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REGULARITIES OF VARIATION OF SPHERICAL TENSOR IN CRYSTALS OF POLYCRYSTALLINE MATERIAL UNDER TORSION ACTION

Vasile Marina[1], Viorica Marina[2]
[1] Ministry of Education, Chisinau, Moldova, vasilemarina21@yahoo.com
[2] Technical University of Moldova, Chisinau, Moldova, marina_viorica@yahoo.com

Abstract: *The laws of fluctuations of spherical stress tensors in cubic lattice crystals are investigated in function of their orientation in polycrystalline single-phase materials. It is shown that interactions among crystals in conglomerate of pollycrystals lead at local volume stresses/strains appearance even at pure macroscopic shear. The interval of changing of spherical stress/strain tensors is comparable with macroscopic module of deviator of stresses/strains and depends on anisotropy coefficient of crystals.*
Based on established laws it is possible to explain the row of experimental thermo mechanical effects, for example, energy dissipation which is connected with concept of internal friction. According to this model the conditions of destructions of polycrystalline materials could be described at general load using at local level simple strength criteria's: maximum normal stress/strain.
Keywords: *stress, strain, symmetry, structure, crystals.*

1. THE CONSTITUTIVE EQUATIONS OF THE MODEL

The polycrystalline aggregate at macroscopical level $(V > V_0)$ initially has been considered homogeneous and isotropic, and at microscopical level $(V < V_0)$, microheterogeneous and anisotropic. The volumes element V_0 is composed by an infinite multitude of subelements cinematically interrelated and having different thermomecanical properties.

In order to create an useful system of constitutive equations it is necessary to concomitantly study the material behavior at the level of material particle, structure element and conglomerate. We note $\tilde{t}_{ij}, \tilde{d}_{ij}$ the stresses and strains at material level and t_{ij} and d_{ij} at conglomerate level, based on geometric and equilibrium equations, on homogeneity conditions at conglomerate level, we obtain the relationships

$$t_{ij} = \frac{1}{\Delta V_0} \int_{\Delta V_0} \tilde{t}_{ij} dV = \left\langle \tilde{t}_{ij} \right\rangle, \qquad d_{ij} = \left\langle \tilde{d}_{ij} \right\rangle, \tag{1}$$

$$\left\langle \tilde{t}_{ij} \tilde{d}_{ij} \right\rangle = \left\langle \tilde{t}_{nm} \right\rangle \left\langle \tilde{d}_{nm} \right\rangle = t_{pq} d_{pq}. \tag{2}$$

The (1) and (2) relations can be presented under one singe expression

$$\left\langle \left(\tilde{t}_{ij} - t_{ij}\right)\left(\tilde{d}_{ij} - d_{ij}\right) \right\rangle = 0. \tag{3}$$

If the stress $\left(\tilde{t}_{ij}\right)$ and strain $\left(\tilde{d}_{ij}\right)$ tensors are discomposed to spherical deviators and tensors

$$\tilde{t}_{ij} = \tilde{\sigma}_{ij} + \tilde{\sigma}_0 \delta_{ij}, \qquad \tilde{d}_{ij} = \tilde{\varepsilon}_{ij} + \tilde{\varepsilon}_0 \delta_{ij}, \tag{4}$$

the (3) relation obtained shape

$$\left(\tilde{\sigma}_{ij}-\sigma_{ij}\right)\left(\tilde{\varepsilon}_{ij}-\varepsilon_{ij}\right)+3\left(\tilde{\sigma}_0-\sigma_0\right)\left(\tilde{\varepsilon}_0-\varepsilon_0\right)=0\,. \qquad (5)$$

At writing (5) relation was admitted that scalar product between fluctuations of stress and strain tensors are canceled for any thermomecanic processes.

