not agree with the metric:

$$ {}^*K_{kij} \equiv {}^*\nabla_k g_{ij} = \frac{\partial g_{ij}}{\partial x^k} - {}^*\Gamma^q_{ik} g_{qj} - {}^*\Gamma^q_{jk} g_{qi} \neq 0. \tag{2.1} $$

We show that the metric coupling enters into the affine metric additively. Cyclic permutation of the indices in (2.1) yields

$$ {}^*\nabla_j g_{ki} = \frac{\partial g_{ki}}{\partial x^j} - {}^*\Gamma_{kj,i} - {}^*\Gamma_{ij,k}, \qquad {}^*\nabla_i g_{jk} = \frac{\partial g_{jk}}{\partial x^i} - {}^*\Gamma_{ji,k} - {}^*\Gamma_{ki,j}, \tag{2.2} $$

where ${}^*\Gamma_{ij,k} = {}^*\Gamma^s_{ij} g_{sk}$. Subtracting (2.1) from both relations in (2.2), we obtain

$$ 2S_{ij,k} = 2\Gamma_{ij,k} + {}^*\Gamma_{ik,j} - {}^*\Gamma_{ki,j} + {}^*\Gamma_{jk,i} - {}^*\Gamma_{kj,i} - ({}^*\Gamma_{ij,k} + {}^*\Gamma_{ji,k}); \tag{2.3} $$

$$ S_{ij,k} = \frac{1}{2}({}^*\nabla_j g_{ki} + {}^*\nabla_i g_{jk} - {}^*\nabla_k g_{ij}). \tag{2.4} $$

The object $S_{ij,k}$ is called a segmentary-curvature tensor [5] (a coupling-defect tensor according to the terminology of [4]). The functions $\Gamma_{ij,k}$ are determined from (1.9):

$$ \Gamma_{ij,k} = \Gamma^s_{ij} g_{sk}. \tag{2.5} $$

The antisymmetric part of the coupling determines the covariant components of the twisting tensor

$$ {}^*C_{ij,k} = \frac{1}{2}({}^*\Gamma_{ij,k} - {}^*\Gamma_{ji,k}), \qquad {}^*C^k_{ij} = {}^*C_{ij,s} g_{sk}. \tag{2.6} $$

From (2.3) and (2.6), we obtain a representation for ${}^*\Gamma_{ij,k}$ in the form [4, 5]

$$ {}^*\Gamma_{ij,k} = \Gamma_{ij,k} - S_{ij,k} + {}^*C_{ik,j} + {}^*C_{jk,i} + {}^*C_{ij,k}. \tag{2.7} $$

Formula (2.7) shows that an arbitrary affine coupling can be resolved into metric and nonmetric components.

For the affine-metric characteristics, the transfer equations can be obtained by a minimum modification of the corresponding transfer equations for the Euclidean model of elastic continuum, i.e., by introducing additional sources for the metric tensor and the coupling objects into (1.4) and (1.11):

$$ \frac{\mathcal{D} g_{ij}}{\mathcal{D}t} = \frac{dg_{ij}}{dt} + g_{ik}\frac{\partial v^k}{\partial x^j} + g_{jk}\frac{\partial v^k}{\partial x^i} = 2E_{ij}; \tag{2.8} $$

$$ \frac{\mathcal{D}\,{}^*\Gamma^k_{ij}}{\mathcal{D}t} = \frac{d}{dt}{}^*\Gamma^k_{ij} + {}^*\Gamma^k_{sj}\frac{\partial v^s}{\partial x^i} + {}^*\Gamma^k_{is}\frac{\partial v^s}{\partial x^j} - {}^*\Gamma^s_{ij}\frac{\partial v^k}{\partial x^s} = -\frac{\partial^2 v^k}{\partial x^i \partial x^j} - E^k_{ij}. \tag{2.9} $$

The structure of the sources E_{ij} and E^k_{ij} depends on the character of the dissipative processes during deformation. Since

$$ \frac{\mathcal{D} A_{ij}}{\mathcal{D}t} = \frac{1}{2}\Big(\frac{\partial v_i}{\partial x^j} + \frac{\partial v_j}{\partial x^i}\Big), \tag{2.10} $$

relations (1.14) and (2.10) imply that $\mathcal{D}\pi_{ij}/\mathcal{D}t = E_{ij}$. The source E_{ij} characterizes the processes of plastic deformation in the material.

