Metallophysics and Advanced Technologies
Металофіз. новітні технол.
Metallofiz. Noveishie Tekhnol.
2024, vol. 46, No. 6, pp. 591–608
https://doi.org/10.15407/mfint.46.06.0591
Reprints available directly from the publisher

PACS numbers: 02.70.Dh, 46.15.-x, 46.50.+a, 62.20.D-, 62.20.mm, 83.80.Fg

Analysis of Extreme Values of Stress and Strain Invariants in Multiphase Polycrystals

V. Yu. Marina and V. I. Marina

Technical University of Moldova,
168 Shtefan cel Mare Blvd.,
MD-2004 Kishinev, Moldova

The limits of change in stress/strain invariants in the phases of polycrystalline materials with cubic lattices are investigated. The relationship between the local and macroscopic parameters is established on the basis of the following principles: averaged connections, orthogonality of fluctuations of the stress and strain tensors, extremum of discrepancy between the macroscopic measures and suitable average values of microscopic analogues. General expressions for extreme values of stress/strain deviator invariants for the polycrystal phases are obtained. The non-monotonic nature of changes in the extreme values of the invariants of stress/strain deviators and volumetric stresses/strains depending on the phase concentration is revealed. In case of a two-phase polycrystal, as the harder phase increases, the invariants first increase, reaching their maximum value at a concentration of less than 5%, and then, monotonically decrease. Volumetric macrostress has a nonlinear effect on the patterns of changes in volumetric stresses in the grains of a polycrystalline material.

Key words: stress, strain, invariants, averaged connections, orthogonality, anisotropy.

Досліджуються межі зміни інваріянтів напруження/деформації у фазах полікристалічних матеріялів з кубічними ґратницями. Взаємозв'язок між локальними та макроскопічними параметрами встановлюється на основі принципів: середніх зв'язків, ортогональности флюктуацій тензорів напружень і деформацій, екстремуму невідповідности макроскопічних величин з відповідними середніми значеннями мікроскопічних ана-

Corresponding author: Vasilii Iurie Marina
E-mail: vasilemarina21@yahoo.com

Citation: V. Yu. Marina and V. I. Marina, Analysis of Extreme Values of Stress and Strain Invariants in Multiphase Polycrystals, *Metallofiz. Noveishie Tekhnol.*, **46**, No. 6: 591–608 (2024). DOI: 10.15407/mfint.46.06.0591

логів. Одержано загальні вирази для екстремальних значень інваріянтів девіяторів напруження/деформації у полікристалічних фазах. Показано, що за фактора анізотропії, більшого за одиницю, максимальні значення інваріянтів девіяторів напруження виникають у зернах, кристалографічні осі яких співвісні з макросистемою, в якій діягональні компоненти девіятора дорівнюють нулю, а мінімальні — у зернах, кристалографічні осі яких співвісні з главами. Встановлено немонотонний характер змін екстремальних значень інваріянтів девіяторів напружень/деформацій та об'ємних напружень/деформацій від концентрації фаз. Для двофазного полікристалу зі зростанням вмісту більш твердої фази інваріянти спочатку збільшуються, досягаючи найбільшого значення за концентрації, меншої за 5%, а потім монотонно зменшуються. Об'ємне макронапруження нелінійно впливає на закономірності змін об'ємних напружень у зернах полікристалічного матеріялу.

Ключові слова: напруження, деформація, інваріянти, усереднені зв'язки, ортогональність, анізотропія.

(Received 4 December, 2023; in final version, 6 May, 2024)

1. INTRODUCTION

The construction of constitutive equations relating macrostresses t_{ij} and macrostrains d_{ij} based on the known constitutive equations at the level of structural elements, $\tilde{t}_{ij} = \tilde{d}_{ij}$ is one of the main problems in the mechanics of a deformed solid. There are three main approaches: statistical [1–8], self-consistent [9–16] and direct [3, 10, 17]. Static 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 the other part, on the basis of accepted kinematic (Voigt hypothesis), static (Reuss hypothesis) or intermediate type (Kroener-type hypotheses). Self-consistent models are based on considering a mesolevel element surrounded by a material matrix with effective characteristics, determined iteratively from the properties of mesolevel elements using the adopted procedure for averaging the latter. Direct models consider the solution of a boundary value problem for a set of crystals with a priori given physical equations, which are unknown for irreversible processes. Numerical implementation in direct methods is usually based on the finite element method.

Currently, when studying reversible processes, two-level models are most widespread, in which the relationship between the local and macroscopic parameters is based on linear relationships between stress and strain fluctuations

$$\tilde{d}_{ij} = \tilde{\varepsilon}_{ij} + \tilde{\varepsilon}_0 \delta_{ij},$$

where only the D and B parameters depend on the model. Based on variational methods [9, 10, 18], it was found that the limiting options $B_{ijnm} = \infty$ (homogeneous strain state $\tilde{d}_{ij} = d_{ij}$) and $B_{ijnm} = 0$ (homogeneous stress state $\tilde{t}_{ij} = t_{ij}$) correspond to the upper and lower limits of the effective elastic constants for composite materials of arbitrary structure. Because of this, intermediate options $0 < B_{ijnm} < \infty$ have become widespread.

It was shown in [4] that linear relationships between fluctuations of stress and strain do not agree with the first law of thermodynamics and give overestimated internal stresses in the irreversible region of deformation. In particular, the inequality was established

$$\left\langle \int \tilde{t}_{ij} \dot{\tilde{d}}_{ij} dt \right\rangle < \int \left\langle \tilde{t}_{pq} \right\rangle \left\langle \dot{\tilde{d}}_{pq} \right\rangle dt$$

for any options for changing isotropic tensor B_{ijnm}, with the exception of limiting values: $B_{ijnm} = 0$, $B_{ijnm} = \infty$.

Nonlinear equations for the connection between local and macroscopic parameters are based on three principles formulated in [4, 5, 19]: averaged connections, orthogonality of fluctuations of stress and strain tensors, the extremum of the discrepancy between the macroscopic measure and a suitable average value of the microscopic analogue.

In Refs. [4–7, 19, 20], nonlinear coupling equations were used to describe deformation processes in single-phase polycrystalline materials. In this article, we will analyse the patterns of changes in the limiting values of stress and strain invariants in multiphase polycrystals with cubic lattices.

