GENERAL ENGINEERING AND MECHANICS

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ANALYSIS OF TWO APPROACHES TO DETERMINING THE ELASTICITY CONSTANTS OF POLYCRYSTALLINE MATERIALS

Abstract. *The article compares the results deriving from the relations of transition from microtensions and deformations to macrotensions and deformations proposed by E. Kroner with the respective relations obtained within the structural model built on the basis of Hill relations and principles: average connections; orthoganality of stress and strain tensor fluctuations; the extreme discrepancy of the macroscopic measure with the mean value of the appropriate microscopic analog. It is shown that the macroscopic shear modulus obtained in E.Kroner's model is greater than or equal to the respective value obtained in V.Marina's model. An inequality between the anisotropy coefficient of the cubic lattice of polycrystalline materials and Poisson's ratio is established. Relations are analyzed by which objective macroscopic measures of the energy of volume and shape change in the field of reversible stresses are determined.*
Keywords: *stress, strain, anisotropy, structural model, crystal, polycrystal.*

1. Hill's relationships

The disordered environment characteristic of most materials used in the technics is considered statistically homogeneous. The minimum volume that satisfies this requirement will be denoted by ΔV_0 and the area that delimits it by - ΔS_0. The volume element ΔV_0 is considered to be composed of an infinite number of structural elements which in turn comprise a sufficiently large number of atoms that the conception of the continuous medium remains valid even on a microscopic scale. For a broader description of the behavior of the material, stresses and strains are defined at two levels of the structure. We will note the tensions and deformations at the microscopic scale $\bar{t}_{ij}, \bar{d}_{ij}$, and at the macroscopic level t_{ij}, d_{ij}. Equilibrium equations and geometric equations are satisfied inside the volume element ΔV_0

$$\bar{t}_{ij} + b_i = 0, \quad \bar{d}_{ij} = \frac{1}{2}\left(u_{i,j} + u_{j,i}\right), \tag{1}$$

and the following contour conditions are satisfied on the surface

$$\bar{u}_i / \Delta S_0 = d_{ij} x_{ij}, \; d_{ij} = const., \; p_i^{(n)} / \Delta S_0 = t_{ij} n,$$

$$t_{ij} = const. \tag{2}$$

Under these conditions, the following relations of R. Hill are verified

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

$$d_{ij} = \langle \bar{d}_{ij} \rangle = \frac{1}{\Delta V_0} \int_{\Delta V_0} \bar{d}_{ij} dV, \tag{3}$$

$$\langle \bar{t}_{ij} \bar{d}_{ij} \rangle = \langle \bar{t}_{ij} \rangle \langle \bar{d}_{ij} \rangle = t_{pq} d_{pq}, \tag{4}$$

where $\langle \cdot \rangle$ *- the symbol of mediation in the volume* ΔV_0.

Equations (3) and (4) are necessary, but not sufficient, to determine the stress-strain relationships at the macroscopic scale if the stress-strain stresses are given at the microscopic scale.

2. Relationships between macro and micro stresses and strains in E.Kroner's model

According to E. Kroner's model [1] each grain in the consecutive volume is examined as an inclusion in the "matrix" composed of the remaining grains. The behavior of the polycrystalline material is determined by means of an appropriate mediation procedure on the set of all grains. E. Kroner's approach leads to proportional relations between the fluctuations of stress $\bar{\sigma}_{ij} - \sigma_{ij}$ and strain $\bar{\varepsilon}_{ij} - \varepsilon_{ij}$ deviators

$$\bar{t}_{ij} = \bar{\sigma}_{ij} + \bar{\sigma}_0 \delta_{ij}, \; \bar{d}_{ij} = \bar{\varepsilon}_{ij} + \bar{\varepsilon}_0 \delta_{ij} \; \bar{\sigma}_{ij} - \sigma_{ij} = 3b_2\left(e_{ij} - \bar{\varepsilon}_{ij}\right),$$

$$2b_2 = 2G \frac{7 - 5\upsilon}{8 - 10\upsilon} \tag{5}$$

and between spherical tensor fluctuations

$$\bar{\sigma}_0 - \sigma_0 = (3b_1 + 2b_2)(\varepsilon_0 - \bar{\varepsilon}_0),$$

$$b_1 = 2G\frac{3-5\upsilon}{8-10\upsilon}. \qquad (6)$$

where G – the shear modulus, υ *– the Poisson's ratio.*

Note that equations (5), (6) do not satisfy relation (4) and therefore the transition relations from the microscopic state to the macroscopic state obtained by E.Kroner are not in accordance with the first law of thermodynamics.

