THE FUNDAMENTAL FUNCTION OF ROTATION AT THE MESO-LEVEL IN DEFORMATION AND FRACTURE OF SOLIDS

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ABSTRACT
A large body of experiments has shown that shear band formation and rotation of structural elements at the mesolevel are fundamental to the development of plastic deformation and fracture of solids. The model of a medium, allowing for independent rotation of its fragments, force-induced and couple stresses, and torsion bends is considered for description of plastic deformation at the mesolevel. This model is generalization of Cosserat elastic approach for the plastic deformation. This model leads to a specific scheme of deformation at the mesolevel "shear plus rotation". Numerical simulation of fragment rotation and plastic shear band development in a polycrystalline specimen is presented.

1 INTRODUCTION

There is no question it is the school of V.E. Panin [1-10] who should be credited with brining the concept of scale and structural levels of deformation of loaded solids to mechanics of deformable solids and to physics of plasticity. The detailed, careful and deep study conducted by researchers of this school has done much to understand the mechanisms of deformation and fracture at the mesolevel, to which a key role in the hierarchy of scales is assigned. The fact that the complicated internal structure of solids is certain to affect their macroscopic behavior was realized even in the making of classical physics of plasticity and mechanical theories of plasticity and fracture. However, the classical phenomenology of deformable solids was invariably based on macroscopic notions [3–7].

The central idea of physical mesomechanics that any loaded material is an evolving hierarchically organized system of differently scaled structural elements has made it possible to treat all developed models as models of the corresponding levels of averaging and accuracy of description [3- 4, 7- 8]. We takes into consideration three scale levels: micro, meso and macro [1-8].

The equations which describe deformation processes are differential equations and therefore at the heart of the models of interest is also the idea of a deformable continuum (a particular case is discrete way of description, i.e., molecular dynamics etc., which are not concerned here). The continuum theory of defects is no exception, even though the motion of a single dislocation is the phenomenon of discontinuity transfer (an elementary step). This very important fact allows us to extend the methods of continuum mechanics to the micro- and mesolevels, i.e., to the level of a structured media where manifestations of discontinuity of elementary acts are essential. In mechanics, such methods received the name "methods of uninterrupted approximation". One of the first theories of this type was the theory of asymmetric elasticity suggested by brothers Cosserat in 1909 [11]. It was unfairly forgotten for several decades and was given rebirth by Truesdell and Toupin in 1960 [12, 13]. Actually, in Cosserat's model an attempt was made to account for inelastic phenomena and for the presence of the internal structure of a material by using the theory of elasticity. We shall take a closer look at Cosserat's model and its modification to describe the inelastic behavior of structured media at the mesolevel.

2. FROM THE EQUATIONS OF THE ASYMMETRIC THEORY OF ELASTICITY TO THE EQUATIONS OF THE ASYMMETRIC THEORY OF PLASTICITY

2.1. Equations of asymmetric elasticity

The approximations of classical theories of elasticity and plasticity are based on idea when resultant surface force vector $\mathbf{P}_n \mathrm{d}S$ is given only (here, $\mathbf{d}S$ is an infinitesimal surface element with the normal $\mathbf{n}$; $\mathbf{P}_n$ is the surface force). Attempts to remove the limits imposed by the symmetric theory were made by Voigt [14]. He supposed that there is a principle moment $\mathbf{M}_n \mathrm{d}S$ (here, $\mathbf{M}_n$ is the moment of forces acting on the surface element area $\mathbf{d}S$ with the normal $\mathbf{n}$). Thus, the couple stresses along with the force stresses were introduced into the model. In the general case, both the force stress tensor and the couple stress tensor are therewith asymmetric. The symmetry of the stress tensor follows from the law of conservation of angular momenta in the classical case, i.e., in the absence of internal moments, surface moments $\mathbf{M}_\mathrm{n}$, and mass moments $\mathbf{Y}$. The introduction of a surface moment into the model not only lifts the symmetry restrictions, it also implies the presence of noncompensated internal moments in a medium. The forgoing suggests that the particles of the medium have six degrees of freedom: three displacements u_i and three independent rotations ω_i $(\mathbf{u} = \{u_i\},\ \boldsymbol{\omega} = \{\omega_i\},\ i = 1, 2, 3)$. The number of motion equations thus becomes equal to six:

$$\sigma_{ji,j} + \rho X_i = \rho \ddot{u}_i, \tag{1}$$

$$\ni_{ijk}\ \sigma_{ji,j} + \mu_{ji,j} + \rho Y_i = J \ddot{\omega}_i. \tag{2}$$

Here, $\ni_{ijk}$ is the Levi-Civita tensor, the systems of equations (1) and (2) expresses, respectively, the law of conservation of momentum and the law of conservation of angular momenta.