2. GENERAL PROVISIONS OF THE CONSTITUTIVE MODEL

Based on the equilibrium equations of continuous medium and geometric Cauchy relations, the following expressions have been established [13, 14]:

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

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

Three equations (1) can be represented as one relation

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

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

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

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

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

Let us establish one fundamental equation for the 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 will establish an expression for 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. It was shown in Ref. [5, 19] that this condition is satisfied by applying the simplest expression to fluctuations of deviatoric quantities

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

where B is an internal parameter, which contains information about the microscopic characteristics of material particles. In what follows, parameter B will be called the heterogeneity parameter.

In accordance with [5, 19], microscopic variables that have a certain physical meaning are divided into two categories: variable averaged values of which depend only on data on the surface of a representative volume and variable averaged values of which depend not only on data on the surface, but also on characteristics structures. In particular, in [5, 19], it is shown that natural macroscopic measures of the energy of change in volume and shape do not coincide with the corresponding averaged micromeasures. It is natural to assume that variables containing information about the characteristics of the microstructure of a material have certain fundamental properties. In [5, 19], a principle was proposed according to which in real interactions the discrepancy between a macroscopic measure and a suitable average value of a microscopic analogue takes on an extreme value. In particular,

$$\Delta = \left\langle \tilde{\sigma}_{ij}\tilde{\varepsilon}_{ij} \right\rangle - \left\langle \tilde{\sigma}_{ij} \right\rangle \left\langle \tilde{\varepsilon}_{ij} \right\rangle = \text{Extremum}\,. \tag{7}$$

Expressions (1), (5)–(7) represent a closed system of equations for the relationship between macro- and microstates. They do not contain references to the properties of the material; therefore, they are valid for describing both reversible and irreversible deformation processes. On their basis, it is possible to construct constitutive equations at the macroscopic level if the constitutive equations at the microscopic level are known.

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

Based on (1), (6) and (7), we analyse the influence of the elastic characteristics of the phases and their volumetric content on the macroscopic elasticity 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} is shear constant (relates shear stress to shear strain), A is anisotropy factor, K is volumetric deformation modulus.

The physical equations of crystals, in the crystallographic co-ordinate 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 into account these expressions in (6), we establish the following relations between local and macroscopic deformations:

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

Here, ε_{ij} is the macroscopic deviator of the deformation tensor in the global co-ordinate system x_i, which coincides with the main system. Let us further agree to denote the elasticity constants of crystals, stress and strain in phase with weight f_k through: $C_k = C_{44,k}, A_k, K_k, \tilde{\sigma}_{ij,k}, \tilde{\varepsilon}_{ij,k}$. Then, macroscopic stresses σ_{ij} and strains ε_{ij} can be expressed through the averaged values of stresses $\langle\tilde{\sigma}_{ij,k}\rangle$ and strains $\langle\tilde{\varepsilon}_{ij,k}\rangle$ in the phases of the polycrystal:

$$\sigma_{ij} = \sum_{k=1}^{n}\langle\tilde{\sigma}_{ij,k}\rangle f_k,\ \varepsilon_{ij} = \sum_{k=1}^{n}\langle\tilde{\varepsilon}_{ij.k}\rangle f_k,\ \sum_{k=1}^{n} f_k = 1\ . \quad (9)$$

Expression (6) for each phase can be represented as

$$\tilde{\sigma}_{ij,k} - \sigma_{ij} = B(\varepsilon_{ij} - \tilde{\varepsilon}_{ij,k})\ . \quad (10)$$

Writing (8) in the global co-ordinate system and taking into account expressions (9), (10), after integration over the orientation factor of the crystal lattice, we obtain

$$\frac{5}{2G+B} = \sum_{k=1}^{n}\left(\frac{3}{2C_{44}+B} + \frac{2A_k}{2C_k + A_k B}\right) f_k \,. \tag{11}$$

The expression for the extremum of the discrepancy between measures Δ (7) can be represented as

$$\Delta = \sum_{k=1}^{n} \left\langle \tilde{\sigma}_{ij,k} \tilde{\varepsilon}_{ij,k} \right\rangle f_k - \sigma_{ij}\varepsilon_{ij} = \text{Extremum} \,. \tag{12}$$

Taking into account relations (1) and (10) in (12), we obtain

$$-B\sum_{k=1}^{n} \left\langle (\tilde{\varepsilon}'_{ij,k} - \varepsilon'_{ij})(\tilde{\varepsilon}'_{ij,k} - \varepsilon'_{ij}) \right\rangle f_k = \text{Extremum} \,. \tag{13}$$

Substituting into (13), expressions (8) for each phase and taking into account that $\tilde{\varepsilon}'_{ij,k}\tilde{\varepsilon}'_{ij,k} = \tilde{\varepsilon}_{ij,k}\tilde{\varepsilon}_{ij,k}, \varepsilon'_{ij}\varepsilon'_{ij} = \varepsilon_{ij}\varepsilon_{ij}$ are invariant quantities, after integrating over the crystal lattice orientation factor, we find:

$$-\frac{\sigma_{nm}\varepsilon_{nm}B}{10G}\sum_{k=1}^{n}\left[2\left(\frac{(B+2G)A_k}{2C_k + A_k B}\right)^2 + 3\left(\frac{B+2G}{2C_k + B}\right)^2 - 5\right] f_k = \text{Extremum} \,. \tag{14}$$

Based on system (11), (14), it is possible to establish patterns of change in the shear modulus G and inhomogeneity parameter B in multiphase materials.

The patterns of changes in parameters G and B scales $X \cdot 10^{-4}$ MPa depending on the volumetric content of the harder phase f ($f_2 = f$, $f_1 = f$)

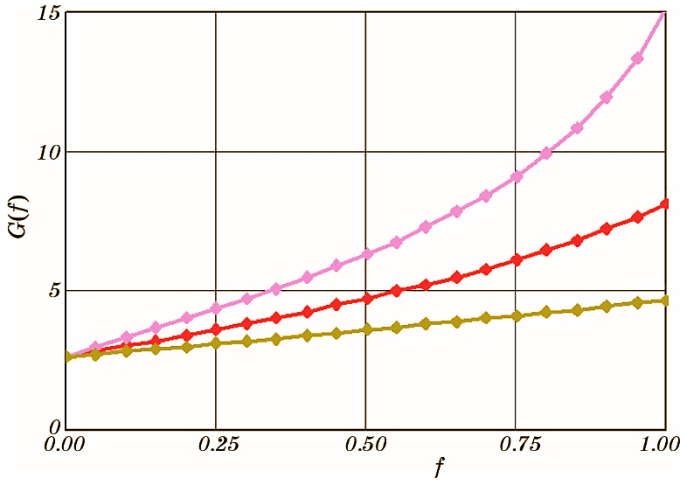

Fig. 1. The influence of volumetric content of harder phase on the alloy shear modulus.

