READING THE POSSIBILITIES TO DECODE THE MICROSTRUCTURE CHARACTERISTICS FROM MACROEXPERIENCE

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ABSTRACT

The paper present the problem of practical application of relationships between the structure and proprieties. Here, it is emphasised that the symmetry elements of crystal lattice, the phases weight and the type of interatomic bond create measurable effects at macroscopic level. On this basis we succeed to formulated not only the direct problem, i.e. to deduce the constitutive equations at macroscopic level by means of constitutive equations at microscopic level, but the inverse problem, which, beside the practical importance, has a great methodological significance too. The knowledge possibilities in both directions allow us to adequately describe the material behavior as a function of external action development. The study is concentrated on the non-linear effects provoqued by the differences between the symmetry elements at macroscopic and microscopic level, prorogued by the differences between the symmetry elements at macroscopic and microscopic level, respectively, and also by the presence of several phases in the studied material, which are generated in the field of elastic strains.

KEYWORDS: Mathematical modelling, Micro-mechanics, macro-mechanics, Structure, Proprieties

1. The principles of transition from micro-stresses and strains to macrostresses and strains

In order to create a 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 $\widetilde{t}_{ij}$, $\widetilde{d}_{ij}$, the stresses and strains at material particle level and t_{ij} and d_{ij} at conglomerate level; based on geometric and equilibrium equations and on homogeneity conditions at conglomerate level, we obtain the relationships [1]:

$$t_{ij} = \frac{1}{\Delta V_0} \int_{\Delta V_0} \widetilde{t}_{ij} dV = \left\langle \widetilde{t}_{ij} \right\rangle ,$$

$$d_{ij} = \left\langle \widetilde{d}_{ij} \right\rangle ; \tag{1.1}$$

$$\left\langle \widetilde{t}_{ij} \widetilde{d}_{ij} \right\rangle = \left\langle \widetilde{t}_{nm} \right\rangle \left\langle \widetilde{d}_{nm} \right\rangle = t_{pq} d_{pq} \tag{1..2}$$

Beside the equations (1.1), (1.2), it is possible to deduce another relationship, which simultaneously satisfies the geometric and equilibrium equations [2]

$$\widetilde{t}_{ij} - t_{ij} = \widetilde{A}_{ijnm} \left(\widetilde{d}_{nm} - d_{nm} \right) - \left\langle \widetilde{A}_{ijnm} \left(\widetilde{d}_{nm} - d_{nm} \right) \right\rangle \tag{1.3}$$

where the tensor $\widetilde{A}_{ijnm}$ depends on the material point coordinates.

If the stress $\widetilde{t}_{ij}$ and strain $\widetilde{d}_{ij}$ tensors are decomposed to spherical deviators and tensors:

$$\widetilde{t}_{ij} = \widetilde{\sigma}_{ij} + \widetilde{\sigma}_0 \delta_{ij} \qquad \widetilde{d}_{ij} = \widetilde{\varepsilon}_{ij} + \widetilde{\varepsilon}_0 \delta_{ij}, \quad \text{then}$$

$$\sigma_{ij} = \left\langle \widetilde{\sigma}_{ij} \right\rangle, \quad \sigma_0 = \left\langle \widetilde{\sigma}_0 \right\rangle, \ \varepsilon_{ij} = \left\langle \widetilde{\varepsilon}_{ij} \right\rangle,$$

$$\varepsilon_0 = \left\langle \widetilde{\varepsilon}_0 \right\rangle, \ \left\langle \widetilde{\sigma}_{ij} \widetilde{\varepsilon}_{ij} \right\rangle \neq \left\langle \widetilde{\sigma}_{nm} \right\rangle \left\langle \widetilde{\varepsilon}_{nm} \right\rangle,$$

$$\left\langle \widetilde{\sigma}_0 \widetilde{\varepsilon}_0 \right\rangle \neq \left\langle \widetilde{\sigma}_0 \right\rangle \left\langle \widetilde{\varepsilon}_0 \right\rangle \tag{1.4}$$

From (1.4) it results that the macroscopic values of some physical parameters are not the same with the similar microscopic values. The difference between these parameters, named incongruity [2,3]

$$\Delta = \left\langle \widetilde{\sigma}_{ij} \widetilde{\varepsilon}_{ij} \right\rangle - \left\langle \widetilde{\sigma}_{ij} \right\rangle \left\langle \widetilde{\varepsilon}_{ij} \right\rangle$$

depends only on the conglomerate surface data, but on its structure too.