The solutions of the kinematic equations (2.8) and (2.9) with known functions E_{ij} and E^k_{ij} give the metric tensor and the coupling coefficients. Within the framework of the geometrical approach, the complete set of coupling components is determined by relation (2.7). Do the solutions of Eqs. (2.8) and (2.9) give this complete set? The answer is positive, and it is formulated as follows: relations (2.7) are the integrals of Eqs. (2.8) and (2.9) for arbitrary E_{ij} and E^k_{ij}.

To prove this statement, we write the transfer equation for the functions appearing on the left-hand and right-hand sides of (2.7). The equation for the affine coupling ${}^*\Gamma_{ij,k}$ follows from (2.8) and (2.9) and has the form

$$\frac{\mathcal{D}\,{}^*\Gamma_{ij,k}}{\mathcal{D}t} = \frac{d}{dt}\,{}^*\Gamma_{ij,k} + {}^*\Gamma_{sj,k}\frac{\partial v^s}{\partial x^i} + {}^*\Gamma_{is,k}\frac{\partial v^s}{\partial x^j} + {}^*\Gamma_{ij,s}\frac{\partial v^s}{\partial x^k} = 2\,{}^*\Gamma^l_{ij}E_{lk} - E^l_{ij}g_{lk} - \frac{\partial^2 v^l}{\partial x^i \partial x^j}g_{lk}. \tag{2.11}$$

The covariant components of the metric coupling $\Gamma_{ij,k}$ are calculated by (2.5). Hence and from (1.11) one obtains the transfer equation

$$\frac{\mathcal{D}\Gamma_{ij,k}}{\mathcal{D}t} = D_{ij,k} - \frac{\partial^2 v^l}{\partial x^i \partial x^j}g_{lk}, \qquad D_{ij,k} = \frac{\partial E_{ki}}{\partial x^j} + \frac{\partial E_{kj}}{\partial x^i} - \frac{\partial E_{ij}}{\partial x^k}. \tag{2.12}$$

We consider the covariant derivatives (2.1) in the coupling-defect tensor (2.4). In accordance with (2.8), the function $\partial g_{ij}/\partial x^k$ satisfies the equation

$$\frac{\mathcal{D}}{\mathcal{D}t}\frac{\partial g_{ij}}{\partial x^l} = 2\frac{\partial E_{ij}}{\partial x^l} - g_{is}\frac{\partial^2 v^s}{\partial x^l \partial x^j} - g_{js}\frac{\partial^2 v^s}{\partial x^l \partial x^i}. \tag{2.13}$$

Combining (2.13) with the transfer equations (2.11), we obtain the evolution equation for ${}^*K_{kij}$:

$$\frac{\mathcal{D}\,{}^*K_{kij}}{\mathcal{D}t} = \frac{d}{dt}\,{}^*K_{kij} + {}^*K_{sij}\frac{\partial v^s}{\partial x^k} + {}^*K_{ksj}\frac{\partial v^s}{\partial x^i} + {}^*K_{kis}\frac{\partial v^s}{\partial x^j}$$
$$= 2\frac{\partial E_{ij}}{\partial x^k} - 2\,{}^*\Gamma^l_{ik}E_{lj} - 2\,{}^*\Gamma^l_{jk}E_{li} + E^l_{ik}g_{lj} + E^l_{jk}g_{li}. \tag{2.14}$$

Using the definition of the covariant derivative [3] for a tensor of rank two, we write the right-hand side of (2.14) in the covariant form

$$\frac{\mathcal{D}\,{}^*K_{kij}}{\mathcal{D}t} = 2\,{}^*\nabla_k E_{ij} + E^l_{ik}g_{lj} + E^l_{jk}g_{li}. \tag{2.15}$$

Inasmuch as the operator $\mathcal{D}/\mathcal{D}t$ preserves the tensorial nature of the quantities, it follows from (2.15) that the sources E^k_{ij} are the tensor objects.