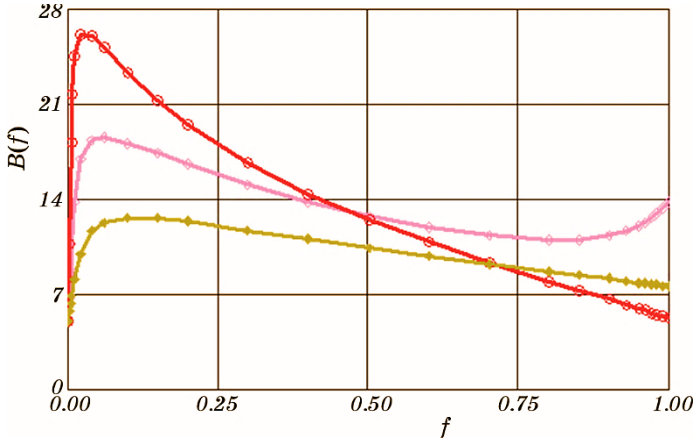

Fig. 2. The influence of volumetric content of the harder phase on the alloy heterogeneity parameter.

were studied using examples of three two-phase materials: Al–Fe, Al–W, Al–Cu, having the following elastic characteristics [21]:

$$M\sigma(f,\mathrm{k}) \le \sqrt{\tilde{I}_{2\sigma,k} / I_{2\sigma}}, \sqrt[3]{\tilde{I}_{3\sigma,k} / I_{3\sigma}} \le N\sigma(f,k)A_k,$$

$$\mathrm{Fe}(A_1 = 2.417,\ C_2 = 11.6c), \mathrm{W}(A_1 = 0.99,\ C_2 = 15.14c),$$

$$\mathrm{Cu}(A_2 = 3.209,\ C_2 = 7.54c), c = 10^4\,\mathrm{MPa}.$$

The results of numerical studies for the shear modulus are presented in Fig. 1. The curve marked in red corresponds to Al–Fe alloy, in lilac corresponds to Al–W alloy, and in brown corresponds to Al–Cu alloy. According to Fig. 1, macroscopic shear modulus $G = G(f)$ increases monotonically with increasing f.

Diagrams for the parameter $B = B(f)$ presented in Fig. 2 have a more complex appearance compared to the diagram $G = G(f)$. For all studied materials, a nonmonotonic dependence of the heterogeneity parameter on f.

4. ANALYSIS OF LIMITING VALUES OF STRESS/STRAIN INVARIANTS IN POLYCRYSTALLINE PHASES

The patterns of changes in the limiting values of stress/strain invariants in single-phase polycrystalline materials with a cubic lattice were studied in [7]. The analysis showed that, along with the main macroscopic co-ordinate system $x_i^{(m)}$, in which the non-diagonal components of the deviator are equal to zero (main co-ordinate system), there is also a system $x_i^{(n)}$, in which the diagonal components are cancelled (auxil-

iary system). To determine the position of the auxiliary co-ordinate system $x_i^{(n)}$ relative to the main system $x_i^{(m)}$, a parameter of the type of stress tensor deviator is introduced into consideration

$$d = \sigma_1/\sigma_3\,, |\sigma_1| \geq |\sigma_2| \geq |\sigma_3|, -0.5 \leq d \leq 0\,. \tag{15}$$

Indices for the eigenvalues σ_1, σ_2, σ_3 of the stress deviator σ_{ij} are assigned based on the condition that inequality (15) is satisfied. The form of the stress tensor deviator d can be expressed in terms of deviator invariants σ_{ij}

$$\frac{\sqrt[3]{-d(d+1)}}{\sqrt{2(d^2+d+1)}} = \pm\frac{\sqrt[3]{I_{3\sigma}}}{\sqrt{I_{3\sigma}}},\ I_{2\sigma} = \sigma_{ij}\sigma_{ij},\ I_{3\sigma} = \det|\sigma_{ij}\sigma_{ij}|\,.$$

In this equality, the sign '+' corresponds to a positive value of the component $\sigma_1 > 0$ and the sign '–' to a negative value $\sigma_1 < 0$. The orientation of the auxiliary co-ordinate system $x_i^{(n)}$ relative to the main system $x_i^{(m)}$ is determined by the following values of the Euler angles [7]

$$\varphi = \frac{\pi}{2},\ \theta = \frac{\pi}{4},\ \psi(d) = \arccos\left(\sqrt{\frac{1+d}{2+d}}\right),\ \frac{\pi}{4} \leq \psi(d) \leq \frac{\pi}{4} + 0.17\,. \tag{16}$$

The relationship between the deviator components in the auxiliary co-ordinate system $x_i^{(n)}$ and the main values is determined by the equalities [7]

$$\sigma_{12}^{(n)} = \sigma_{21}^{(n)} = -\sigma_3,\ \sigma_{32}^{(n)} = \sigma_{23}^{(n)} = \sigma_{13}^{(n)} = \sigma_{31}^{(n)} = \pm\sqrt{-\sigma_1\sigma_2/2}\,.$$

According to (23), there are simple relations between the deviator components of any symmetric tensor in co-ordinate systems with zero diagonal components and zero non-diagonal components. The sign '–' corresponds to the value $\sigma_1 > 0$, and the sign '+' corresponds to the value $\sigma_1 < 0$. The listed properties for single-phase polycrystals are also preserved in the case of multiphase polycrystals.