According to the proposed principle, during the real interactions, the incongruity Δ reaches the extreme value [2,3]:

$$\langle \widetilde{\sigma}_{ij} \widetilde{\varepsilon}_{ij} \rangle - \langle \widetilde{\sigma}_{ij} \rangle \langle \widetilde{\varepsilon}_{ij} \rangle = Extr. \qquad (1.5)$$

In expressions (1.1)- (1.5) are established direct relationships between stresses and strains at microscopic and macroscopic level. We observe that the relationships (1.1) and (1.2) do not depend on the real material structure, and (1.4) and (1.5) depend on the structure parameters. In order to obtain a correct model, we must also take into account the self-coordination phenomenon of the conglomerate deformation process. The structure elements in conglomerate loose some particular proprieties for common proprieties. As a result, it is not possible to pass directly from constitutive equations at microscopic level to macroscopic level. The self-coordination processes of thermal-mechanical interactions is emphasised by means of stresses and strains at structure elements level:

$$\bar{t}_{ij} = \langle \widetilde{t}_{ij} \rangle_{\Delta\bar{V}}, \qquad \bar{d}_{ij} = \langle \widetilde{d}_{ij} \rangle_{\Delta\bar{V}},$$

where $\Delta\bar{V}$ is the volume of considered structure element. The relationships (1.1)- (1.3) can be written at structure elements level too. Thus, the stress and strain tensors at material particle level can be presented as follows:

$$\widetilde{t}_{ij} = t_{ij} + \Delta\bar{t}_{ij} + \Delta\widetilde{t}_{ij}, \qquad \Delta\bar{t}_{ij} = \bar{t}_{ij} - t_{ij},$$
$$\Delta\widetilde{t}_{ij} = \widetilde{t}_{ij} - \bar{t}_{ij}$$
$$\widetilde{d}_{ij} = d_{ij} + \Delta\bar{d}_{ij} + \Delta\widetilde{d}_{ij},$$
$$\Delta\bar{d}_{ij} = \bar{d}_{ij} - d_{ij}, \qquad \Delta\widetilde{d}_{ij} = \widetilde{d}_{ij} - \bar{d}_{ij},$$

where $\Delta\widetilde{t}_{ij}, \Delta\widetilde{d}_{ij}$ represent the stress and strains variations in the material particles within the considered structure element $(\bar{t}_{ij} = const, \bar{d}_{ij} = const)$ and $\Delta\bar{t}_{ij}, \Delta\bar{d}_{ij}$ the stresses and strains variations in the conglomerate at structure element level. We consider that between the two types of variation there is a well determined correlation: the variations within the structure element are determinate by the proprieties variation. One can observe that:

$$t_{ij} = \langle \bar{t}_{ij} \rangle_{\Omega}, \qquad d_{ij} = \langle \bar{d}_{ij} \rangle_{\Omega}, \qquad (1.6)$$

and for the variations between the stress and strain tensors we can write the relationships:

$$\widetilde{t}_{ij} - \bar{t}_{ij} = \widetilde{A}_{ijnm} \left(\widetilde{d}_{nm} - \bar{d}_{nm} \right),$$
$$\bar{t}_{ij} - t_{ij} = \bar{A}_{ijnm} \left(\bar{d}_{nm} - d_{nm} \right) \qquad (1.7)$$

In the reversible range, $\widetilde{A}_{ijnm} = \bar{c}_{ijnm}$, where $\bar{c}_{ijnm}$ represents the elasticity constants, which are different from a particle to another within considered structure element.

