ELASTICITY CONSTANTS IN THE CASE OF POLYCRYSTALLINE MATERIALS WITH MULTIPLE PHASES

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Abstract. The patterns of change in elastic constants in multiphase polycrystalline materials with cubic lattices are investigated. The relationship between local and macroscopic parameters is established based on the principles of averaged bonds, orthogonality of stress and strain tensor fluctuations, and the extremum of the discrepancy between macroscopic measures and the appropriate average values of microscopic analogues. A closed system of equations has been established for determining macroscopic elastic constants and the parameter of deformation and stress heterogeneity. Numerical studies of the influence of phase elastic characteristics and volume content on the values of macroscopic elastic constants are presented.

Key words: extremum, discrepancy of measures, multiphase polycrystal, stress, strain, anisotropy.

1. INTRODUCTION

One of the main tasks of the mechanics of deformed solids is to construct determining equations linking macro-stresses t_{ij} and macro-deformations d_{ij}, based on known determining equations at the level of structural elements $\tilde{t}_{ij} - \tilde{d}_{ij}$. There are three main approaches: statistical [4, 5, 16, 18, 19, 21], self-consistent [2, 3, 5, 7, 9–12], and direct [1, 19, 23]. Statistical models include models that consider elements of the lowest scale level with a sufficient degree of independence from each other; the transition to a higher scale for some characteristics is carried out by averaging, for others – on the basis of accepted hypotheses of a kinematic (Voigt hypothesis), static (Reiss hypothesis) or intermediate type (Kroner-type hypotheses).

The first intermediate approach was proposed by Kroner. It is based on the so-called self-consistent scheme, in which the real interaction of numerous

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structural elements with each other is replaced by the interaction of each structural element with the surrounding matrix, which has unknown averaged properties

$$\tilde{t}_{ij} - t_{ij} = B_{ijnm}\left(d_{nm} - \tilde{d}_{nm}\right) \quad , \; B_{ijnm} = D\delta_{ij}\delta_{nm} + BI_{ijnm},$$

where only the parameters B and D depend on the model. Based on variational methods [5–8, 21], it was established that the limiting variants $B_{ijnm} = \infty$ (homogeneous deformed state $\tilde{d}_{ij} = d_{ij}$) and $B_{ijnm} = 0$ (homogeneous stressed state $\tilde{t}_{ij} = t_{ij}$) correspond to the upper and lower limits of effective elastic constants for composite materials of arbitrary structure. Because of this, the intermediate variants $0 < B_{ijnm} < \infty$ have become widely used.

The basic flaw in Kroner's model is that it does not satisfy the first law of thermodynamics. For the first time, a model that simultaneously reflects the inhomogeneity of stress and deformation states that satisfy the laws of thermodynamics was developed by Prof. Marina V., [3–5].

2. GENERAL EQUATIONS OF THE CONSTITUTIVE MODEL MARINA

Based on the equations of equilibrium of a continuous medium and Cauchy's geometric relations, the following expressions are established

$$t_{ij} = \left\langle \tilde{t}_{ij} \right\rangle = \frac{1}{\Delta V_0} \int\limits_{\Delta V_0} \tilde{t}_{ij} \mathrm{d}V, \quad d_{ij} = \left\langle \tilde{d}_{ij} \right\rangle, \quad \left\langle \tilde{t}_{ij}\tilde{d}_{ij} \right\rangle = t_{pq} d_{pq}, \tag{1}$$

where, $\tilde{t}_{ij}, \tilde{d}_{ij}$ are the stress and strain tensors at each point in the domain ΔV_0 respectively, $\langle . \rangle$ is the volume averaging sign ΔV_0. In deriving (1), it is assumed that the boundary conditions $\tilde{u}_{i/S_0} = u_i = d_{ij}x_j$, $d_{ij} = const.$, $p^{(n)}_{i/S_0} = t_{ij}n_j$, $t_{ij} = const.$ are satisfied on the surface S_0.