Let us pass in (9) from the components of strain deviators to the components of stress deviators, we obtain the relations

$$\tilde{\sigma}_{ij,k} = \begin{cases} M\sigma_k \tilde{r}_{in}\tilde{r}_{jm}\sigma_{nm}, i = j, \\ N\sigma_k \tilde{r}_{in}\tilde{r}_{jm}\sigma_{nm}, i \neq j, \end{cases}\quad \tilde{r}_{ij} = \tilde{r}_{ij}(\varphi, \theta, \psi)\,, \tag{17}$$

$$\mathrm{M}\,\sigma_k = \frac{2G+B}{2C_k + A_k B}\frac{C_k}{G}, \mathrm{N}\sigma_k = \frac{2G+B}{2C_k+B}\frac{C_k}{G}, \tag{18}$$

where φ, θ, ψ are the Euler angles (they specify the orientation of the orthogonal axes of crystallites relative to the main macroscopic co-

ordinate system). Note that, in (17), (18), both individual characteristics of phases (C_k, A_k) and global characteristics (B, G) appear, which depend both on the elastic characteristics of the phases and on their volumetric content.

Based on (16)–(18) and taking into account the fact that, along with the main co-ordinate system, there is also an auxiliary co-ordinate system, for alloys with cubic crystal lattices, the theorems can be formulated.

Theorem 1. The maximum values of stress deviator invariants ($A_k > 1$) arise in grains whose crystallographic axes are coaxial with the macrosystem in which the diagonal components are equal to zero, and the minimum values occur in grains whose crystallographic axes are coaxial with the main co-ordinate system. When $A_k < 1$, the opposite picture is observed.

Theorem 2. The types of deviators of stress/strain tensors in crystals with extreme values of invariants, in each phase of a polycrystalline material, coincide with the macroscopic form, *i.e.*,

$$\frac{\sqrt[3]{\det\left|\tilde{\sigma}_{ij,k}\right|}}{\sqrt{\tilde{\sigma}_{ij,k}\tilde{\sigma}_{ij,k}}} = \frac{\sqrt[3]{\det\left|\sigma_{ij}\right|}}{\sqrt{\sigma_{ij}\sigma_{ij}}}, \frac{\sqrt[3]{\det\left|\tilde{\varepsilon}_{ij,k}\right|}}{\sqrt{\tilde{\varepsilon}_{ij,k}\tilde{\varepsilon}_{ij,k}}} = \frac{\sqrt[3]{\det\left|\varepsilon_{ij}\right|}}{\sqrt{\varepsilon_{ij}\varepsilon_{ij}}}.$$

According to the theorems formulated, the relationship between the extreme values of the stress/strain deviator invariants and the corresponding macroscopic invariants $A_k > 1$ is determined by the relations

$$\begin{aligned} &\min\sqrt{\tilde{\sigma}_{ij,k}\tilde{\sigma}_{ij,k}} = M\sigma_k\sqrt{\sigma_{ij}\sigma_{ij}}, \min\det\left|\tilde{\sigma}_{ij,k}\right| = M\sigma_k^3\det\left|\sigma_{ij}\right|, \\ &\max\sqrt{\tilde{\sigma}_{ij,k}\tilde{\sigma}_{ij,k}} = N\sigma_k\sqrt{\sigma_{ij}\sigma_{ij}}, \max\det\left|\tilde{\sigma}_{ij,k}\right| = N\sigma_k^3\det\left|\sigma_{ij}\right|, \end{aligned} \tag{19}$$

$$\max\sqrt{\tilde{\varepsilon}_{ij,k}\tilde{\varepsilon}_{ij,k}} = N\varepsilon_k\sqrt{\varepsilon_{ij}\varepsilon_{ij}}, \max\det\left|\tilde{\varepsilon}_{ij,k}\right| = N\varepsilon_k^3\det\left|\varepsilon_{ij}\right|, N\varepsilon_k = \frac{(2G+B)A_k}{2C_k + A_kB},$$

$$\min\sqrt{\tilde{\varepsilon}_{ij,k}\tilde{\varepsilon}_{ij,k}} = M\varepsilon_k\sqrt{\varepsilon_{ij}\varepsilon_{ij}}, \min\det\left|\tilde{\varepsilon}_{ij,k}\right| = M\varepsilon_k^3\det\left|\varepsilon_{ij}\right|, \mathrm{M}\varepsilon_k = \frac{2G+B}{2C_k+B}. \tag{20}$$

If $A_k < 1$, then, in (19), (20), min and max change places.

Let us consider the patterns of changes in the limiting values of deviators stress moduli and strain tensors in the phases of Al–Fe and Al–Cu alloys depending on the volumetric content of the 'solid' phase $f_2 = f$. For two-phase polycrystals, relations (18) can be represented in the form

$$\begin{aligned} M\sigma_k &= M\sigma(f,k) = \frac{2G(f)+B(f)}{2C_k + A_kB(f)}\frac{C_k}{G(f)}, \\ \mathrm{N}\sigma_k &= N\sigma(f,k) = \frac{2G(f)+B(f)}{2C_k + B(f)}\frac{C_k}{G(f)}, \end{aligned} \tag{21}$$

where the index k, for elastic characteristics C_k, A_k, is assumed to be equal to unity $k = 1$ for the soft phase and $k = 2$ for the harder phase. Figure 3 shows diagrams of changes in parameters (21) for the Al–Fe alloy. Curves *1* and *2* describe patterns of changes $N\sigma(f, 2)$, $M\sigma(f, 2)$ in the Fe phase, and curves *2* and *4* show patterns of change $N\sigma(f, 1)$, $M\sigma(f, 1)$ in Al phase respectively. For a better perception of the limits of change in the relative values of stress invariants in the grains of each phase, $M\sigma(f,k) \le \sqrt{\tilde{I}_{2\sigma,k}}/I_{2\sigma}$, $\sqrt[3]{\tilde{I}_{3\sigma,k}}/I_{3\sigma} \le N\sigma(f,k)$ the areas between the parameter values $M\sigma(f, k)$ in $N\sigma(f, k)$ the grain system are shaded (red colour corresponds to Fe phase, brown corresponds to Al). From (19), (21) it follows that the specificity of changes pattern in the maximum values of invariants $\tilde{I}_{2\sigma,k}$ in k phase is influenced by only one constant C_k. $\tilde{I}_{3\sigma,k}$ pattern of changes in the minimum values of invariants $\tilde{I}_{2\sigma,k}$ is $\tilde{I}_{3\sigma,k}$ influenced by two constants k of the phase: C_k, A_k. In this case, the width of the zone of change in the limiting values of invariants increases with increasing phase anisotropy factor A_k.