3. Relationships between macro and micro stresses and strains in V. Marina's model

The structural model developed by V. Marina [2] is built on R. Hill`s relationships (3), (4) and three additional principles. According to the first principle: *the interactions between sub-elements (structural elements) are formed only under the influence of the average bonds*. This principle reflects the phenomenon of self-coordination of deformations in the volume ΔV_0. The second principle states: *the fluctuations of the stress tensors are orthogonal to the fluctuations of the strain tensors*, ie

$$(\bar{t}_{ij} - t_{ij})(\bar{d}_{ij} - d_{ij}) = 0. \qquad (7)$$

Note that expression (7) satisfies relation (4) and as a result verifies the first law of thermodynamics. If in (7) the stresses and stresses are decomposed into deviators and spherical tensors, then the first type of relationship between the microscopic states and the macroscopic state is obtained

$$(\bar{\sigma}_{ij} - \sigma_{ij})(\bar{\varepsilon}_{ij} - \varepsilon_{ij}) + 3(\bar{\sigma}_0 - \sigma_0)(\bar{\varepsilon}_0 - \varepsilon_0) = 0. \qquad (8)$$

The structure of the relationship between the fluctuations of the stress and strain tensor deviators is admitted by E.Kroner's relationship type (5)

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

where $B \neq 2d_2$ *- internal parameter that reflects the inhomogeneities of the stress and strain fields in* ΔV_0*. The third principle refers to the discrepancies between some* *macroscopic measures with their appropriate microscopic analogies. For example,* $\langle \bar{\sigma}_{ij}\bar{\varepsilon}_{ij} \rangle \neq \langle \bar{\sigma}_{ij} \rangle \langle \bar{\varepsilon}_{ij} \rangle$, $\langle \bar{\sigma}_0 \bar{\varepsilon}_0 \rangle \neq \langle \bar{\sigma}_0 \rangle \langle \bar{\varepsilon}_0 \rangle$ *according to the principle stated in [2]: in all real interactions the discrepancies between the macroscopic measurements with the appropriate microscopic analogies obtain extreme values*

$$\langle \bar{\sigma}_{ij}\bar{\varepsilon}_{ij} \rangle - \langle \bar{\sigma}_{ij} \rangle \langle \bar{\varepsilon}_{ij} \rangle = Extr. \tag{10}$$

Relationships (3), (8) - (10) form a complete system of equations on which basis the constitutive equations can be deduced at the macroscopic scale if the constitutive equations at the microscopic scale are known.

4. Comparison of the calculation relations of the macroelasticity constants for polycrystalline materials with cubic lattice

In the case polycrystalline materials with cubic lattice, the microscopic compression modulus coincides with the macroscopic compression modulus $3K = c_{11} + 2c_{12}$, where through c_{ij} the elasticity constants of the crystals in the coordinate crystallographic system are noted. Therefore, the difference in the calculation relations appears only for the shear module *G*. Because in both models relations (3) are used, based on the physical relations at crystal level, and the replacement of the volume integration operation with the integration according to the crystal orientation factor a common relationship is obtained

$$\frac{5}{2G+B} = \frac{3}{2c_{44}+B} + \frac{2}{c_{11}-c_{12}+B}. \tag{11}$$

E. Kroner's model for the calculation of *B* parameter uses the solution obtained by J. D. Eshelby regarding the problem of spherical inclusion (relation (5)) in the isotropic matrix. In the case of V. Marina's model, the calculation of parameter *B* is performed based on expression (10). In [2] the formula was obtained

$$B = \sqrt{\frac{c_{44}(c_{11}-c_{12})[4c_{44}+3(c_{11}-c_{12})]}{3c_{44}+c_{11}-c_{12}}}, \quad A = \frac{2c_{44}}{c_{11}-c_{12}}, \tag{12}$$

$$G = \sqrt{\frac{c_{44}(c_{11}-c_{12})[3c_{44}+c_{11}-c_{12}]}{4c_{44}+3(c_{11}-c_{12})}} = \sqrt{G_R G_V}, \tag{13}$$

where A is denoted by the anisotropy coefficient of the crystal, G_R *– the shear modulus obtained by R. Reuss in the hypothesis* $B=0$*,* G_V *- the shear modulus obtained by W. Voigt (*$B=\infty$*).*

In Kroner's model, the shear modulus is determined from the following equation

$$G_k^3+\frac{1}{8}(5c_{11}+4c_{12})G_k^2-\frac{1}{8}(7c_{11}-4c_{12})G_k-\frac{1}{8}(c_{11}+2c_{12})(c_{11}-c_{12})c_{44}=0 \quad (14)$$

Table 1 presents the experimental results obtained in the works for 6 materials [3,4] and theoretical calculated based on relations (13) and (14).