The fundamental relationships (1.2), (1.5) can be expressed by the variation of stress and strain tensors at the two structure levels and by the variation of respective deviators, they become:

$$\langle \Delta\bar{t}_{ij} \Delta\bar{d}_{ij} \rangle_{\Omega} + \langle \langle \Delta\widetilde{t}_{ij} \Delta\widetilde{d}_{ij} \rangle_{\Delta\bar{V}} \rangle_{\Omega} = 0,$$
$$\langle \Delta\bar{\sigma}_{ij} \Delta\bar{\varepsilon}_{ij} \rangle_{\Omega} + \langle \langle \Delta\widetilde{\sigma}_{ij} \Delta\widetilde{\varepsilon}_{ij} \rangle_{\Delta\bar{V}} \rangle_{\Omega} = Extr.$$
$$(1.8)$$

One can be emphasised that for each structure element:

$$\langle \Delta\widetilde{t}_{ij} \Delta\widetilde{d}_{ij} \rangle_{\Delta\bar{V}} \geq 0.$$

As a result, the scalar product of stresses and strains variation at structure elements level is obtained with negative sign.

$$\langle \Delta\bar{t}_{ij} \Delta\bar{d}_{ij} \rangle_{\Omega} \leq 0.$$

The integration in (1.6), (1.7) is performed according to orientation factor or to another parameter; in (1.8) was neglected the therm $\langle \bar{A}_{ijnm} \left(\bar{d}_{nm} - d_{nm} \right) \rangle_{\Omega}$. It is important to notice that in relationship (1.5) it is not possible to pass from the components of the deviator of stress and strain tensors at microscopic level to the deviator components of stress and strain tensors at structure element level, because

$$\langle \widetilde{\sigma}_{ij} \widetilde{\varepsilon}_{ij} \rangle_{\Delta\bar{V}} \neq \langle \widetilde{\sigma}_{nm} \rangle_{\Delta\bar{V}} \langle \widetilde{\varepsilon}_{nm} \rangle_{\Delta\bar{V}}.$$

Thus, the expression (1.5), which is an information carrier about structure element, has an extremely important physical significance. The tensor $\bar{A}_{ijnm}$ reflect, only those details of the interaction between the considered structure element with the other structure elements in conglomerate, which influence the material behavior at macroscopic level.

The structure of tensor $\bar{A}_{ijnm}$ and its dependence on the integration parameter (in special case, on the orientation factor Ω) is established from the condition that in statistical approximation the relationships (1.5)- (1.8) from a complete system of equations; on its base are deduced the constitutive equations at macroscopic level by means of constitutive equations at microscopic level.

If the relationships between stresses and strains at structure element level are know, then from (1.6)- (1.8) we can express $\bar{t}_{ij}$ and $\bar{d}_{ij}$ by local thermal-mechanical characteristics, the tensor $\bar{A}_{ijnm}$ components and the stresses and strains at macroscopic level. The problem of defining the distribution of fields $\widetilde{d}_{ij}$, $\widetilde{t}_{ij}$ in the structure elements

is considerably simplified knowing the stress and strain average values in the structure elements, with the precision of tensor $\overline{A}_{ijnm}$. Thus, in relationship (1.5), beside the mechanical characteristics at microscopic level, will be present also parameters which describe the structure elements shape and size. The $\overline{A}_{ijnm}$ components are determined from (1.5) and (1.7). If the components of $\overline{A}_{ijnm}$ tensor are know, then we establish the constitutive equations at macroscopic level from (1.6) - (1.8).

Further on, we will refer to some examples, which demonstrate the examined model efficiency. We will limit to the case of isotropic materials at macroscopic level, in statistical approximation, i.e. the relationships (1.8) will be written as follows:

$$\left\langle \left(\overline{t}_{ij} - t_{ij} \right)\left(\overline{d}_{ij} - d_{ij} \right) \right\rangle = 0 ,$$

$$\left\langle \left(\overline{\sigma}_{ij} - \sigma_{ij} \right)\left(\overline{\varepsilon}_{ij} - \varepsilon_{ij} \right) \right\rangle = Extr. \qquad (1.9)$$