The three equations (1) can be represented as a single relation

$$\left\langle \left(\tilde{t}_{ij} - t_{ij}\right)\left(\tilde{d}_{ij} - d_{ij}\right) \right\rangle = 0. \tag{2}$$

From (2) it follows that the average value of the scalar product of the fluctuations of the stress and strain tensors in a representative volume is zero. In [13–15], it was assumed that relation (2) holds for each material particle. This statement is formulated as a postulate about the orthogonality of the fluctuations of the stress and strain tensors in each element of the structure

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

By decomposing the stress and strain tensors in (3) into deviatoric and spherical components, we obtain

$$\begin{gathered}\tilde{t}_{ij}=\tilde{\sigma}_{ij}+\tilde{\sigma}_0\delta_{ij}, \quad \tilde{d}_{ij}=\tilde{\varepsilon}_{ij}+\tilde{\varepsilon}_0\delta_{ij}, \quad t_{ij}=\sigma_{ij}+\sigma_0\delta_{ij}, \\ d_{ij}=\varepsilon_{ij}+\varepsilon_0\delta_{ij},\end{gathered} \tag{4}$$

we establish one fundamental equation of connection between macro- and microstates

$$(\tilde{\sigma}_{ij}-\sigma_{ij})(\varepsilon_{ij}-\tilde{\varepsilon}_{ij})=3(\tilde{\sigma}_0-\sigma_0)(\tilde{\varepsilon}_0-\varepsilon_0). \tag{5}$$

We establish the expression for the fluctuations of stress and strain deviators based on the condition of equality of the mechanical work of the system of structural elements and the body element. In [15], it is shown that this condition is satisfied by applying to fluctuations The expression for fluctuations of stress and strain deviators is established based on the condition of equality of mechanical work of the system of structural elements and the body element. For deviator values, the simplest expression is

$$\tilde{\sigma}_{ij}-\sigma_{ij}=B(\varepsilon_{ij}-\tilde{\varepsilon}_{ij}), \tag{6}$$

where B is an internal parameter containing information about the microscopic characteristics of material particles. Hereinafter, we will refer to parameter B as the heterogeneity parameter.

We will establish an expression for the fluctuations of stress and strain deviators based on the condition of equality of the mechanical work of the system of structural elements and the body element

$$\Delta=\left\langle\tilde{\sigma}_{ij}\tilde{\varepsilon}_{ij}\right\rangle-\left\langle\tilde{\sigma}_{\mathrm{ij}}\right\rangle\left\langle\tilde{\varepsilon}_{ij}\right\rangle=\mathrm{Extr.} \tag{7}$$

Expressions (1), (5), and (7) represent a closed system of equations describing the relationship between macro- and microstates. They do not contain references to material properties and are therefore valid for describing both reversible and irreversible deformation processes. Based on them, it is possible to construct determining equations at the macroscopic level if the determining equations at the microscopic level are known. Note that in multi-element models, averaging is performed not by volume, but by a set of realisations, i.e. it is considered legitimate to use the ergodic hypothesis. In the elastic region, the values t_{ij}, d_{ij} are determined by averaging over the crystal lattice orientation factor.

3. DETERMINATION OF MACROSCOPIC ELASTIC CONSTANTS OF MULTIPHASE POLYCRYSTALLINE MATERIALS AND THE HETEROGENITY PARAMETER

Based on (1), (6) and (7), we will analyse the influence of the elastic characteristics of phases and their volume content on the macroscopic elastic constants and the heterogeneity parameter. When analysing the behaviour of crystals with a cubic lattice, we will use three independent elastic parameters that have a clear physical meaning: c_{44} – shear constant (relates shear stress to shear strains), A – anisotropy factor, K – bulk modulus of elasticity. The physical equations of crystals in the crystallographic coordinate system x_i' have the form $\sigma_{ij}' = 2c_{44}\tilde{\varepsilon}_{ij}'/A$ if $i = j$ and $\sigma_{ij}' = 2c_{44}\tilde{\varepsilon}_{ij}'$ if $i \neq j$, $\sigma_0 = 3K\varepsilon_0$. Taking these expressions into account in relation (6), we establish the following relationships between local and macroscopic deformations