Figure 4 shows diagrams of changes in parameters (21) for the Al–Cu alloy. The region of changes in values $\sqrt{\tilde{I}_{2\sigma,k}}/I_{2\sigma}$, $\sqrt[3]{\tilde{I}_{3\sigma,k}}/I_{3\sigma}$ in the Cu phase is shaded in red, and in the Al phase is shaded in purple. From those 4 diagrams presented in Fig. 3 and expressions (19), (21), it is clear that the dependences of changes in extreme values of invariants of deviators of stress tensors in alloys are non-monotonic to the function f. With an increase in the volumetric content of the harder phase $M\sigma(f, k)$, the parameters $N\sigma(f, k)$ first increase, reaching their highest value at $f = f_* = 0.034$, in the case of Al–Fe and $f = f_* = 0.06$ in the case of

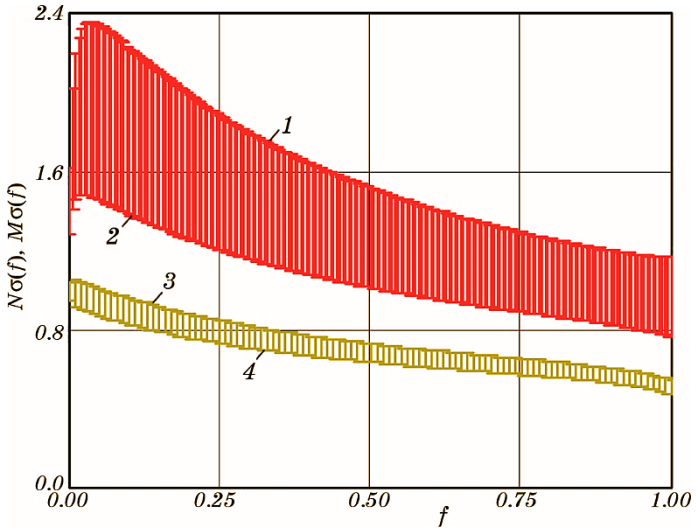

Fig. 3. Effect of volumetric Fe content on parameters reflecting the limits of change in stress invariants in Al–Fe alloy.

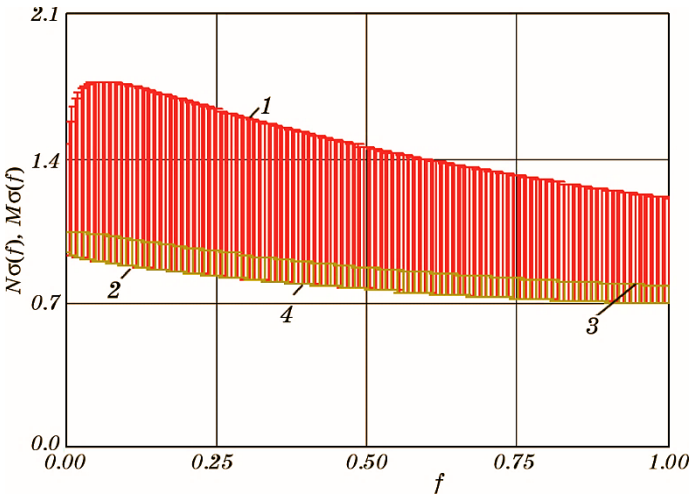

Fig. 4. The influence of the volumetric Cu content on parameters reflecting the limits of change in stress invariants in Al–Cu alloy.

Al–Cu alloy, and then decrease monotonically. For the soft phase, a violation of monotonicity is observed only in the diagram $M\sigma' \sim f$ (the highest value is achieved at $f = 0.01$). In the Al–Fe alloy, the highest values of invariants $\max \tilde{\sigma}/\sigma = N\sigma(0.034, 2) = 2.32$ arise $\max \tilde{I}_{3\sigma}/I_{2\sigma} = 2.32^3 = 12.49$ in the Fe phase at $f = 0.034$, and in the Al–Cu alloy, $\max \tilde{\sigma}/\sigma = N\sigma(0.06, 2) = 1.77$, $\max \tilde{I}_{3\sigma}/I_{2\sigma} = 5.55$ in the Cu phase at $f = 0.06$. Calculations carried out for other alloys showed that as the ratio increases, C_2/C_1 the value $f = f_*$ in the solid phase decreases and $N\sigma(f_*, k)$ increases.

According to Figure 3 in Al–Fe alloy, the zone of change in stress invariants in the Fe phase ($A_2 = 2.41$) is greater than in the Al phase ($A_1 = 1.215$). In this case, the zone of changes in the local invariants of stress tensor deviators in the Fe phase does not intersect with the corresponding zone of the Al phase. The Al–Cu alloy variant shown in Fig. 4 looks different. Since A_2 the width of the zone of change in stress invariants increases with growth at a fixed value f, options are possible when the corresponding zones intersect. From Figure 4, it is clear that, in the case of the Al–Cu alloy (Cu:Al = 3.209), the zone of invariants changes in the Al phase completely transforms into the zone of the Cu phase.

The dependence of the stress-tensor deviator modulus on the orientation factor of the crystallographic co-ordinate system $\tilde{\sigma}(\varphi = \theta, \theta, \psi)$ in the Fe phase ($f = 0.4$) of the Al–Fe alloy under uniaxial tension ($t_1 = 12$ MPa) is shown in Fig. 5. Horizontal planes in Fig. 5 establishes the limits of change in the deviator modulus of the stress tensor in Fe phase crystals under the given test conditions.

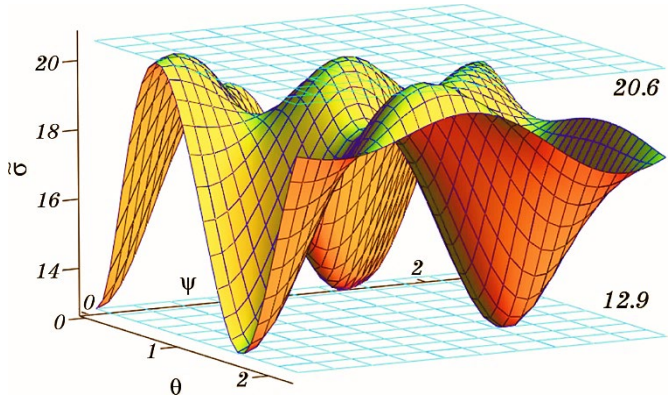

Fig. 5. Dependence of the stress-tensor deviator modulus on the orientation of the crystallographic co-ordinate system in the Fe phase ($f = 0.4$) of the Al–Fe alloy under uniaxial tension ($t_1 = 12$ MPa).