Note that the system of equations (1) and (2), as in the classical case, assumes that any macroscopic particle of a deformable continuum is infinitesimal and thus the classical theory of asymmetric elasticity does not handle with the characteristic length [11, 15].

In the case of asymmetric elasticity, the law of conservation of energy for an arbitrary volume V bounded by the surface S has the form [15]:

$$\int_V \{\dot{E} - [\sigma_{ji}(v_{i,j} - \ni_{kji}\ \dot{\omega}_k) - \mu_{ji}\dot{\omega}_{i,j}] - q_{i,i}\}\mathrm{d}V. \tag{3}$$

Denoting

$$\gamma_{ji} = u_{i,j} - \ni_{kji}\ \omega_k,\ \ \kappa_{ji} = \omega_{i,j}, \tag{4}$$

we obtain expressions for deformations which are convenient to rewrite in the form:

$$\dot{\gamma}_{ji} = v_{i,j} - \ni_{kji}\ \dot{\omega}_k,\ \ \dot{\kappa}_{ji} = \dot{\omega}_{i,j}. \tag{5}$$

Expressions (4) or (5) hold true only locally, $\dot{\gamma}_{ji}$ is the asymmetric strain rate tensor, $\dot{\kappa}_{ji}$ is the bending-torsion rate tensor, and q_i are the heat flux vector components. Thus the law of energy conservation (13) elucidates the meaning of the introduced deformation (4). In this law expressions $\sigma_{ji} d\gamma_{ji}$ and $\mu_{ji} d\kappa_{ji}$ should therewith have the meaning of work of asymmetric force stresses in the increments of "deformations", $d\gamma_{ji}$, which are asymmetric as well, and the meaning of work of couple stresses in the increments $d\kappa_{ji}$ $\kappa_{ji} \neq \kappa_{ij}$ [15].

Now, the law of conservation of energy is written in the differential form:

$$\dot{E} = \sigma_{ji}\dot{\gamma}_{ji} + \mu_{ji}\dot{\kappa}_{ji} - q_{i,i}. \tag{6}$$

Thus, the system of equations (1) and (2), which expresses the laws of conservation of momentum and angular momenta, together with the law of conservation of energy (6) and with the equation

$$\dot{\rho} + \rho \dot{u}_{i,i} = 0, \tag{7}$$

which expresses the law of conservation of mass, and also with constitutive equations (which are yet to be written) and additional equations (5) give a closed system of dynamic equations of the asymmetric theory of elasticity.

The independent rotations ω_i are therewith produced by noncompensated internal moments, i.e., by internal motion at lower scale levels. Thus, it becomes apparent that in essence the equations of asymmetric elasticity should describe inelastic effects.

This fact gave grounds to a great number of attempts at applying Cosserat's approach to construct models of the asymmetric theory of plasticity on the macrolevel. The application of these equations to macroscopic objects could not, however, meet with success, since the conclusions made from such theories were not confirmed by macroscopic experiments. Another disadvantage of such macroscopic theories of asymmetric plasticity is complete indeterminancy in the so-called "moment moduli" as in macroscopic parameters which cannot be determined experimentally similar to the moduli of elasticity of a symmetric medium.

The constitutive equations of asymmetric elasticity can be presented in the form [15, 16]:

$$\begin{aligned} &\sigma_{ji} = (\mu + \alpha)\gamma_{ji} + (\mu - \alpha)\gamma_{ij} + (\lambda\gamma_{kk} - \nu\theta)\delta_{ij}, \\ &\mu_{ji} = (\gamma + \varepsilon)\kappa_{ji} + (\gamma - \varepsilon)\kappa_{ij} + \beta\kappa_{kk}\delta_{ij}, \\ &S = \nu\gamma_{kk} + m\theta, \; \theta = T - T_0, \end{aligned} \tag{8}$$

In these equations, λ and μ are Lame's constants, α, γ, β, ε are moment "moduli", $\nu = a_{\mathrm{t}}(3\lambda + 2\mu)$, a_{t} is the coefficient of linear thermal expansion.

2.2. Equations of the theory of asymmetric plasticity

Entertaining the main idea of physical mesomechanics about hierarchical structural organization of a medium, we shall think that at the macrolevel of averaged description the internal moments are always compensated and any theory of an elastoplastic medium (except for particular cases) invariably gives symmetric stress and strain tensors.

At the mesolevel, all structural elements significant for study are defined explicitly. The noncompensated internal moments are due to microscale internal motion, nonuniform strain-induced defect distribution, and collective processes. This locally ordered internal motion is taken into account in the averaged manner by the development of independent rotations whose driving forces are couple stresses and asymmetric components of force stresses. Such an asymmetric theory is essentially gradient and implies in an implicit manner that there is a characteristic internal scale l at the mesoscale.