At reversible processes the subelements, from which the polycrystalline conglomerate is composed, are selected only after orientation factor, which are characterized by those tree Euler's angels θ,ψ,ϕ, videlicet

$$\tilde{\sigma}_{ij}=\tilde{\sigma}_{ij}(\theta,\psi,\phi,s),\ \tilde{\varepsilon}_{ij}=\tilde{\varepsilon}_{ij}(\theta,\psi,\phi,s),\ \tilde{\sigma}_0=\tilde{\sigma}_0(\theta,\psi,\phi,s),\ \tilde{\varepsilon}_0=\tilde{\varepsilon}_0(\theta,\psi,\phi,s), \qquad (6)$$

where by s - the solicitation factor at macroscopical level is noticed.

In the irreversible processes materials are also selected after irreversible strain tensor p_{ij}.

Each subelement can be identified with all the material particles in the volume V_0, which have the same the same tensor of irreversible deformations. The total amount of material particles having the same tensor of irreversible deformations determines the weight of the given subelement in the volume V_0. The composition of material particles in each subelements is unchanged during all forming processes of the conglomerate. The stress deviators at the level of subelements in reversible processes we will note through $\bar{\sigma}_{ij},\bar{\varepsilon}_{ij}$. Starting with this definition relation (5) for polycrystalline materials with cubic lattice $\sigma_0=K\varepsilon_0$, $\tilde{\sigma}_0=K\tilde{\varepsilon}_0$ will be written in following way

$$\left(\tilde{\varepsilon}_0-\varepsilon_0\right)^2=\frac{1}{3K}\left(\tilde{\sigma}_{ij}-\sigma_{ij}\right)\left(\varepsilon_{ij}-\tilde{\varepsilon}_{ij}\right)=\frac{1}{3K}\left(\tilde{\sigma}'_{ij}-\sigma'_{ij}\right)\left(\varepsilon'_{ij}-\bar{\varepsilon}'_{ij}+\bar{e}'_{ij}-\tilde{e}'_{ij}\right), \qquad (7)$$

where through $\tilde{\sigma}'_{ij},\bar{\varepsilon}'_{ij},...$ – the components of those deviators are noted in crystallographic system of coordinates; $\bar{e}'_{ij},\tilde{e}'_{ij}$ - deviators of reversible strains at the level of subelement and material particle of some orientation of crystallographic system of coordinates.

The interactions between two subelements result from interactions among particles belonging to different kinds of subelements. Therefore, the interactions among subelements have a nonparticular character. It's obvious that not all the details of interactions among particles influence the behavior at microscopical level.

The notion of subelement has been defined as a lot of material points which belong to different monocrystals (crystallites). The stress-state of every material point of the given subelement depends of it's network (Ω) – orientation too.

The selection of particles in the inner of subelement in function of Ω orientation – factor permits a more detailed analysis of stress-and strain-state at microscopical level.

We propose the following kinetical relations for a subelement

$$\tilde{\sigma}_{ij}-\bar{\sigma}_{ij}=B(\bar{\varepsilon}_{ij}-\tilde{\varepsilon}_{ij}), \qquad (8)$$

where $\tilde{\sigma}_{ij},\tilde{\varepsilon}_{ij}$ - are components of stress/strain deviators in material particles which have the same values of components irreversible strain deviator, $\bar{\sigma}_{ij},\bar{\varepsilon}_{ij}$ - are average values of components of stress/strain deviators in material particles (subelements) which have the same values of components irreversible strain deviator; B - a constant which is an information carrier about structure elements, has an extremely important physical significance.

The cinematical interactions among the material particles which belong to giving subelement are focused in base of relationship

$$\bar{\sigma}_{ij}-\sigma_{ij}=D(\varepsilon_{ij}-\bar{\varepsilon}_{ij}), \qquad (9)$$

where $\sigma_{ij},\varepsilon_{ij}$ - macroscopic components of stress/strain deviators; D – the material constant.