From (2.4) and (2.15), one obtains the following equation for the coupling-defect tensor $S_{ij,k}$:

$$\frac{\mathcal{D}S_{ij,k}}{\mathcal{D}t} = {}^*\nabla_i E_{jk} + {}^*\nabla_j E_{ik} - {}^*\nabla_k E_{ij} + \frac{1}{2}(E^l_{ij} + E^l_{ji})g_{lk} - \frac{1}{2}(E^l_{ik} - E^l_{ki})g_{lj} - \frac{1}{2}(E^l_{jk} - E^l_{kj})g_{li}.$$

Passing from covariant to classical derivatives and the coupling coefficients, we obtain

$$\frac{\mathcal{D}S_{ij,k}}{\mathcal{D}t} = \frac{\partial E_{ki}}{\partial x^j} + \frac{\partial E_{kj}}{\partial x^i} - \frac{\partial E_{ij}}{\partial x^k} - ({}^*\Gamma^l_{ij} + {}^*\Gamma^l_{ji})E_{lk} + 2\,{}^*C^l_{jk}E_{li} + 2\,{}^*C^l_{ik}E_{lj}$$
$$+\frac{1}{2}(E^l_{ij} + E^l_{ji})g_{lk} - \frac{1}{2}(E^l_{ik} - E^l_{ki})g_{lj} - \frac{1}{2}(E^l_{jk} - E^l_{kj})g_{li}. \tag{2.16}$$

We need now an equation for the twisting tensor (2.6). From (2.6), (2.8), and (2.11), we have

$$\frac{\mathcal{D}\,{}^*C^k_{ij}}{\mathcal{D}t} = \frac{d}{dt}\,{}^*C^k_{ij} + {}^*C^k_{sj}\frac{\partial v^s}{\partial x^i} + {}^*C^k_{is}\frac{\partial v^s}{\partial x^j} - {}^*C^s_{ij}\frac{\partial v^s}{\partial x^k} = -\frac{1}{2}(E^k_{ij} - E^k_{ji}),$$
$$\frac{\mathcal{D}\,{}^*C_{ij,k}}{\mathcal{D}t} = \frac{d}{dt}\,{}^*C_{ij,k} + {}^*C_{sj,k}\frac{\partial v^s}{\partial x^i} + {}^*C_{is,k}\frac{\partial v^s}{\partial x^j} + {}^*C_{ij,s}\frac{\partial v^s}{\partial x^k} = -\frac{1}{2}(E^l_{ij} - E^l_{ji})g_{lk} + 2\,{}^*C^l_{ij}E_{lk}. \tag{2.17}$$

The proof of the statement that the solutions of the evolution equations (2.8) and (2.9) have the general integral (2.7) reduces now to the standard calculation: applying the operator $\mathcal{D}/\mathcal{D}t$ to both sides of (2.7) and using Eqs. (2.11), (2.12), (2.16), and (2.17), we obtain the required result.

To write the equation of state for a material within the framework of the affine-metric model, one should consider the internal energy as a function of the entropy and tensorial geometrical characteristics of internal interactions

$$U = U(s, \varepsilon_{ij}, {}^*C^k_{ij}, {}^*K_{kij}, {}^*R^k_{ijq}). \tag{2.18}$$

The last argument of the function of the internal energy (2.18) coincides with the coupling-curvature tensor

$${}^*R^k_{ijq} = \frac{\partial\, {}^*\Gamma^k_{ij}}{\partial x^q} - \frac{\partial\, {}^*\Gamma^k_{iq}}{\partial x^j} + {}^*\Gamma^k_{\alpha q}\, {}^*\Gamma^\alpha_{ij} - {}^*\Gamma^k_{\alpha j}\, {}^*\Gamma^\alpha_{iq}.$$

The transfer equation for this tensor follows from (2.9):

$$\frac{\mathcal{D}\, {}^*R^k_{ijq}}{\mathcal{D}t} = \frac{d}{dt}\, {}^*R^k_{ijq} + \frac{\partial v^p}{\partial x^i}\, {}^*R^k_{pjq} + \frac{\partial v^p}{\partial x^j}\, {}^*R^k_{ipq} + \frac{\partial v^p}{\partial x^q}\, {}^*R^k_{ijp} - \frac{\partial v^k}{\partial x^p}\, {}^*R^p_{ijq} = -\, {}^*\nabla_q E^k_{ij} + {}^*\nabla_j E^k_{iq} - 2E^k_{il}\, {}^*C^l_{jq}, \tag{2.19}$$

where the definition [3] of the covariant derivative was used for the tensor E^k_{ij}:

$${}^*\nabla_q E^k_{ij} = \frac{\partial E^k_{ij}}{\partial x^q} - {}^*\Gamma^l_{iq} E^k_{lj} - {}^*\Gamma^l_{jq} E^k_{il} + {}^*\Gamma^k_{lq} E^l_{ij}.$$