Let us postulate that the total strain rate and bending-torsion rate are the sum of elastic and plastic components:

$$\begin{aligned} &\dot{\gamma}^{\mathrm{T}}_{ji} = \dot{\gamma}^{\mathrm{e}}_{ji} + \dot{\gamma}^{\mathrm{p}}_{ji}, \\ &\dot{\kappa}^{\mathrm{T}}_{ji} = \dot{\kappa}^{\mathrm{e}}_{ji} + \dot{\kappa}^{\mathrm{p}}_{ji}. \end{aligned} \tag{9}$$

Now, constitutive equations (8) will take the relaxation form:

$$\begin{aligned} &\dot{\sigma}_{ji} = \lambda(\dot{\gamma}^{\mathrm{T}}_{kk} - \dot{\gamma}^{\mathrm{p}}_{kk})\delta_{ij} + (\mu + \alpha)(\dot{\gamma}^{\mathrm{T}}_{ji} - \dot{\gamma}^{\mathrm{p}}_{ji}) + (\mu - \alpha)(\dot{\gamma}^{\mathrm{T}}_{ij} - \dot{\gamma}^{\mathrm{p}}_{ij}), \\ &\dot{\mu}_{ji} = \beta(\dot{\kappa}^{\mathrm{T}}_{kk} - \dot{\kappa}^{\mathrm{p}}_{kk})\delta_{ij}(\gamma + \varepsilon)(\dot{\kappa}^{\mathrm{T}}_{ji} - \dot{\kappa}^{\mathrm{p}}_{ji}) + (\gamma - \varepsilon)(\dot{\kappa}^{\mathrm{T}}_{ij} - \dot{\kappa}^{\mathrm{p}}_{ij}). \end{aligned} \tag{10}$$

In equations (10), the increments in elastic force stresses and couple stresses are invariably proportional to the increments in total strains and bending-torsions and the stresses relax as the plastic components of the increments in strains and bends-torsions develop [17].

Within the framework of the model developed, the stage of elastic deformation ensures zero moment "moduli" and the theory is reduced to symmetric equations of the Hooke's elastic medium. In the course of inelastic deformations, these moment "moduli" becomes no longer equal to zero and increase as the microscale internal motion gets more and more nonuniform.

Thus, as already mentioned [2, 8, 17, 18], the moment "moduli" characterize local development of mesoscale inelastic deformations, rather than being macroscopic constants of a material, and it is worth applying these parameters only to the mesolevel. In this case, it would be appropriate to present them in the form of some functions (linear functions as is the simplest variant) of cumulative plastic deformation $\varepsilon_k^{\mathrm{p}}$ stored in a given local volume (in a point of continuum at the mesolevel) of a loaded medium:

$$\varepsilon_k^{\mathrm{p}} = \int_0^{\varepsilon} \left| \mathrm{d}\varepsilon^{\mathrm{p}} \right| = \int_0^{t} \left| \dot{\varepsilon}^{\mathrm{p}} \right| \mathrm{d}t. \qquad (11)$$

Here, $\dot{\varepsilon}^{\mathrm{p}}$ means the intensity of plastic deformation.

Of particular importance is the problem of limitations of force and couple stresses. Leaving this challenging and incompletely understood problem untouched, we shall dwell briefly on two simplest possibilities how to do so:

1. To introduce into consideration a generalized or combined plasticity criterion where both the force and couple stresses are involved in one expression. This requires normalization and reduction of the stresses to the dimensionless form or an explicit introduction into consideration the length parameter $[\mu_{ji}] = [\sigma_{ji}][L]$.

2. To limit only the force stresses, by using, e.g., von-Mises plasticity criterion where one should average the asymmetric shear stresses $s_{ij}s_{ij}$ at $i \neq j$, e.g., as follows:

$$\left[\frac{3}{2} \left(s_{xx}^2 + s_{yy}^2 + s_{zz}^2 + \frac{1}{4}(s_{xy} + s_{yx})^2 + \frac{1}{4}(s_{xz} + s_{zx})^2 + \frac{1}{4}(s_{yz} + s_{zy})^2 \right) \right]^{1/2} \leq K_1. \qquad (12)$$

Here, s_{ij} are the force stress deviator tensor components. If condition (12) is fulfilled, we should additionally limits the couple stresses by writing an expression similar to (12) for them:

$$\left[\frac{3}{2} \left(\mu_{xx}^2 + \mu_{yy}^2 + \mu_{zz}^2 + \frac{1}{4}(\mu_{xy} + \mu_{yx})^2 + \frac{1}{4}(\mu_{xz} + \mu_{zx})^2 + \frac{1}{4}(\mu_{yz} + \mu_{zy})^2 \right) \right]^{1/2} \leq K_2. \qquad (13)$$

Because the momentum $\mathbf{M} = \mathbf{F}\ell$ and the rotation of a medium element induces shear deformation at its boundaries, the constant K_2 in (13) can be chosen to correspond to the quantity $\tau^*\ell$, where τ^* is the yield limit of a material in pure shear.