The material is considered isotropic at macroscopic level and the $\overline{A}_{ijnm}$ tensor will be present as follows:

$$\overline{A}_{ijnm} = \overline{A}_0 V_{ijnm} - \overline{A}_1 D_{ijnm} , \quad V_{ijnm} = \frac{1}{3}\delta_{ij}\delta_{nm} ,$$

$$D_{ijnm} = I_{ijnm} - V_{ijnm} \qquad (1.10)$$

From (1.10) and (1.8) is results:

$$\overline{\sigma}_{ij} - \sigma_{ij} = \overline{A}_I \left(\varepsilon_{ij} - \overline{\varepsilon}_{ij} \right);$$

$$\Delta\overline{\sigma}_{ij} = -\overline{A}_1 \Delta\overline{\varepsilon}_{ij} \qquad (1.11)$$

$$\overline{\sigma}_0 - \sigma_0 = \overline{A}_0 \left(\overline{\varepsilon}_0 - \varepsilon_0 \right); \quad \Delta\overline{\sigma}_0 = \overline{A}_0 \Delta\overline{\varepsilon}_0 \quad (1.12)$$

Taking into account (1.11), (1.12) and (1.7) we obtain:

$$\left\langle 3\overline{A}_0 \left(\Delta\overline{\varepsilon}_0 \right)^2 - \overline{A}_1 \Delta\overline{\varepsilon}_{ij}\Delta\overline{\varepsilon}_{ij} \right\rangle = 0 \qquad (1.13)$$

2. Polycrystalline materials with cubic lattice

The relationships (1.2), (1.3) are automatically verified for the critical cases, that is the W.Voight`s $(\overline{d}_{ij} = d_{ij})$ and R.Reuss`s $(\overline{t}_{ij} = t_{ij}, A_0 = A_1 = 0)$ models. However, for the intermediate variants, the expression (1.13) imposes severe constraints not only to the ratio A_0/A_1, but to the structure of relationships between the stress and strain variations too.

Because $(\Delta\overline{\varepsilon}_0)^2 \geq 0, \Delta\overline{\varepsilon}_{ij}\Delta\overline{\varepsilon}_{ij} \geq 0$, it

results that $\dfrac{\overline{A}_0}{\overline{A}_1} > 0$ and consequently, the

E.Kroner`s model:

$$\overline{A}_1 = G\frac{7 - 5\nu}{4 - 5\nu}, \quad \overline{A}_0 = -4G$$

is in a qualitative contraction with the fundamental relationship (1.13). We can observe that for the polycrystallines monophasic materials with cubic lattice ($\overline{\sigma}_0 = K\overline{\varepsilon}_0$, $\sigma_0 = K\varepsilon_0$), the spherical tensor variations cannot be determined based on the relationship (1.12), which is reduced to the expression:

$$\left(K - \overline{A}_0 \right)\left(\overline{\varepsilon}_0 - \varepsilon_0 \right) = 0 \qquad (2.1)$$

Indeed, from (1.13) it results that for $\overline{\varepsilon}_0 = \varepsilon_0$ we obtain $\overline{\varepsilon}_{ij} = \varepsilon_{ij}$, i.e. the Voight`s model. A complete system of equations, supposing that $\overline{t}_{ij} \neq t_{ij}$, $\overline{d}_{ij} = d_{ij}$, is obtained only if it is assumed that in (2.1) and (1.13):

$$\overline{A}_0 = K, \left(\overline{\varepsilon}_0 - \varepsilon_0 \right)^2 = \frac{A_1}{3K}\left(\overline{\varepsilon}_{ij} - \varepsilon_{ij} \right)\left(\overline{\varepsilon}_{ij} - \varepsilon_{ij} \right)$$

$$(2.2)$$

Thus, for some materials, the relationships between the stress and strain variations are determined based on the expressions (1.11) and (1.12). In the case of polycrystalline polyphasic materials with cubic lattice, from (1.12) we obtain:

$$\Delta\overline{\varepsilon}_0 = \overline{\varepsilon}_0 - \varepsilon_0 = \frac{K_f - K}{K^f - \overline{A}_0^f}\varepsilon_0, \quad K_f \neq K$$

$$(2.3)$$

where K^f is the compression modulus in the phase no. "f", and $\overline{A}_0^f$ is the internal parameter, which characterises the spherical tensor field unhomogeneity inside the considered phase. For the spherical tensor variations, from (1.13) and relationships:

$$\overline{\sigma}^f = K^f\overline{\varepsilon}_0 , \qquad \sigma_0 = K\varepsilon_0 ,$$

it is obtained the expression:

$$3\left(K^f\overline{\varepsilon}_0 - K\varepsilon_0 \right)\left(\overline{\varepsilon}_0 - \varepsilon_0 \right) = A_1^f\left(\overline{\varepsilon}_{ij}^f - \varepsilon_{ij} \right)\left(\overline{\varepsilon}_{ij}^f - \varepsilon_{ij} \right)$$

$$(2.4)$$

If $\varepsilon_0 \neq 0, K^f \neq K = const$., than from (1.13) and (2.3) we obtain the following relationship:

$$3\overline{A}_0^f \left(\frac{K^f - K}{K^f - \overline{A}_0^f} \right)^2 \varepsilon_0^2 = A_1^f\left(\overline{\varepsilon}_{ij}^f - \varepsilon_{ij} \right)\left(\overline{\varepsilon}_{ij}^f - \varepsilon_{ij} \right)$$

$$(2.5)$$

from which it results that the parameter $\overline{A}_0^f$ varies from a particle to another and also within the each phase in the case of polycrystalline polyphasic materials.

In the relationships (2.4) there are only invariant parameters; because of this, it is appropriate to calculate the scalar product of the variations of strain tensor deviator within the crystallographic system of

coordinates $x`_i$ for each structure element. For the polycrystalline materials with cubic lattice, within the crystallographic system of coordinates it is obtained the following expression:

$$\left(\bar{\varepsilon}'_{ij} - \varepsilon'_{ij}\right)\left(\bar{\varepsilon}'_{ij} - \varepsilon'_{ij}\right) = \left(\frac{2G - c^f_{11} + c^f_{12}}{c^f_{11} - c^f_{12} + A^f_1}\right)^2 \left[(\varepsilon'_{11})^2 + (\varepsilon'_{22})^2 + (\varepsilon'_{22})^2\right] + \quad + 2\left(\frac{2G - 2c^f_{44}}{2c^f_{44} + A^f_1}\right)^2 \left[(\varepsilon'_{12})^2 + (\varepsilon'_{13})^2 + (\varepsilon'_{23})^2\right]$$

(2.6)

To write the expressions (2.6) there were taken into account the relationships between stresses and strains within the crystallographic system of coordinates:

$$\bar{\sigma}'_{11} = \left(c_{11} - c_{12}\right)\bar{\varepsilon}'_{11}, \ldots; \bar{\sigma}'_{12} = 2c_{44}\bar{\varepsilon}'_{12},$$ (2.7)

After the substitution of these expressions and formula $\bar{\sigma}'_{ij} = 2G\varepsilon'_{ij}$ in (1.11), we obtain:

$$\bar{\varepsilon}'_{11} = \frac{(A_1 + 2G)\varepsilon'_{11}}{c_{11} - c_{12} + A_1}, \quad \bar{\varepsilon}'_{12} = \frac{(A_1 + 2G)\varepsilon'_2}{2c_{44} + A_1}, \quad (2.8)$$

Within the overall system of coordinates $\varepsilon'_{ij} = \bar{a}_{in}\bar{a}_{jm}\varepsilon_{nm}$ and, as a result, the relationship (2.6) get the form:

$$\left(\bar{\varepsilon}'_{ij} - \varepsilon'_{ij}\right)\left(\bar{\varepsilon}'_{ij} - \varepsilon'_{ij}\right) = \left(\frac{2G - c^f_{11} + c^f_{12}}{c^f_{11} - c^f_{12} + A^f_1}\right)^2 \left(\sum_{i=1}^{3} \bar{a}_{in}\bar{a}_{im}\bar{a}_{iq}\bar{a}_{ik}\right)\varepsilon_{nm}\varepsilon_{qk} +$$

$$+ \left(\frac{2G - 2c^f_{44}}{2c^f_{44} + A^f_1}\right)^2 \left(\sum_{i\neq j=1}^{3} \bar{a}_{in}\bar{a}_{jm}\bar{a}_{iq}\bar{a}_{jk}\right)\varepsilon_{nm}\varepsilon_{qk}$$

(2.9)