$$\tilde{\varepsilon}_{11}' = \frac{(B+2G)\tilde{r}_{1n}\tilde{r}_{1m}\varepsilon_{nm}}{B+2C_{44}/A},\ldots,\quad \tilde{\varepsilon}_{ij}' = \frac{(B+2G)\tilde{r}_{in}\tilde{r}_{jm}\varepsilon_{nm}}{B+2C_{44}},i \neq j,$$
$$r_{ij} = \cos(x_i', x_j), \tag{8}$$

hereby ε_{ij} is the macroscopic deviator of the deformation tensor in the global coordinate system x_i, which coincides with the principal system.

Based on (8), (7) after a series of transformations, we obtain a system of equations [23]

$$\frac{5}{2G+B} = \sum_{k=1}^{n}\left(\frac{3}{2C_k+B} + \frac{2A_k}{2C_k+A_kB}\right)f_k, \tag{9}$$

$$-\sigma_{nm}\varepsilon_{nm}\frac{B}{10G}\sum_{k=1}^{n}\left[2\left(\frac{(B+2G)A_k}{2C_k+A_kB}\right)^2 + 3\left(\frac{B+2G}{2C_k+B}\right)^2 - 5\right]f_k = \text{Extr.} \tag{10}$$

In the case of single-phase polycrystalline materials, system (9), (10) has a simple analytical solution [13]

$$G_M = \sqrt{G_V G_R}, \quad B = 2C_{44}\sqrt{\frac{2A+3}{A(3A+2)}}, \tag{11}$$

where c_{11}, c_{12}, c_{44} are the elastic constants of the crystals, A is the crystal anisotropy coefficient.

For the compression modulus in the examined model, the following relationship results

$$K_M(f)=\sqrt{K_1K_2\frac{K_2 f+K_1(1-f)}{K_1 f+K_2(1-f)}},\quad K_k=\frac{1}{3}(C_{11,k}+2C_{12,k}), \tag{12}$$

where K_1, K_2 denotes the compression modulus of single-phase materials, K_M – the compression modulus for two-phase materials.

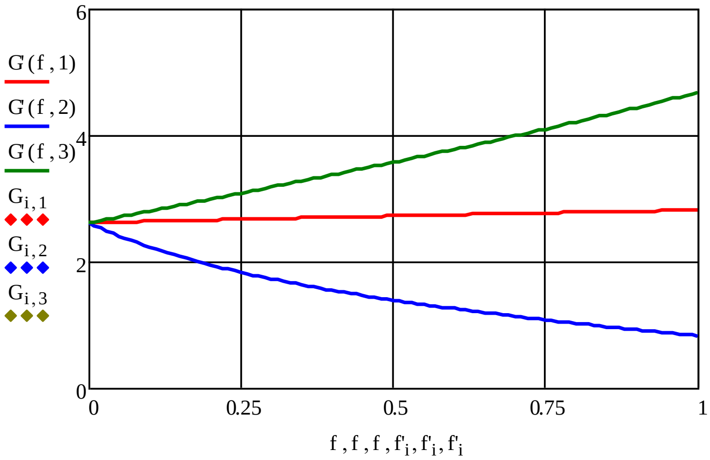

Fig. 1 – Influence of phase proportions on shear modulus value.

In the case of multiphase polycrystals, system (8), (10) has only a numerical solution. Note that the extremum of the discrepancy of measures (10) is determined under the condition $\sigma_{nm}\varepsilon_{nm}=const.$ The patterns of change in parameters G and B on scales $X\cdot 10^{-4}$ MPa depending on the volume content of the harder phase f ($f_2= f, f_1=1-f$) were studied using three two-phase materials: *Al-Th, AL-Pl,* Al-Cu. The results of numerical studies for the shear modulus are presented in Fig. 1. The curve marked in red corresponds to the alloy *Au-Fe*, blue to *Au-Al*, and green to Au-Cu. According to Fig. 1, the macroscopic shear modulus $G=G(f)$ monotonically increases with the growth of f .