5. ANALYSIS OF THE LIMITING VALUES OF THE FIRST STRESS/STRAIN INVARIANT IN POLYCRYSTAL PHASES

The patterns of changes in volumetric stresses and strains are established on the basis of the postulate about the orthogonality of stress and strain fluctuations (5). If the postulate about the orthogonality of stress and strain fluctuations is extended to each phase, then, Eq. (5), taking into account (10), can be represented in the form

$$(\tilde{\sigma}_{0,k} - \sigma_0)(K\tilde{\sigma}_{0,k} - K_k\sigma_0) = \frac{KK_k}{B}(\tilde{\sigma}'_{ij,k} - \sigma'_{ij})(\tilde{\sigma}'_{ij,k} - \sigma'_{ij}). \qquad (22)$$

The quantities $\tilde{\sigma}'_{ij,k} - \sigma'_{ij}$ will be determined based on (17):

$$\tilde{\sigma}'_{ij,k} - \sigma'_{ij} = \begin{cases} (M\sigma_k - 1)\tilde{r}_{in}\tilde{r}_{jn}\sigma_{nm}, i = j, \\ (N\sigma_k - 1)\tilde{r}_{in}\tilde{r}_{jn}\sigma_{nm}, i \neq j. \end{cases} \qquad (23)$$

When the orientation of the crystallographic co-ordinate system of the crystal coincides with the main macroscopic co-ordinate system, relation (30) taking into account (23) takes the form

$$(\sigma m_k - \sigma_0)(K\sigma m_k - K_k\sigma_0) = \frac{KK_k}{B}(M\sigma_k - 1)^2\sigma_{ij}\sigma_{ij}, \qquad (24)$$

where through σm_k denotes the volumetric stress in the grain whose crystallographic system is coaxial with the macrosystem $x_i^{(m)}$. The volumetric stress $\tilde{\sigma}_{0,k}$ in the grain, whose crystallographic system is coaxial with the co-ordinate system $x_i^{(n)}$ (22), will be denoted by σn_k. In this case, we have

$$(\sigma n_k - \sigma_0)(K\sigma n_k - K_k\sigma_0) = \frac{KK_k}{B}(N\sigma_k - 1)^2\sigma_{ij}\sigma_{ij}. \qquad (25)$$

From (24), (25), we establish formulas for extreme values of volumetric stresses in a set of polycrystal grains

$$\sigma m(f,k) = \frac{K_k + K(f)}{2K(f)}\sigma_0 \pm \sqrt{\left(\frac{K_k - K(f)}{2K(f)}\sigma_0\right)^2 + \frac{K_k(M\sigma(f,k)-1)^2\sigma_{ij}\sigma_{ij}}{B(f)}}, \qquad (26)$$

$$\sigma n(f,k) = \frac{K_k + K(f)}{2K(f)}\sigma_0 \pm \sqrt{\left(\frac{K_k - K(f)}{2K(f)}\sigma_0\right)^2 + \frac{K_k(N\sigma(f,k)-1)^2\sigma_{ij}\sigma_{ij}}{B(f)}}. \qquad (27)$$

Writing (26) and (27), there were used notations: $\sigma m(f,\ k) = \sigma m_k$, $\sigma n(f,\ k) = \sigma n_k$. Both roots of equations (26), (27) have a physical meaning. According to (26), (27), the extreme values of volumetric stresses in the phases of a polycrystal depend on the elastic characteristics of the crystals and macroscopic stresses: σ_0, $\sigma = \sqrt{\sigma_{ij}\sigma_{ij}}$. Volume stresses in crystals of arbitrary orientation are determined from (22) taking into account (23).

The patterns of changes in volumetric stresses depending on the volumetric content of the harder phase f were studied for alloys: Al–Fe, Al–W, Al–Cu. Figure 6 shows diagrams $\sigma n \sim f$ (curve *1* refers to the Fe phase, and curve *3*—Al) and $\sigma m \sim f$ (curve *2*—Fe, curve *4*—Al) for pure macroscopic shear ($\sigma_0 = 0$, $\sigma = 10$ MPa). The region of possible changes in volumetric stresses in grains of the Fe phase is shaded in red, and Al is shaded in brown. Since in this case solutions (34), (35) differ only in sign, Fig. 6 shows only positive values of the diagrams

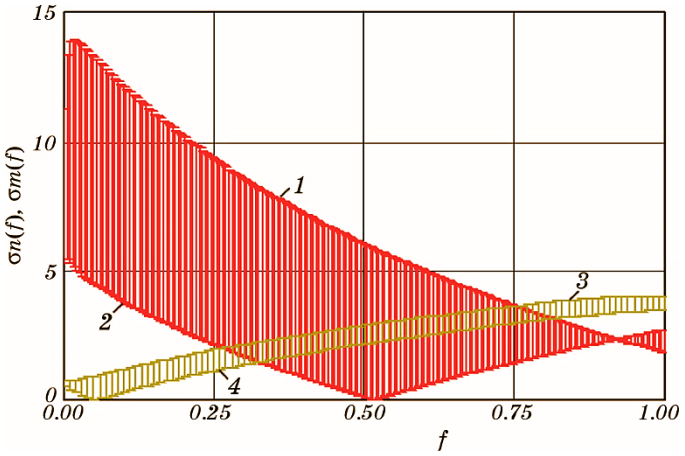

Fig. 6. The influence of the volumetric Fe content on the limits of change in volumetric stresses in the Al–Fe alloy under pure shear.