From (2.9) it results that the scalar product of the variations of strain tensor deviator depends on: the crystals elasticity constants $c^f_{11}, c^f_{12}, c^f_{44}$, which varie form a phase to another; the internal parameter A^f_1 (reflects the unhomogeneity of $\bar{\varepsilon}^{ij}$ field in the conglomerate); it is worth too considering the variant when $A^f_1 = A_1$ or $A^f_1 = A_1 f\left(\psi_f, A^f\right)$ (where A^f is the anisotropy coefficient of "f" phase and ψ_f the phase weight); the crystallographic axes orientation $\bar{x}`_i$, $\bar{a}_{ij} = \cos\left(\bar{x}'_i, x_j\right)$; the values of the

components of strain tensor deviator ε_{ij} (at macroscopic level). In the considered phase crystals, the variations of the strain tensor deviator change from a crystal to another only function of crystallographic axes orientation.

In (2.9), G and A^f_1 are unknown parameters. To calculate them, we`ll use the relationships (1.6), (1.9), (1.11), (2.8) and (2.9). We can observe that the relationships (2.8) within the overall system of coordinates could be written like an unique expression:

$$\bar{\varepsilon}_{ij} = \left[\frac{A^f_1 + 2G}{c^f_{11} - c^f_{12} + A^f_1}\sum_{n=1}^{3}\bar{a}_{ni}\bar{a}_{nj}\bar{a}_{nk}\bar{a}_{nq} + \frac{A^f_1 + 2G}{2c^f_{44} + A^f_1}\sum_{m\neq n=1}^{3}\bar{a}_{ni}\bar{a}_{mj}\bar{a}_{nk}\bar{a}_{mq}\right]\varepsilon_{kq}$$ (2.10)

Substituting (2.10) in (1.6) and taking into account the relationships:

$$\left\langle\bar{a}_{ni}\bar{a}_{nj}\bar{a}_{nk}\bar{a}_{nq}\right\rangle_\Omega = \frac{1}{15}\left(\delta_{ij}\delta_{kq} + \delta_{ik}\delta_{jq} + \delta_{iq}\delta_{jk}\right)$$

(2.11)

we will obtain:

$$\left\langle\bar{a}_{ni}\bar{a}_{nk}\bar{a}_{mj}\bar{a}_{mq}\right\rangle_\Omega = \frac{2}{15}\delta_{ik}\delta_{jqk} - \frac{1}{15}I_{ikjq}, \quad (2.12)$$

where ψ_f is the "f" phase weight and N-phases number. To deduce the formula (2.13), it was considered that the material particles distribution is homogeneous from a statistical point of view, during each phase. Substituting (1.11) in (1.9) and taking into account the relationship (2.9) in the obtained expression, after integration, we find:

$$\left\{ \sum_{f=1}^{N} \frac{A_1^f}{5} \left[2 \left(\frac{2G - c_{11}^f + c_{12}^f}{c_{11}^f - c_{12}^f + A_1^f} \right)^2 + 3 \left(\frac{2G - 2c_{44}^f}{2c_{44}^f + A_1^f} \right)^2 \right] \psi_f \right\} \frac{1}{2G} = Extr \qquad (2.14)$$

Based on the relationships (2.13) and (2.14), we determine the unknown constants 2G and A_1^f values. If A_1^f is known, then from the relationships (2.5) and (2.9) we calculate the parameter $\overline{A}_0^f$ values and from (2.3) after integration:

$$\left\langle \frac{K_f - K}{K^f - \overline{A}_0^f} \right\rangle = 0 \qquad (2.15)$$

we establish the compression modulus K values. We can observe that form (2.5) and (2.9) it results that $\overline{A}_0^f$ depends not only on the crystal's elasticity constants, but on the deformation degree too. Consequently, we determine that the compression modulus at macroscopic level will depend on the deformation degree in the case of polyphonic materials with cubic lattice.