The diagrams for the parameter $B=B(f)$ $B=B(f)$ shown in Fig. 2 are more complex than the diagram $G=G(f)$. For all the materials studied, a non-monotonic dependence of the parameter heterogeneity on f has been established. The following pattern is observed: at low values of f, the parameter B increases to a certain maximum value, and then, depending on the values of the elastic characteristics of the phases, a monotonic decrease is observed. For some materials, a decrease in the heterogeneity parameter B is observed only in the organic interval of change $f\,(f_* < f < f_0)$. At $f > f_0$, a new increase in the heterogeneity parameter B is observed.

The shear modulus varies monotonically depending on the phase ratio.

In Fig 2 it is shown graph of the parameter of non-homogeneity of stress and strain distribution in the same phases.

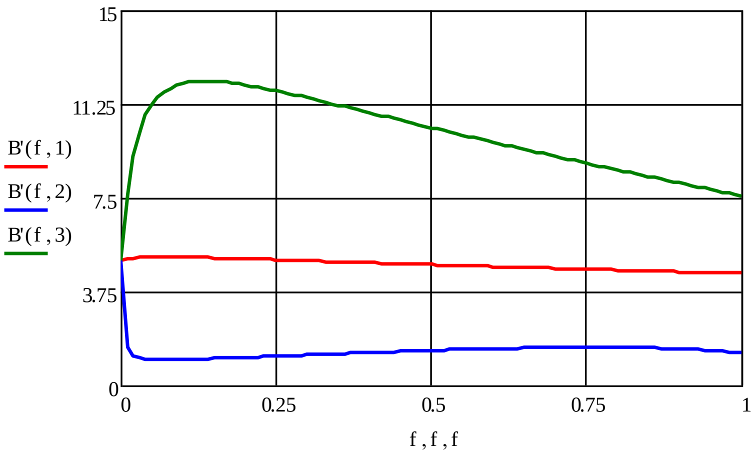

Fig. 2 – Influence of phase weight on the non-homogeneity parameter *B*.

Parameter B changes depending on the weight of the non-monotonic phases.

Figures 3, 4, 5 present the influences of the phase weight on the compression modulus (Fig. 3), the modulus of elasticity (Fig. 4) and the Poisson's coefficient (Fig. 5).

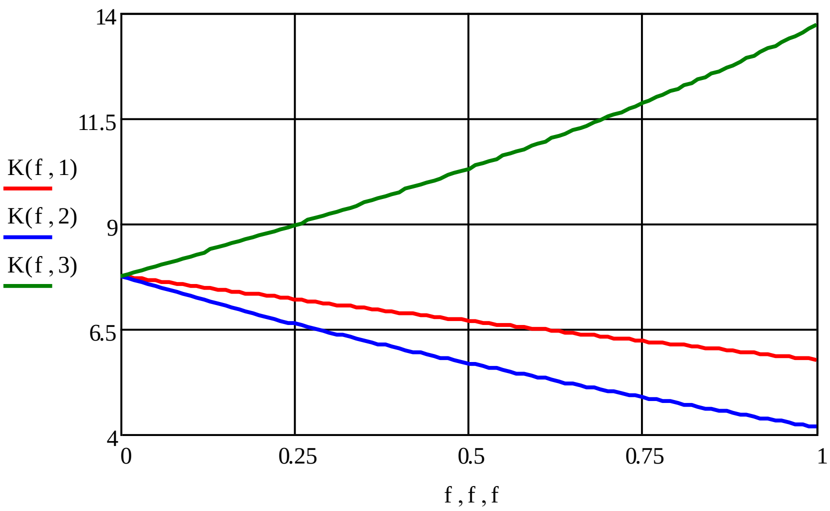

Fig. 3 – Influence of phase weight on the compression modulus.