Taking the postulate that unloading is elastic, the force and couple stresses are calculated by elastic formulae of the already asymmetric elasticity with functions of the moment "moduli" attained in each local region, depending on the value of the accumulated inelastic deformations.

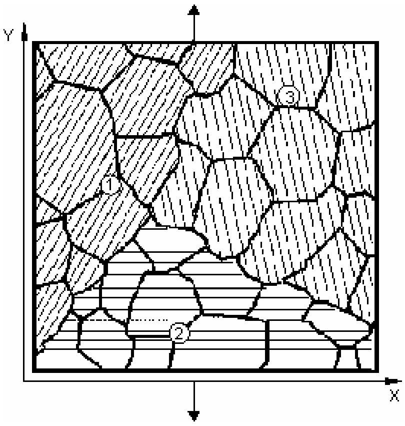
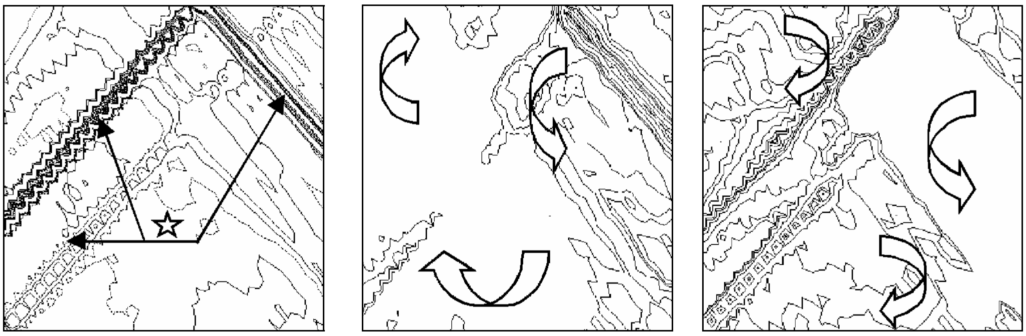


Figure 1: Map of polycrystalline mesovolumes with grain conglomerates [21]

3. Simulation of the mechanical behavior of submicrocrystalline materials

It is well known that in submicrocrystalline materials mesostructural elements are misoriented to a great extent and their inelastic deformation are essentially associated with grain-boundary defect flows [19, 20]. The idea is naturally conceived that the application of the asymmetric theory with developed microscale internal motion to these materials is quite efficient. in the case of two-dimensional plane flow with: $u_1 \neq 0$, $u_2 \neq 0$, $u_3 = 0$, $\Omega_3 \neq 0$, $\omega_3 \neq 0$, $\Omega_1 = \Omega_2 = \omega_1 = \omega_2 = 0$.

Figure 1 shows the initial map of specimens with conglomerates of grains of different sizes. The susceptibility to the development of independent rotations for grains of each of three conglomerates is given nearly the same, but considerably different in going from one conglomerate to another. The results of calculations for the formation of localized deformation are presented in Fig. 2. In this figure, the direction of rotation of the strain-induced blocks is shown by arrows, the contours of blocks are shown by isolines. All calculations in this section have been preformed according to the simplified model reported in [17, 21]. Some of the blocks rotate clockwise, while the others rotate anticlockwise. The boundary of the rotating structural elements is determined by localized deformation bands which are not closely related neither to the conglomerate boundaries nor to the grain boundaries. Some rotations bring about the formation of tension zones, resulting in fracture by the opening mechanism separation (where the rotations are oppositely directed (clock- and anticlockwise)).



(*a*) (*b*) (*c*)

Figure 2: Isolines of the plastic strain intensity (*a*), negative (clockwise) (*b*) and positive (anticlockwise) (*c*) rotations of the mesovolumes shown in Fig. 1. The star indicates the bands of localized deformation. The directions of rotation of the strain-induced blocks are shown by arrows.

Of interest is the case where adjacent elements rotate in one direction, but with different speeds and at different angles. Such zones can be seen in Fig. 2(*b*, *c*). In this event, a slip of blocks is observed and fracture will follow the mechanism of shear. If the band of localized deformation at the upper left corner (Fig. 2(*c*)) is considered to be the nucleus of a crack, opening will dominate in its upper part and shear in its lower part. Such combined fracture is observed most frequently. We hope the proposed method of simulation will be useful and efficient in predicting the deformation properties of UFG materials, nanomaterials and composites.

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