Table 1

Experimental and theoretical elasticity constants

Element	Monocrystal, 10^4MN/m^2			Polycrystal, 10^4MN/m^2		
	c_{11}	c_{12}	c_{44}	$G_{\exp}$	G_K	G_M
Ni	24,65	14,7	12,5	8,46	8,69	8,57
Au	18,6	15,7	4,2	2,77	2,81	2,72
W	5,1	19,8	15,1	15,14	15,14	15,14
CdTe	5,35	3,68	1,99	1,38	1,42	1,40
Mo	46	17,6	11	12,19	12,19	12,18
-Fe	23,7	14,1	11,6	7,85	8,21	8,11

Table 1 shows that the theoretical results obtained in the two models are in good agreement with the experimental data. It is observed that the difference between the results obtained using formula (13) is closer to the experimental data than those calculated from equation (14). A broader analysis of the dependence of the value of the shear modulus on the model used in the calculation is obtained by passing from the dimensional parameter *B* to the dimensionless parameter *b* defined by the relation $b=B/2G$. Taking into account this presentation in formula (11) after a series of transformations we obtain

$$G=\frac{2b(3c_{44}+c_{11}-c_{12})-[4c_{44}+3(c_{11}-c_{12})]}{20b}+\frac{\sqrt{[2b(3c_{44}+c_{11}-c_{12})-[4c_{44}+3(c_{11}-c_{12})]]^2}}{20b}+$$

$$+\frac{\sqrt{200b[c_{44}(c_{11}-c_{12})]}}{20b}. \quad (15)$$

This relation can be further simplified if the constants $c_{11} - c_{12}$ are expressed by the constant c_{44} and the coefficient of anisotropy *A*, relation (12)

$$G = \frac{1}{10bA}\left[b(3A+2)-3-2A\right] + \frac{1}{10bA}\left[\sqrt{\left[b(3A+2)-3-2A\right]^2 + 100bA}\right]. \qquad (16)$$

Parameter *b* in Kroner's model is determined from (5), and in Marina model - (12) and (13)

$$b_k = \frac{7-5\upsilon}{8-10\upsilon}, \quad b_m = \frac{3+2A}{2+3A}. \qquad (17)$$

We observe that the parameter *b* in Kroner's model depends on the Poisson's ratio, and in Marina's model on the crystal anisotropy coefficient. The laws of variation of the b_K and b_M parameters are illustrated in fig.1. The two diagrams intersect at point *A=1,32*. For $A \geq 2$ the parameter b_K is higher than b_M and therefore the shear modulus $G_K > G_M$.

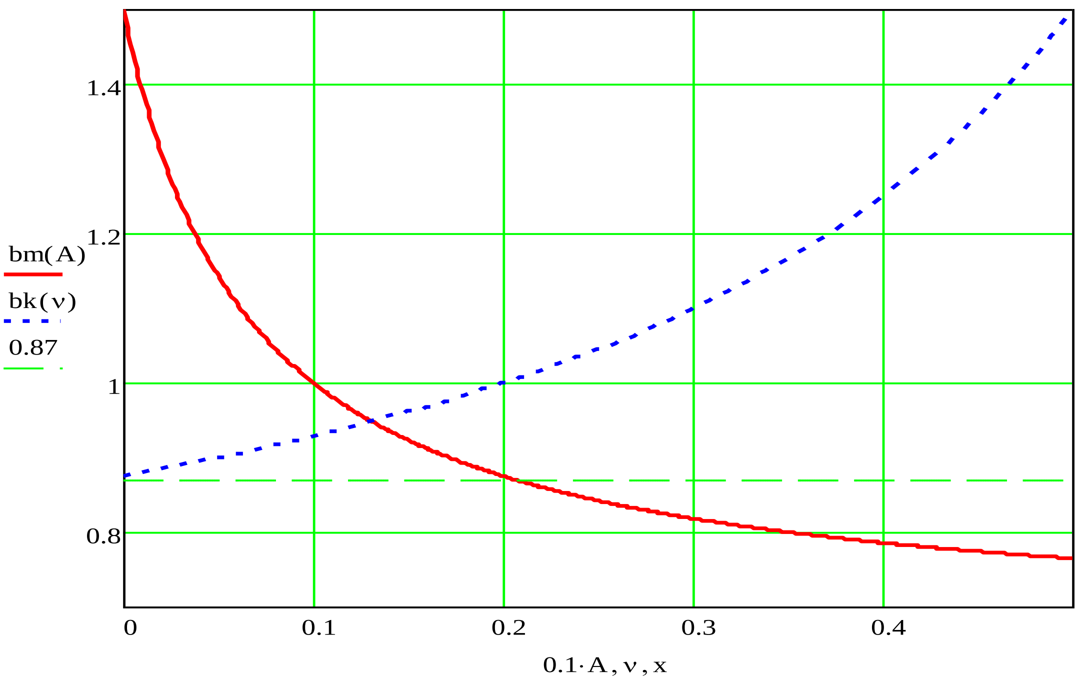

Fig. 1. **Comparison of the legitimacy of variation of the b parameter**

Fig. 2 shows the dependence of the shear modulus ratio G and the elasticity constant c_{44} as a function of *b* parameter and the anisotropy coefficient *A*