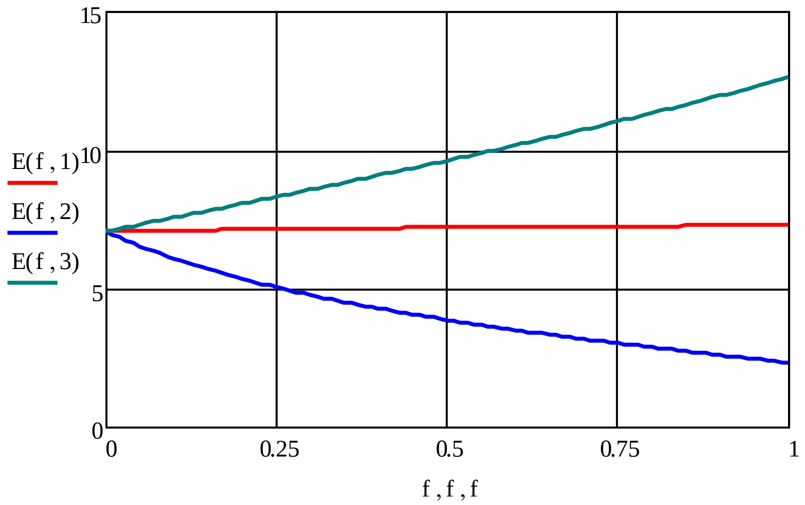

Fig. 4 – Influence of phase weight on the modulus of elasticity.

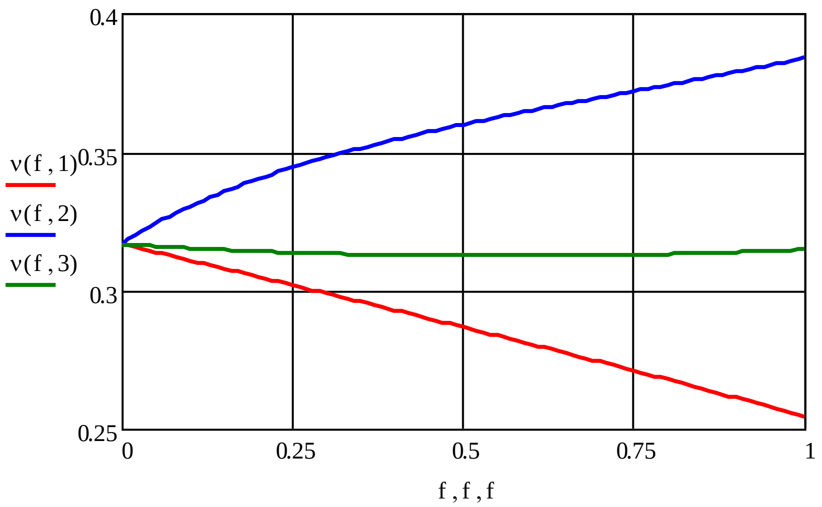

Fig. 5 – Influence of phase weight on the Poisson's coefficient

The red lines indicate the elastic constants E, K, ν, G and non-homogeneity parameter B for the Al-Th alloy, the blue ones indicate *Al-Pl*, and the green ones indicate Al-Cu. These alloys have the following elastic properties [24]:
Al$(A_1 = 1.215,\ C_{44} = C_1 = 2.85 \cdot c)$; Th$(A_2 = 3.621, C_2 = 4,78 \cdot c)$
Pl$(A_2 = 3.892, C_2 = 1.44 \cdot c)$; Cu$(A_2 = 3.209, C_2 = 7.54 \cdot c)$,
where $c = 10^4\,MPa$.

The physical and technical constants of elasticity change monotonically depending on the phase weight f . The parameter of non-homogeneity of the distribution of stresses and strains changes according to non-monotonic laws for all the alloys studied. Thus, the fluctuations of stresses and strains in the representative volume of the material are more sensitive to the influence of phase weight.

4. CONCLUSIONS

1. A system of equations has been established for determining the macroscopic shear modulus and the parameter of alloy heterogeneity in multiphase polycrystals.
2. The influence of phase weight for various multiphase materials in polycrystals has been investigated.
3. It was shown that the elasticity constants change monotonically depending on the phase ratio, while the inhomogeneity parameter of the stress and strain distribution changes according to non-monotonic laws, demonstrating that the fluctuations of stresses and strains are more sensitive to the influence of phase weight.

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