For a material that contains no defect structures in the initial state when the tensors ${}^*R^l_{ijq}$, ${}^*C^k_{ij}$, and ${}^*K_{ijk}$ vanish, the process of their occurrence during deformation is connected with energy dissipation. Therefore, when formulating the constitutive equations of the material, it is necessary to specify the internal energy (2.18) and the dissipative function. From the viewpoint of a qualitative analysis of these processes, the use of relation (1.14) between reversible and irreversible strains is of considerable significance. As a rule, the relation takes this form for small strains. For finite strains, there is no generally accepted relation. The more complicated nonlinear relations between the tensors A_{ij}, ε_{ij}, and π_{ij} compared to (1.14) are discussed in the literature (see [9] and references therein). However, from the phenomenological viewpoint, relation (1.14) can also be applied to arbitrary finite strains, since it leads only to a change of the variables in the internal energy (2.18). However, this change does not affect the choice of the affine-metric characteristics ${}^*R^l_{ijq}$, ${}^*C^k_{ij}$, and ${}^*K_{ijk}$ in (2.18), because their structure is determined by the dissipative processes in the material.

We mentioned above that these processes are characterized by the dissipative function, which in the framework of the assumptions of nonequilibrium thermodynamics is the bilinear form of thermodynamic force and flow: $D(X) = X_i Y^i$ ($D \geqslant 0$). A further generalization of this structure is connected with introduction of the following dissipative potential $\Phi(X)$ [10]:

$$\Phi(X) = \int_0^1 D(\lambda X)\frac{d\lambda}{\lambda}, \qquad \frac{\partial \Phi}{\partial X_i} = Y^i.$$

Let the internal energy (2.18) and the dissipative potential $\Phi = \Phi(E_{ij}, E^k_{ij}, e_{ij}, T)$ be specified. The equations of state of the material can be written in the form

$$\begin{gathered}
\sigma^j_i = (\delta_{ik} - 2\varepsilon_{ik})\rho\frac{\partial U}{\partial \varepsilon_{kj}} + \rho\Big(\frac{\partial U}{\partial\, {}^*C^i_{kl}}\, {}^*C^j_{kl} + 2\frac{\partial U}{\partial\, {}^*C^k_{lj}}\, {}^*C^k_{il}\Big) - \rho\Big(\frac{\partial U}{\partial\, {}^*K_{jkl}}\, {}^*K_{ikl} + 2\frac{\partial U}{\partial\, {}^*K_{kjl}}\, {}^*K_{kil}\Big) \\
+\rho\Big(\frac{\partial U}{\partial\, {}^*R^i_{kpq}}\, {}^*R^j_{kpq} - \frac{\partial U}{\partial\, {}^*R^k_{jpq}}\, {}^*R^k_{ipq} - 2\frac{\partial U}{\partial\, {}^*R^k_{pjq}}\, {}^*R^k_{piq}\Big) + \frac{\partial \Phi}{\partial e_{ij}}, \\
\rho\frac{\partial U}{\partial \varepsilon_{ij}} + 2\rho\frac{\partial U}{\partial\, {}^*K_{ksj}}({}^*\Gamma^i_{sk} + {}^*\Gamma^i_{ks}) - \frac{\partial}{\partial x^k}\Big(\rho\frac{\partial U}{\partial\, {}^*K_{kij}}\Big) = \frac{\partial \Phi}{\partial E_{ij}}, \\
\rho\frac{\partial U}{\partial\, {}^*C^k_{ij}} - 2\rho\frac{\partial U}{\partial\, {}^*K_{jis}} g_{sk} - 2\frac{\partial}{\partial x^q}\Big(\rho\frac{\partial U}{\partial\, {}^*R^k_{ijq}}\Big) - 2\rho\Big(\frac{\partial U}{\partial\, {}^*R^k_{ljq}}\, {}^*\Gamma^i_{lq} - \frac{\partial U}{\partial\, {}^*R^l_{ijq}}\, {}^*\Gamma^l_{kq}\Big) = \frac{\partial \Phi}{\partial E^k_{ij}}.
\end{gathered} \tag{2.20}$$