Because $\bar{\varepsilon}_{ij}-\tilde{\varepsilon}_{ij}=\bar{e}_{ij}-\tilde{e}_{ij}$, where $\tilde{e}_{ij}$ reversible strain in exanimate material particle, but $\bar{e}_{ij}$ the average value of reversible strains in system of material particles with the same value of irreversible strains, the following relationships are obtained

$$\tilde{\sigma}'_{ij}(A,\theta,\psi,\varphi,\sigma_{nm}) = \begin{cases} M1(A)\tilde{a}_{in}(\theta,\psi,\varphi)\tilde{a}_{jm}(\theta,\psi,\varphi)\overline{\sigma}_{nm}, \; i=j \\ N1(A)\tilde{a}_{in}(\theta,\psi,\varphi)\tilde{a}_{jm}(\theta,\psi,\varphi)\overline{\sigma}_{nm}, \; i \neq j \end{cases}, \tag{10}$$

$$\tilde{e}'_{ij}(A,\theta,\psi,\varphi,\varepsilon_{nm}) = \begin{cases} M(A)\tilde{a}_{in}(\theta,\psi,\varphi)\tilde{a}_{jm}(\theta,\psi,\varphi)\overline{e}_{nm}, \; i=j \\ N(A)\tilde{a}_{in}(\theta,\psi,\varphi)\tilde{a}_{jm}(\theta,\psi,\varphi)\overline{e}_{nm}, \; i \neq j \end{cases}, \tag{11}$$

where

$$M1(A) = \frac{5(1+A)}{2+3A+\sqrt{A(2+3A)(3+2A)}}, \tag{12}$$

$$N1(A) = \frac{5(1+A)\sqrt{A}}{\sqrt{(2+3A)(3+2A)}+(2+3A)\sqrt{A}}, \tag{13}$$

$$M(A) = \frac{5(1+A)\sqrt{A}}{(2A+3)\sqrt{A}+\sqrt{(2+3A)(3+2A)}}, \tag{14}$$

$$N(A) = \frac{5(1+A)}{2A+3+\sqrt{A(2+3A)(3+2A)}}, \tag{15}$$

$$\left[a_{ij}(\theta,\psi,\varphi)\right] = \begin{bmatrix} \cos\varphi\cos\psi & \cos\varphi\sin\psi+\cos\theta\cos\psi\sin\varphi & \sin\theta\sin\varphi \\ -\cos\psi\sin\varphi & -\sin\psi\sin\varphi+\cos\theta\cos\psi\cos\varphi & \sin\theta\cos\varphi \\ \sin\theta\sin\psi & -\sin\theta\cos\psi & \cos\theta \end{bmatrix}, \tag{16}$$

where A anisotropy coefficient $A = \dfrac{2c_{44}}{c_{11}-c_{12}}$, c_{11}, c_{12}, c_{44} - elastic constants in crystallographic system of coordinates x'_i.

In case of proportional loading we have

$$\frac{\overline{\sigma}_{ij}}{\overline{\sigma}} = \frac{\overline{\varepsilon}_{ij}}{\overline{\varepsilon}} = \frac{\sigma_{ij}}{\sigma} = \frac{\varepsilon_{ij}}{\varepsilon}, \quad \overline{\sigma} = \sqrt{\overline{\sigma}_{ij}\overline{\sigma}_{ij}}, \; \overline{\varepsilon} = \sqrt{\overline{\varepsilon}_{ij}\overline{\varepsilon}_{ij}}, \quad \sigma = \sqrt{\sigma_{ij}\sigma_{ij}}, \; \varepsilon = \sqrt{\varepsilon_{ij}\varepsilon_{ij}}, \tag{17}$$

In base of (10) relationship for deviator components of stress and strain tensors in subelements the following relationships are obtained

$$\overline{\sigma}_{ij} = \overline{\sigma}\frac{\sigma_{ij}}{\sigma}, \quad \overline{\varepsilon}_{ij} = \overline{\varepsilon}\frac{\sigma_{ij}}{\sigma}. \tag{18}$$