$$G'' = \frac{G}{c_{44}} = \frac{1}{10bA}\left[b(3A+2)-3-2A\right]+\frac{1}{10bA}\left[\sqrt{\left[b(3A+2)-3-2A\right]^{2}+100bA}\right]. \quad (18)$$

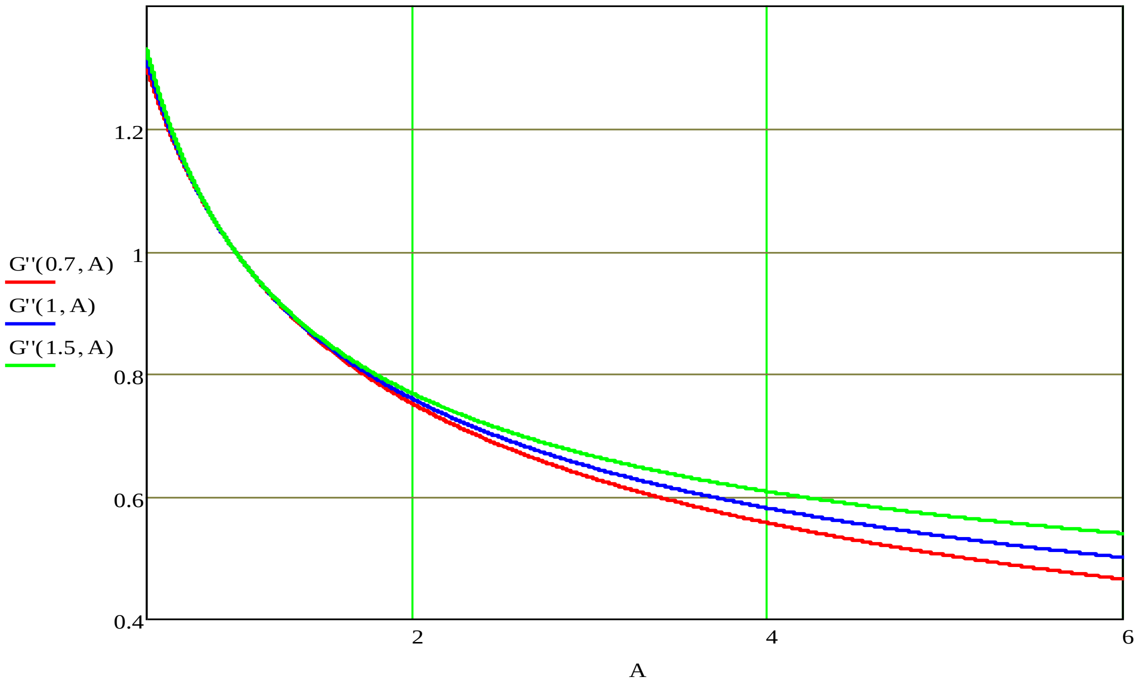

Fig. 2. **Remarkable features of coefficient variation** G''

One of the remarkable properties of the relation (18) consists in the fact that for values of the anisotropy coefficient *A<1,32* the shear modulus does not depend on the parameter *b* (fig.2). It turns out that on this segment $G_K = G_M$. The analysis of this relation over the whole range of variation of *A* leads us to the following inequality

$$G_K \geq G_M . \quad (19)$$

Thus, the shear modulus obtained in the Kroner model is greater than or equal to the shear modulus obtained in the Marina model. The inequality (19) is confirmed on the basis of the experimental data presented in Table 1.

3. CONCLUSIONS

The proportionality parameters between the fluctuations of stresses and strains obtained in the Kroner - b_K and Marina b_M - model were compared. It has been shown that $b_K \geq b_M$. It has been shown that the shear modulus of the polycrystalline material is proportional to the elastic constant c_{44} of the single crystal. The proportionality coefficient depends on only two variables: *A* and *b*. It has been shown that the shear modulus obtained in the Kroner model is greater than or equal to the shear modulus obtained in the Marina model.

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