The standard analysis within the framework of nonequilibrium thermodynamics allows one to calculate the components J^k of the defect-flow vector:

$$J^k = \rho E_{ij}\frac{\partial U}{\partial\, {}^*K_{kij}} - 2E^l_{ij}\rho\frac{\partial U}{\partial\, {}^*R^l_{ijk}}. \tag{2.21}$$

Inasmuch as the defects do not go outside the boundary S, the normal component of the defect-flow vector vanishes at the boundary: $n_k J^k = 0$. Since the sources E_{ij} and E^l_{ij} are independent, hence and from (2.21) we have the boundary conditions in the form

$$\rho \frac{\partial U}{\partial {}^*K_{kij}} n_k \Big|_S = 0, \qquad \rho \frac{\partial U}{\partial {}^*R^l_{ijk}} n_k \Big|_S = 0. \tag{2.22}$$

The components of the metric tensor and the coupling objects satisfy the second-order equations in the spatial variable; therefore, for 6 functions g_{ij} and 27 objects ${}^*\Gamma^k_{ij}$, relations (2.22) provide the complete set of 33 necessary boundary conditions.

3. Elastoplastic Model with Disclinations. To show the influence of the internal stresses associated with defect structures in a specimen on its behavior during plastic deformation, we consider an affine-metric model which includes only disclinations. For this non-Euclidean model, the coefficients of affine coupling ${}^*\Gamma_{ij,k}$ remain symmetric relative to the lower indices and the coupling matches the metrics. From (2.7), it follows that the affine coupling coincides with the metric coupling $\Gamma_{ij,k}$, the latter being calculated by the relations (1.9) and (2.5), in which the metrics are determined by the solution of Eq. (2.8). The internal energy has the form $U = U(s, \varepsilon_{ij}, R_{lijq})$, where the elastic strain tensor is determined in terms of metrics (1.3) and (2.8), while the transfer equation (2.19) for the covariant components of the Riemann tensor is written in the form

$$\frac{\mathcal{D}R_{lijq}}{\mathcal{D}t} = \frac{d}{dt}R_{lijq} + \frac{\partial v^p}{\partial x^l}R_{pijq} + \frac{\partial v^p}{\partial x^i}R_{lpjq} + \frac{\partial v^p}{\partial x^j}R_{lipq} + \frac{\partial v^p}{\partial x^q}R_{lijp}$$
$$= \nabla_q\left(\nabla_i E_{jl} - \nabla_l E_{ij}\right) + \nabla_j\left(\nabla_l E_{iq} - \nabla_i E_{ql}\right) + 2E_{lp}g^{ps}R_{sijq}.$$

We consider a theoretical variant by setting $D = D(T, E_{ij})$. In this case, we have

$$D = E_{nj}\Big(\rho\frac{\partial U}{\partial \varepsilon_{nj}} - H^{nj}\Big),$$
$$H^{nj} = \Big[-4\frac{\partial^2}{\partial x^l \partial x^q}\rho J^{lnjq} + 4\frac{\partial}{\partial x^q}\rho(J^{nlpq}\Gamma^j_{lp} + J^{qlpj}\Gamma^n_{lp} - J^{nlpj}\Gamma^q_{lp}) - 2\rho J^{lkpq}(\Gamma^n_{lp}\Gamma^j_{kq} - \Gamma^n_{lq}\Gamma^j_{kp})\Big], \tag{3.1}$$
$$J^{lijq} = \frac{\partial U}{\partial R_{lijq}}.$$

We rewrite expression (3.1) in the form adopted in the theory of plasticity. To this end, we express the first term in brackets through the stress tensor

$$\sigma^j_i = (\delta_{ik} - 2\varepsilon_{ik})\rho\frac{\partial U}{\partial \varepsilon_{kj}} + 4R_{ilpq}\rho\frac{\partial U}{\partial R_{ljpq}}$$

and use the formula

$$\frac{1}{\Delta}\frac{\partial \Delta}{\partial a_{ik}}a_{kj} = \delta^i_j, \qquad \Delta = \det||a_{ij}||, \qquad a_{ij} = \delta_{ij} - 2\varepsilon_{ij}.$$