The $\overline{\sigma}$ and $\overline{\varepsilon}$ values depend on giving subelement characteristics $\psi, \tau(\psi)$ (ψ - the share of subelements requested after elasticity limit at the moment of achieving threshold crossing from reversible state in irreversible state of subelement with $\tau(\psi)$ elasticity limit and actual values of stress/strain deviator tensors modules σ/ε. If in the plastic domain moment skin pass is $\overline{\sigma} = 2G(\tau(1-\chi)+\chi\overline{\varepsilon})$, then $\overline{\sigma}, \overline{\varepsilon}$ values are determined form the relationships

$$\bar{\varepsilon}(e,e') = \begin{cases} \dfrac{(e' + b\varepsilon')(1+b) - (1-\chi)(e + b\varepsilon)}{(\chi + b)(1+b)} \text{ dacă } e < e' \\ \dfrac{e' + b\varepsilon'}{1+b} \text{ dacă } e \geq e' \end{cases}, \tag{19}$$

$$\bar{e}(e',e) = \begin{cases} \dfrac{(1-\chi)b}{(1+b)(\chi+b)}(e + b\varepsilon(e)) + \dfrac{\chi}{\chi + b}(e' + b\varepsilon(e')) \text{ dacă } e < e' \\ \dfrac{e' + b\varepsilon(e')}{1+b} \text{ dacă } e \geq e' \end{cases}. \tag{20}$$

In (19), (20) thought ε' and e' the actual values of modules of total and elastic strain deviator tensors, but thought ε, e - respective values in the moment of passing from reversible stare in irreversible state of subelements with elastic limit

$$\tau(\psi) = \frac{e + b\varepsilon(e)}{1+b}, \tag{21}$$

in which ψ argument determined skin pass of subelements requested in plastic

$$\psi = \frac{\chi + b}{1-\chi} \frac{\varepsilon_{,e} - 1}{b\varepsilon_{,e} + 1}. \tag{22}$$

2. THE NUMERIC ANALYSIS OF VARIATION OF SPHERICAL TENSOR IN CASE OF SHEAR LOADING

Further we will analyze the variation of spherical tensor after absolute value for policristalline material 40X. Because variations of spherical tensors depend on five variables $\phi, \theta, \psi, r.r`$, at the beginning we will examine the lows of variation of $\tilde{\varepsilon}_0$ in function of one single variable. In fig. 1 the variation of $\tilde{\varepsilon}_0$ is presented in function of orientation angle ψ. The first curve refers at $\tilde{\varepsilon}_0$ variations in the subelement with the smallest elastic limite $\tau = \varepsilon_{nn}$, where ε_{nn} - represents the elastic limit at macroscopic level, curve *2* reflects $\tilde{\varepsilon}_0$ variations in subelement with elastic limit equal to $1{,}5\varepsilon_{nn}$, curve *3* reflects $\tilde{\varepsilon}_0$ variations in subelement with elastic limit equal to $2\varepsilon_{nn}$.