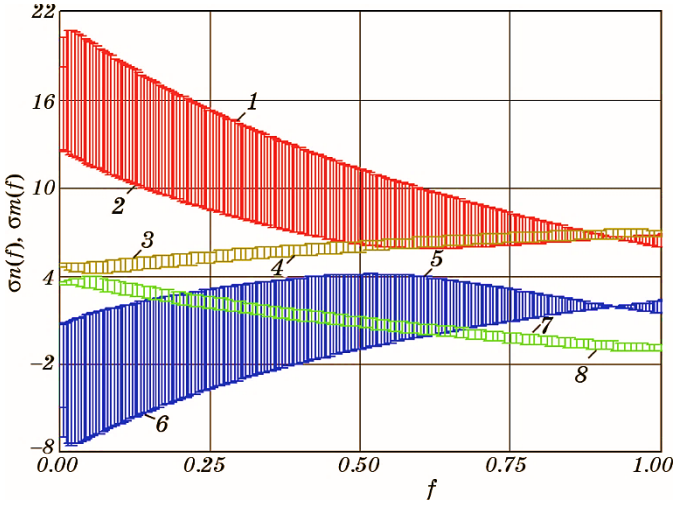

Fig. 7. Effect of volumetric Fe content on the limits of changes in volumetric stresses in the Al–Fe alloy when stretched.

$\sigma m \sim f$, $\sigma n \sim f$.

According to Figure 7, the width of the zone of change in volumetric stresses in the Fe phase is significantly greater than in the Al phase. With the volumetric content of iron $f = f_* = 0.02$ in the solid phase, volumetric stress occurs: $\sigma n(0.02, 1) = \pm 1.4\sigma$. If $f < 0.26$ in all grains of the Fe phase the volumetric stresses are greater than in the Al phase. In $0.26 < f < 0.82$, the range of changes in volumetric stresses in the Fe and Al phases polycrystalline intersect. If $f > 0.75$, the volumetric stresses in the Al phase are greater than in the Fe phase.

Figure 8 presents the results of numerical calculations for the Al–Cu alloy. Diagrams *1* and *2* characterize the limits of changes in invariants in the Cu phase, and diagrams *3*, *4*—in the Al phase. The region of possible changes in volumetric stresses in grains of the Cu phase is shaded in red, and in Al—brown. Diagrams presented in Figs. 7, 8 correspond to alloys in which the properties of solid phases are qualitatively different: the anisotropy coefficient A_2 for Cu is greater than A_2 for Fe and the elastic constant for Cu is less than C_{44} for Fe. As the constant increases, C_2 the largest values of the stress invariants increase, and with an increase in the anisotropy coefficient, A_2 the width of the zone of changes in the invariants increases. From Figures 7, 8, a very remarkable effect stands out: in the harder phase, in the $f = 0.915$ Al–Fe alloy and in the $f = 0.8$ Al–Cu alloy, the volume stress $\tilde{\sigma}_{0.2}$ in the crystals does not depend on the crystal lattice orientation factor. A similar effect is impossible in a single-phase polycrystal, except in the case of $A = 1$. This effect occurs when in equations (26), (27) the equali-

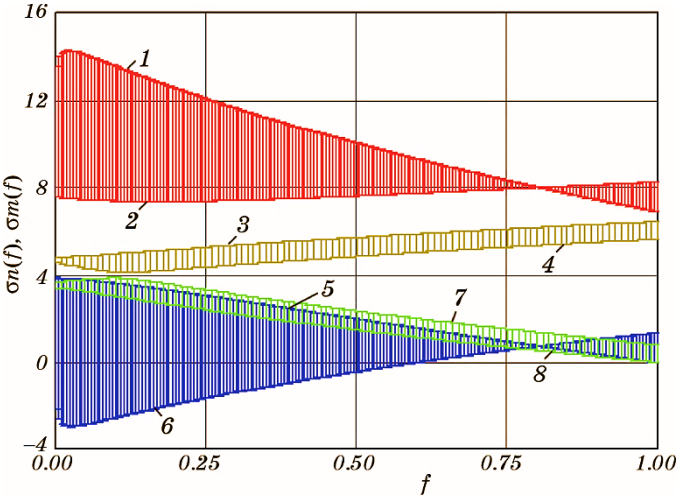

Fig. 8. Effect of volumetric Cu content on the limits of changes in volumetric stresses in the Al–Cu alloy under tension.

ty

$$(N\sigma_k - 1)^2 = (M\sigma_k - 1)^2, N\sigma_k - 1 = 1 - M\sigma_k .$$

Consequently, for a certain group of alloys there is a concentration of the solid anisotropic phase $f = f_*$ at which volumetric stresses are the same as in the isotropic phase. From (26) and (27), it follows that volumetric macrostress σ_0 has a nonlinear effect on the patterns of changes in volumetric stresses in the grains of a polycrystalline material. Let us consider the regions of changes in volumetric stresses $\tilde{\sigma}_0$ in crystals soft two-phase polycrystals: Al–Fe and Al–Cu under uniaxial loading. Figure 7 presents the results of numerical studies for the Al–Fe alloy, and in Fig. 8—results for Al–Cu. For a better perception of the results, a unified diagram notation system and the same external influence conditions are used: $\sigma_0 = 4.08$ MPa, $\sigma = 10$ MPa. Diagrams marked with odd numbers refer to curves $\sigma n \sim f$, and with odd numbers $\sigma m \sim f$. Diagrams marked with numbers *3*, *4*, *7*, *8* belong to the soft phase (Al) a diagrams *1*, *2*, *5*, *6*—to the solid phase (Fe or Cu). Curves marked with numbers *1*–*4* correspond to '+' sign in formulas (26) and (27), and *5*–*8*—to '–' sign.

The areas of changes in volumetric stresses $\tilde{\sigma}_0$ in the harder phase are shaded red when there is a '+' sign in (26), (27) and blue when there is a negative sign. In the Al phase, in Figs. 7, 8, the region of changes in volumetric stresses $\tilde{\sigma}_0$ is shaded brown for '+' sign in (26), (27) and green for '–' sign. If the macroscopic volume stress $\sigma_0 > \sqrt{K(f) / B(f)}(N_\sigma(f,k) - 1)\sigma$, then, in all grains of this from, this

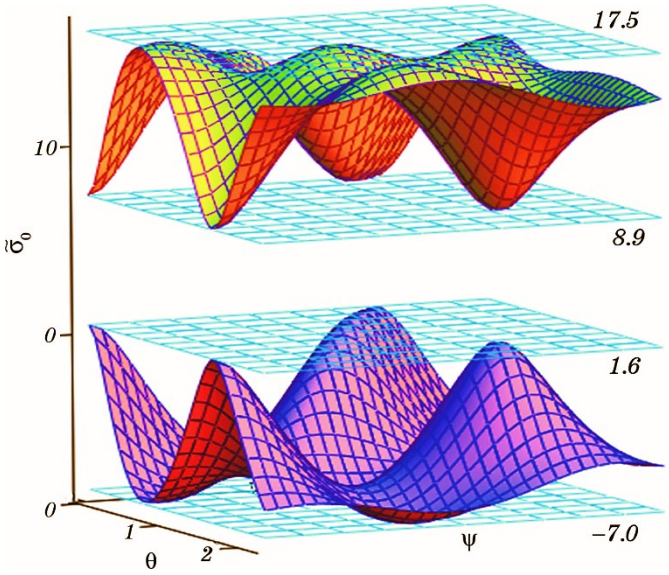

Fig. 9. Dependence of volumetric stresses in the Fe phase ($f = 0.4$, Al–Fe alloy) during tension on the orientation of the crystallographic co-ordinate system.

phase $\tilde{\sigma}_0 > 0$.