Then,

$$D = E_{nj}\frac{\partial \ln \Delta}{\partial a_{ni}}\Big(\sigma^j_i - 4R_{ilpq}\rho\frac{\partial U}{\partial R_{ljpq}} - a_{ik}H^{kj}\Big) \equiv v^s_i(\sigma^i_s - \tau^i_s).$$

It is usually assumed that plastic strains do not change the volume of material. We require that $v^i_i = 0$ and express the rate of energy dissipation in the form

$$D = v^i_k s^k_i, \qquad s^k_i = (\sigma^k_i - \tau^k_i) - \frac{1}{3}\delta^k_i(\sigma^l_l - \tau^l_l). \tag{3.2}$$

Let D be the function of the first degree of homogeneity in v^k_i, i.e., $D(\lambda v^k_i) = |\lambda| D(v^k_i)$. We use the Mises yield criterion for the material. Then, $D = \tau_0\sqrt{v_i^j v_j^i}$ and $s_i^j = \tau_0(v_i^j/\sqrt{v_m^n v_n^m})$, which is equivalent to the relations

$$v_i^j = \lambda\frac{\partial f}{\partial s_j^i}, \qquad f = s_i^k s_k^i - \tau_0^2.$$

As a result, the rate of plastic strain can be written in the form

$$E_{ij} = \lambda\frac{\partial f}{\partial s_k^i}(\delta_{kj} - 2\varepsilon_{kj}).$$

For elastic strains, we obtain

$$\frac{\mathcal{D}\varepsilon_{ij}}{\mathcal{D}t} = \begin{cases} e_{ij} & \text{if} \quad s_i^k s_k^i < \tau_0^2, \\ e_{ij} - E_{ij} & \text{if} \quad s_i^k s_k^i = \tau_0^2. \end{cases} \tag{3.3}$$

In the case of small elastic strains and the absence of defects, we have $\tau_i^j = 0$ in (3.2). This implies the well-known equations of an ideal rigid-plastic medium $e_{ij} = E_{ij}$. The allowance for the contribution from the defects to the dissipation results in a translational transfer of the yield surface in the stress space and hardening of the material.

The above generalization of the internal geometrical structure of the material with a transition from the Euclidean to Riemannian geometry leads to a geometrically closed class of models of elastoplastic materials. Within the framework of the model considered, any strains do not alter the qualitative character of interaction between the particles in the material.

4. Discussion. The extension of the classical theory of elasticity to the broad class of elastoplastic materials the internal interactions in which are of affine-metric structure allows one to construct geometrically closed complete thermomechanical models of these materials. The use of the formalism of nonequilibrium thermodynamics makes it possible to model the interaction between the defects and to relate these defects to the macroscopic properties of the material during deformation. In addition, concretization of the dissipative characteristics of materials must be based on experimental data.

We make a few remarks concerning the physical interpretation of the quantities used in the theory. We note primarily that the equilibrium equations of a specimen with defects are a generalization of the well-known physical equilibrium models of elastic continuum with dislocations (see, e.g., [11]). The presence of dislocations leads to a replacement of all the affine-metric characteristics on the right-hand side of (1.12) or (2.20) by a singularity of a certain form. As a result, elastic strains occur, which correspond to a defect-induced plastic strain and leads to the nonzero internal energy of this specimen.

The use of the affine-metric characteristics to describe the defects was proposed by Kondo and Bilby [12, 13]. The affine-metric theories used to describe disordered systems were classified by Grachev et al. [6, 7]. However, their correspondence to the generally accepted physical models requires a special discussion. In particular, the model of an elastoplastic body considered in Sec. 3 contains no dislocations according to this classification. Nevertheless, a theory with $U = U(s, \varepsilon_{ij}, R_{lijq})$ can be constructed that takes into account dislocations determined in terms of the Burgers vector $\boldsymbol{b}$. In Euler variables, the components of this vector are calculated via the transformation matrix $p_i^\alpha = p_i^\alpha(\boldsymbol{x}, t)$ which relates the coordinates of the points of the medium dx^k after deformation to the initial coordinates $d\xi^\alpha$ for an infinitesimal element of the medium [14]: $d\xi^\alpha = p_k^\alpha dx^k$. The components of the Burgers vector are $b^\alpha = -\oint p_k^\alpha dx^k$ for any closed contour [2, p. 184]. The dislocation-density tensor $B^{i\alpha}$ is determined by the relation