If we refer only to monophasyc polycrystalline materials, then form (2.13), (2.14), they result the relationships:

$$A_1 = \sqrt{\frac{c_{44}(c_{11} - c_{12})[4c_{44} + 3(c_{11} - c_{12})]}{3c_{44} + c_{11} - c_{12}}},$$

$$(2.16)$$

$$G = \sqrt{\frac{c_{44}(c_{11} - c_{12})(3c_{44} + c_{11} - c_{12})}{4c_{44} + 3(c_{11} - c_{12})}} = \sqrt{G_V G_R}$$

$$(2.17)$$

$$\frac{\langle \overline{\sigma}_{ij} \overline{\varepsilon}_{ij} \rangle - \langle \overline{\sigma}_{ij} \rangle \langle \overline{\varepsilon}_{ij} \rangle}{\langle \overline{\sigma}_{nm} \rangle \langle \overline{\varepsilon}_{nm} \rangle} = -6 \left(\frac{A-1}{5\sqrt{A} + \sqrt{(2+3A)(3+2A)}} \right)^2, \qquad (2.18)$$

$$A = \frac{2c_{44}}{c_{11} - c_{12}}, \quad \langle \overline{\sigma}_0 \overline{\varepsilon}_0 \rangle - \sigma_0 \varepsilon_0 = 2 \left(\frac{A-1}{5\sqrt{A} + \sqrt{(2+3A)(3+2A)}} \right)^2 \sigma_{ij} \varepsilon_{ij}, \qquad (2.19)$$

obtained for the first time in [4]. We mention that G_v and G_R represent the shear modulus values, obtained by W.Voight (1928) and A.Ress (1929). The relationship (2.19) allow us to evaluate the influence of anisotropy factor A on the energy dissipation under cyclic loads in elastic field. Based on the relationships (2.16), (2.17) and the formula for anisotropy factor, we establish the following relationships:

$$\frac{A_1}{2G} = \frac{2A+3}{3A+6} \qquad (2.20)$$

from which it results that the internal parameter A_f, which emphasises the inhomogeneities of strain and stress deviator fields in conglomerate satisfies the inequality

$$G < A_1 < \frac{4}{3}G \qquad (2.21)$$

If the microscopic characteristics are unknown, then one can assume that $A_1 \approx 1{,}1G$. This type of relationships are useful for numerical computations, performed based on the expressions (2.13) and (2.14), in the case of polycrystalline polyphasic materials.
We observe that the A_1 values, obtained within the studied model are always smaller than A_k^1 values, which result from E.Kroner`s model $\nu = 0 \div 0.5$.

$$1.75G < A_1^{(k)} < 3G \qquad (2.22)$$

According to expression (2.18), for *N=1* it is obtained the relationship:

$$G = \frac{5c_{44}(c_{11} - c_{12}) + (c_{11} - c_{12} + 3c_{44})A_1}{4c_{44} + 3(c_{11} - c_{12}) + 5A_1}$$

$$(2.23)$$

from which it results that the shear modulus diminishes with A_1 increasing; as a result, the shear modulus obtained from (2.17) is "more microscopic" than the shear modulus determined by E.Kroner`s model. We mention that the A_0 values are different from qualitative point of view within the 2 models:

$$A_0 = K; A_0^{(k)} = -4G.$$

3. Polycrystalline materials with crystalline lattice symmetry lower than the cubic one

For the polycrystalline materials with crystalline lattice symmetry lower than the cubic one, the variation of spherical tensors $\overline{\sigma}_0, \overline{\varepsilon}_0$ is obtained based on the relationships (1.12). As a result, the formula (1.13) is completely verified.

According to [3], the symmetry elements at microscopic level lead to the appearance of some effects at macroscopic level, based on which one can concludes about material structure. Thus, from studied model it results that each structure element at microscopic level determines effects measurable at macroscopic level. Based on this kind of effects, it becomes real the inverse problem: the decoding of some details about material microstructure from macroexperience. We mention that the inverse problem was considered unreal until establishing these effects. In order formulate the final conclusions, we`ll refer to the computation relationships obtained in [3] for the polycrystalline monophasic materials with crystalline lattice symmetry lower than the cubic one:

$$\left(b_{ijnn}b_{ijmm} - 3b_0^2\right)\left(\frac{A_0}{A_1} + 1 - 60\frac{\mu^2 b^2}{b_0^2}\right) = 3b_{pqkl}b_{pqkl} - b_{pqkk}b_{pqll} - 60b^2 \tag{3.1}$$

the b_{ijnm} tensor is determined based on the relationships:

$$\frac{b_{ijnn}b_{ijmm} - 3b_0^2}{b(1 - 2A_1 b)}A_0 = Extr, \tag{3.2}$$

where

$$b_0 = \frac{1}{3}b_{kknn}, \quad b = \frac{1}{30}\left(3b_{knkn} - b_{kknn}\right), \quad \mu^2 = \frac{\varepsilon_0^2}{\varepsilon_{pq}\varepsilon_{pq}} \tag{3.3}$$