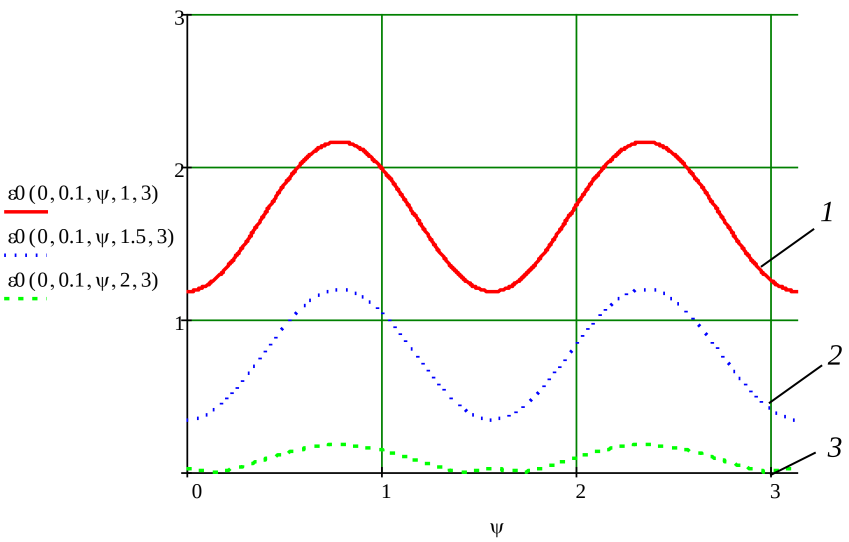


Figure.1. Variation of $\varepsilon 0$ in function of ψ

In fig.2 is given $\tilde{\varepsilon}_0$ dependence in function of strain deviator tensor modules at macroscopic level for four subelements with elastic limits ε_{nn}, $1{,}2\varepsilon_{nn}$, $1{,}4\varepsilon_{nn}$, $1{,}6\varepsilon_{nn}$.

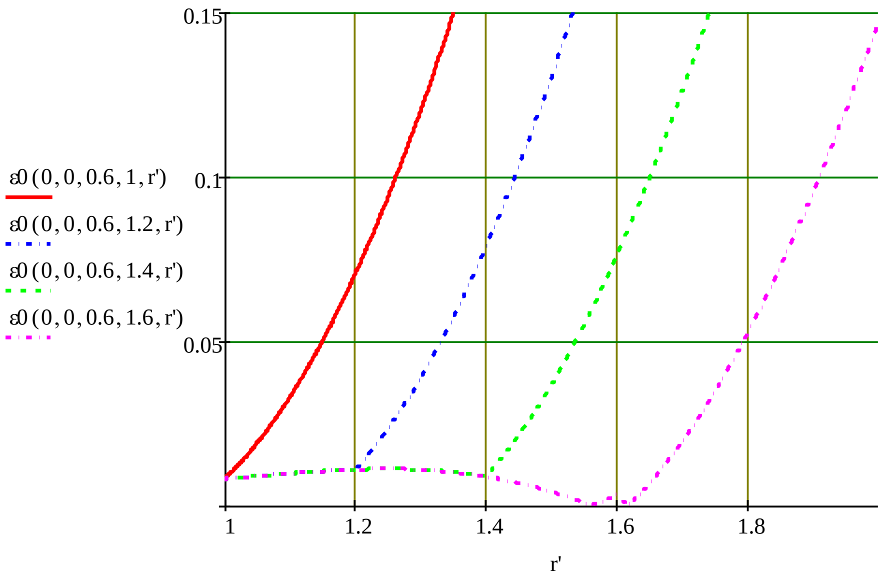


Figure.2. Variation of $\varepsilon 0$ in function of $r`$

In fig.1 and 2 is used the notation $\varepsilon 0 = \tilde{\varepsilon}_0 / \varepsilon_{nn}$.

In figures 3-5 the $\tilde{\varepsilon}_0$ variations are presented in function of two variables. So, in fig.3 the $\tilde{\varepsilon}_0 = \tilde{\varepsilon}_0(\phi,\theta,0{,}1{,}2)$ is given, in fig.4 $\tilde{\varepsilon}_0 = \tilde{\varepsilon}_0(\phi,0{,}0{,}3{,}2,r`)$, but in fig.5 $\tilde{\varepsilon}_0 = \tilde{\varepsilon}_0(0{,}5,\theta,0{,}3{,}2,r`)$.