$$B^{i\alpha} = -\varepsilon^{ikj}C_{kj}^\alpha, \qquad C_{kj}^\alpha \equiv \frac{1}{2}\left(\frac{\partial p_j^\alpha}{\partial x^k} - \frac{\partial p_k^\alpha}{\partial x^j}\right), \tag{4.1}$$

where ε^{ikj} is the Levi-Civita symbol, and the objects C_{kj}^α characterize the deviation of the mapping p_k^α from diffeomorphism. We assume that the metric elastic-strain tensor g_{ij} has the form $g_{ij} = p_i^\alpha p_j^\alpha$. Actually, this relation determines the choice of a possible parametrization, for which the intrinsic metric tensor does not coincide with the complete strain tensor, i.e., the Almansi tensor A_{ij}, but possesses an algebraic structure that corresponds to the classic theory of elasticity. Calculating $\Gamma_{ij,k}$ for the above model with disclinations, we obtain

$$\Gamma_{ij,k} = \frac{1}{2}p_k^\alpha\left(\frac{\partial p_j^\alpha}{\partial x^i} + \frac{\partial p_i^\alpha}{\partial x^j}\right) + p_i^\alpha C_{jk}^\alpha + p_j^\alpha C_{ik}^\alpha.$$

From this relation and (4.1), it is seen that this model contains dislocations. It is clear that the separation of them in affine-metric objects is determined by a relation between the experimentally observed discontinuity of the diffeomorphic structure of the strain field (the functions p_k^α) and the intrinsic metric structure (the tensor g_{ij}). Obviously, ε_{ij} and R_{lijq} are expressed in terms of the generalized distortions as well. The transfer equations for them can be written in the form

$$\frac{dp_i^\alpha}{dt} + p_l^\alpha \frac{\partial v^l}{\partial x^i} = I_i^\alpha.$$

Moreover, E_{ij} are connected with I_i^α by the relations $E_{ij} = (p_i^\alpha I_j^\alpha + p_j^\alpha I_i^\alpha)/2$. We set $I_i^\alpha = \gamma^{\alpha\beta}p_i^\beta$; then $E_{ij} = \gamma^{\alpha\beta}p_i^\alpha p_i^\beta$ and $\gamma^{\alpha\beta}$ can be expressed in stresses and distortions. Thus, to describe the evolution of the generalized distortion, in place of Eqs. (3.3) for elastic strains we have

$$\frac{dp_i^\alpha}{dt} + p_l^\alpha \frac{\partial v^l}{\partial x^i} = \begin{cases} 0 & \text{for} \quad s_i^k s_k^i < \tau_0^2, \\ \gamma^{\alpha\beta}p_i^\beta & \text{for} \quad s_i^k s_k^i = \tau_0^2. \end{cases}$$

From the physical viewpoint, the affine-metric objects are the intrinsic variables. The tensors ε_{ij} and π_{ij} cannot be measured directly. Only the sum of them (or any other representation of A_{ij} in terms of ε_{ij} and π_{ij}) can be measured directly. Nevertheless, the tensor A_{ij} can always be determined if the velocity field is known, since $v^i = du^i/dt$ (u^i is the displacement field). In addition, the tensor A_{ij} is expressed in displacements in a standard way. The above representation for g_{ij} in terms of the generalized distortion p_i^α is not necessary for the model considered. However, this representation is frequently used in the literature [2, 11, 14, 15] to describe dislocations.

The physical interpretation of the model presented in this paper gives an insight into the nature of plastic deformation at the scale levels that are characteristic of various types of defect structure.

The general affine-metric model describes phenomenologically the interaction between the defects and the perturbations induced by these defects in an elastic strain field. At the same time, it allows one to interpret the plastic behavior of the material on the basis of the structure of deformation fields with various levels of measurement resolution.

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