The b_{ijnm} tensor is determined based on the relationships:

$$b_{ijkl}\left(c_{k\ln m} - A_{k\ln m}\right) = I_{ijnm}, \qquad A_{ijnm} = A_0 V_{ijnm} - A_1 D_{ijnm} \tag{3.4}$$

In the system (3.4) c_{klnm} are elasticity constants at microscopic level within the crystalographic system of coordinates. Thus, in the non-linear equation system (3.1), (3.2) are present two unknowns, A_0 and A_1; based on them, from the relationships:

$$b_0 = \frac{1}{3}b_{kknn}, \tag{3.5}$$

$$2b(2G + A_1) = 1, \tag{3.6}$$

we calculate the macro-elasticity constants K and G.

From (2.6), (2.7) it results that A_0 and A_1 depend not only on the microscopic elasticity constants, but on the deformation degree too. As a result, we establish that the relationships between the stresses and stains at macroscopic level are non-linear, if the structure elements have a lower symmetry than the cubic one; the elasticity characteristics K and G at macroscopic level depend

on the deformation degree $\mu^2 = \dfrac{\varepsilon_0^2}{\varepsilon_{pq}\varepsilon_{pq}}$ or stress.

4. Conclusions

From the structural model it results that each structure element at microscopic level determines a measurable effect at macroscopic level. Starting from the established relationships between cause and effect, based on the experience at macroscopic level, we succeed to formulate conclusions about the microstructure of the examined material.
If from macro-experience we establish that the shear (G) and compression (K) moduli are not influenced

by the stress or deformation degree, than we can assert that the examined polycrystalline material is monophasic with cubic crystalline lattice. In the case of polycrystalline polyphasic material with cubic lattice, from macro-experience we find that the shear modulus is not influenced by the stress degree and the compression modulus K depends on the stress/strain degree. If from macro-experience we establish that both elasticity characteristics (K,G) depend on the stress degree, from the proposed model it results that the crystalline lattice symmetry of the examined polycrystalline material is lower than the cubic one; determining the structure of K and G parameters dependence on stress/strain degree, one can establish the details about the symmetry elements of the crystalline lattice and the presence of one or more phases. We mention that the listed effects do not result from other models of transition from the microscopic state to the macroscopic one. Based on the established non-linear effects, one can assert that exists an equivalence between the direct problem, i.e. the deduction of constitutive equations at microscopic level, and the inverse problem, the decoding of thermomechanical characteristics at microscopic level from macro-experience. We can observe that the majority of specialists, until the establishing of mentioned non-linear effects, consider the inverse problem without solution. The existence of inverse solution has a great practical and scientific importance. Because the structure elements in conglomerate modifie some proprieties, the knowledge direction from micro-to macro especially during the irreversible processes, leads to some unavoidable errors in conglomerate behavior description. This finding is available in the case of

inverse problem too, because not all the details of structure elements can be precised from macro-experience. Thus, the knowledge process will become more complete, if the study is performed in both directions. We mention that from macro-experience it can be determined the interatomic bonds type. Thus, in the case of ionic bond (the model of central interaction proposed by Cauchy), besides the symmetry relationships, there are deduced the following expressions [5] too:

$$c_{1122} = c_{1212}, c_{1133} = c_{1313}, c_{2233} = c_{2323}; \qquad (4.1)$$

$$c_{1312} = c_{1132}, c_{1223} = c_{2213}, c_{2331} = c_{3321};$$

Thus, determining, e.g., from macro - experience on a NaCl or KCL crystal that $c_{1122}=c_{1212}$, (for the materials with cubic lattice the 6 relationships (4.1) are reduced to an unique one $c_{11}=c_{44}$, 1~11, 4 ~12) , we establish that the interatomic bond of examined material is an ionic one. For the materials with other bonds type, are not deduced yet supplementary relationships (4.1) type: this problem has a great methodologic importance in the context of stated conclusions.

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