Comparing the limiting diagrams of changes in volumetric stresses (Cu:Al = 3.209) in Al–Fe alloys (Fig. 7) and Al–Cu alloy (Fig. 8), we discover a qualitative difference in the laws of change $\sigma m \sim f$. In the case of the Al–Fe alloy, the lower value of volumetric stress $\sigma m(f)$ decreases (diagrams *2* in Fig. 7, 8) to $f = 0.52$, and then grow in the Al–Cu alloy, volumetric stresses $\sigma m(f)$ increase monotonically with increasing f (diagrams *2*). Note that the largest range of changes in volumetric stress $\tilde{\sigma}_0$ is observed at a low concentration of one of the phases.

The patterns of changes in volumetric stresses depending on the orientation of the crystallographic co-ordinate system $\tilde{\sigma}_0(\varphi = \theta, \theta, \psi)$ in the Fe phase ($f = 0.4$) of Al–Fe alloy under uniaxial tension ($t_1 = 12$ MPa) are shown in Fig. 9. Calculations were carried out based on expressions (22), (23). The roots for volumetric stresses $\tilde{\sigma}_0$ have the form $\tilde{\sigma}_0 = x \pm \sqrt{y}$. A solution obtained with '+' sign is indicated in orange, and a solution with '–' sign is indicated in blue. Horizontal planes in Fig. 9 establish the limits of possible changes in volumetric stresses $\tilde{\sigma}_0$ in the Fe phase of the Al–Fe alloy.

6. CONCLUSION

A system of equations is established to determine the macroscopic shear modulus and the heterogeneity parameter of alloys, whose crys-

tal symmetry is not lower than cubic one. General expressions are obtained for extreme values of invariants of stress/strain deviators in polycrystal phases, which include both individual characteristics of the phases (anisotropy factor and crystal shear constant) and global characteristics B, G. It is shown that, when the anisotropy factor is greater than one, the maximum values of stress deviator invariants appear in grains, the crystallographic axes of which are coaxial with the macrosystem, in which the diagonal components are equal to zero, and the minimum—in grains, the crystallographic axes of which are coaxial with the main co-ordinate system. When the anisotropy factor is less than one, the opposite picture is observed.

It is shown that the invariants of the deviators of the stress tensors undergo nonmonotonic changes with increasing volumetric content of the harder phase. As the harder phase grows, the invariants first increase, reaching their highest value at $f \cong 0.01 \pm 0.06$, and then, decrease monotonically. Thus, the largest deviations of the limiting values of the invariants of the deviators of the stress tensors are observed at very low values of the concentration of the solid phase.

The specificity of the pattern of changes in the maximum values of stress deviator invariants in a separate phase is influenced only by the corresponding crystal shift constant, and the pattern of changes in the minimum values is influenced by both the shift constant and the anisotropy factor.

REFERENCES

1. A. G. Fokin and T. D. Shermergor, *PMTF*, No. 3: 123 (1968) (in Russian).
2. Z. Hashin and S. Shtrikman, *J. Mech. Phys. Solids*, **10**, Iss. 4: 335 (1962).
3. L. P. Khoroshun, B. P. Maslov, E. N. Shikula, and L. V. Nazarenko, *Statisticheskaya Mekhanika i Ehffektivnyye Svoistva Materialov* [Statistical Mechanics and Effective Properties of Materials] (Kiev: Naukova Dumka: 1993) (in Russian).
4. V. Yu. Marina, *Numerical Investigations in Continuum Mechanics* (Kishinev: 1987), p. 47.
5. V. Yu. Marina, *Appl. Mech.*, **6**: 9 (1997).
6. V. Yu. Marina and V. I. Marina, *Metallofiz. Noveishie Tekhnol.*, **42**, No. 3: 415 (2020) (in Russian).
7. V. Yu. Marina, *Mech. Solids*, **58**: 727 (2023).
8. P. V. Trusov, *News of the Russian Academy of Sciences. MTT*, **1**: 69 (2021) (in Russian).
9. J. R. Willis, *J Appl. Mech.*, **50**: 1202 (1983).
10. B. Flipona, C. Kellera, R. Queyb, and F. Barbea, *Int. J. Solids Structures*, **184**: 178 (2020).
11. Z. Hashin and S. Shtrikman, *J. Mech. Phys. Solids*, **10**, Iss. 4: 335 (1962).
12. Z. Hashin, *J. Mech. Phys. Solids*, **50**: 481 (1983).
13. R. Hill, *Proc. Phys. Soc. A*, **65**: 349 (1952).

14. R. Hill, *Progress in Appl. Mech.*, 99 (1963).
15. E. Kroner, *J. Mech. Phys. Solids*, **15**, Iss. 5: 319 (1967).
16. E. Kroner, *Inst. I. Engng. Sci.*, **1**: 261 (1963).
17. P. V. Trusov, A. I. Shveikin, E. S. Nachaeva, and P. S. Volegov, *Phys. Mesomechanics*, **15**: 58 (2012).
18. S. K. Kanun, *PMTF*, No. 4: 194 (1975) (in Russian).
19. V. Yu. Marina, *News of the Academy of Sciences of Moldova. Mathematics Series*, **2**: 16 (1998).
20. V. Yu. Marina and V. I. Marina, *Int. Appl. Mech.*, **57**: 707 (2022).
21. T. D. Shermergor, *Theory of Elasticity of Microinhomogeneous Media* (Moskva: Nauka: 1977) (in Russian).