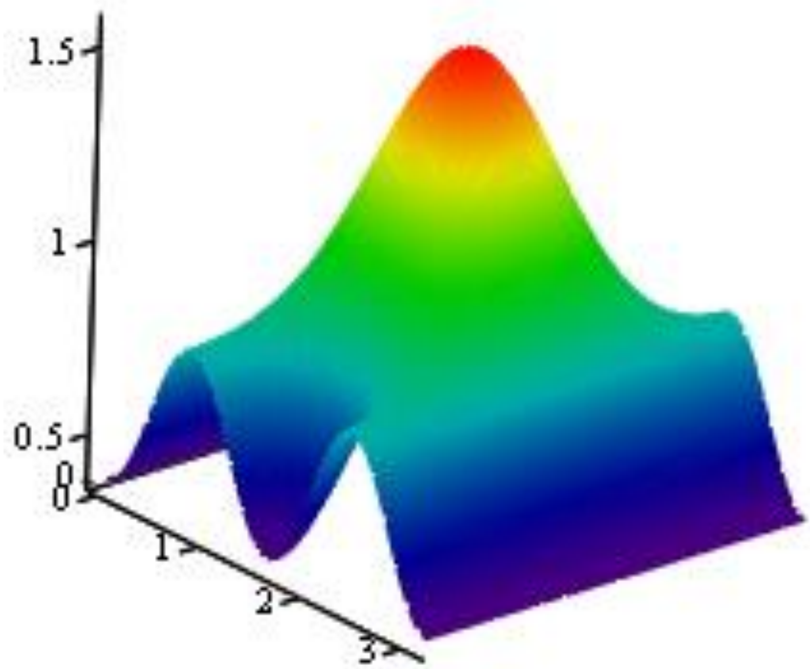
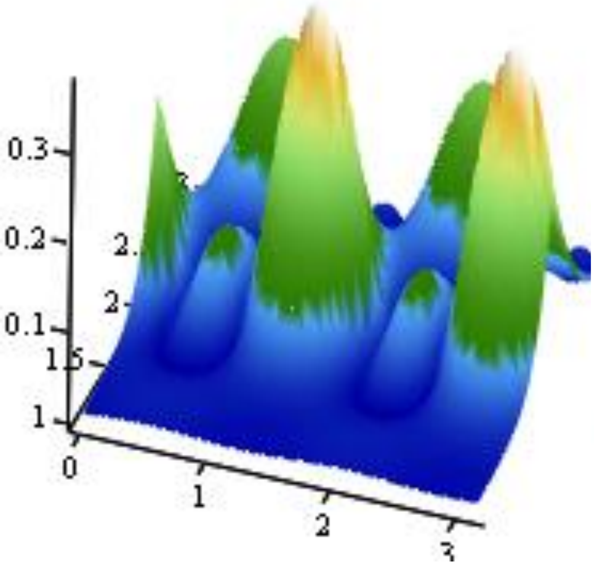


Figure.3. Variation of $\varepsilon 0$ in function of θ,ϕ



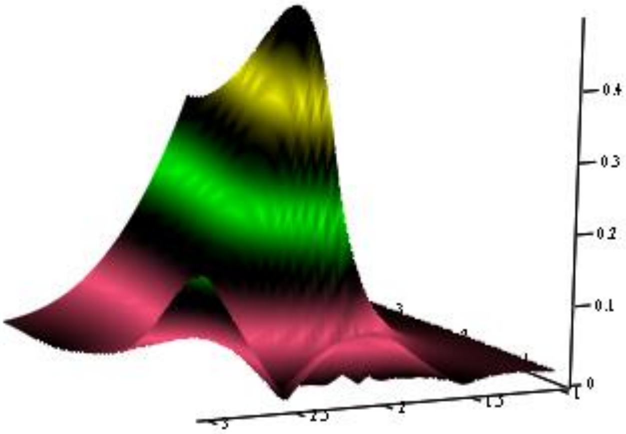


Figure.4. Variation of $\varepsilon 0$ in function of $\phi, r`$ **Figure.5.** Variation of $\varepsilon 0$ in function of $\theta, r`$

3. CONCLUSION

The calculation relationships for spherical tensor variations at microscopical level were deducted in function of stress/strain states at microscopic level and orientation factor of crystallographic system of coordinates.

From examined model result, that in conglomerate exist the subelements, in which spherical tensor at microscopic level it is not equal to zero for any type of loading. In examined cases the maximum values of spherical tensors obtained the same order values like stress/strain deviator tensor at macroscopical level.

This effect allow us to formulate the simple criteria of breaking at microscopic level. If we admit, for example, that breaking in subelement is produced under linear strain d_1 influence, than, at macroscopic will obtain the breaking criteria in which all components of strain tensor and crystal element structure will appear.

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