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ON A GENERAL THEORY OF COMPOSITE MATERIALS AND MICRO-INHOMOGENEOUS ELASTIC MEDIA

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A method is developed to average over the volume the differential equations of equilibrium describing inhomogeneous elastic composite media with markedly different elastic moduli. A chain of macro-equilibrium equations is obtained involving macro tensors of stress couples and other stresses, all of increasing rank. These tensors are in general unisymmetric due to their definition of average quantities with respect to the oriented surface elements. The system of equations reduces to a single equation involving a series of derivatives of stresses of increasing order, averaged over the volume and residual term which is a derivative of stress averaged over the surface. By truncation of the series for an assumed accuracy a differential equation is obtained which is sufficient in the case when a single kinematic quantity is a vector of macro displacement. A structure of equation is derived typical for a gradient in the nonlocal theory of elasticity. Numerical calculations were carried out for a polycrystal provided that averaging over the volume is equivalent to averaging over the number of possible realizations.

A method of averaging over the volume for differential equations of equilibrium in inhomogeneous elastic media is developed in the present paper. The material under consideration is assumed to be a composite, the constituents of which are characterized by various elastic moduli. A chain set of macro-equilibrium equations is obtained, containing macro-tensors of stress, double-stress, etc. These tensors are non-symmetric in general, due to their definitions as some mean values over the surface, in accordance with the original Cauchy's concept. In the case when the displacement vector constitutes the only kinematic variable, the chain set of equations reduces to a single one which contains, however, some additional differential components of subsequently increasing orders, dependent on the order of the theory. Similar analytical expressions are derived in the case of a polycrystal material.

The difference between the present theory and the widely acknowledged approach presented, for example, in the papers [4–7], consists in considering the physical background for the application of different methods of averaging for various state parameters. Only in the case of calculating the mean characteristic of a random distribution of elastic moduli over the volume is statistic averaging performed, i.e. an ensemble averaging over the realization of a random distribution of crystals in the considered volume. If one introduced the hypothesis of an equivalence of all methods of averaging, one would a priori exclude theories of couple stress elasticity from consideration, thus making it impossible to investigate their connection with statistical theories of micro-inhomogeneous materials. On the other hand, in contradition to some well-known theories of couple-stress elasticity [8–10] the relationships between the macro-tensors of stress and strain are introduced in the present paper not by a hypothetic assumption of some elastic potential, but as a result of averaging the constitutive equations valid for the micro-level of description.

1.

Let us introduce two different levels of investigation for the state of stress and strain of the medium: the micro-level described by the coordinates x_i, and the macro-level for which the coordinates X_i are appropriate. Further, let us suppose for the micro-scale, i.e. for an infinitesimal element $ds = dx_1\, dx_2\, dx_3$, the validity of the equations of equilibrium

$$\frac{\partial}{\partial x_j}\sigma_{ij} + f_i = 0, \tag{1.1}$$

where $\sigma_{ij} = \sigma_{ij}(x)$ denotes the microstress tensor, $f_i = f_i(x)$ is the body force vector. Multiplying Eq. (1.1) with x_k, we obtain

$$\sigma_{ik} = \frac{\partial}{\partial x_j}(\sigma_{ij} x_k) - f_i x_k. \tag{1.2}$$

Further multiplication with the Levy-Civitta's alternating tensor ε_{lik} yields the moment of momentum balance equation

$$\frac{\partial}{\partial x_j}(\varepsilon_{lki}\sigma_{ij} x_k) - \varepsilon_{lki} f_i x_k = 0, \tag{1.3}$$

where the symmetry of the stress tensor σ_{ij}, defined in the microscale dV, is taken into account ($\varepsilon_{lki}\,\sigma_{ki} = 0$).

The medium under considration is assumed to be perfectly elastic but inhomogeneous at the micro-level. The stress-strain relation for this medium obeys the Hooke's law

$$\sigma_{ij} = L_{ijkl}\,\varepsilon_{kl}, \tag{1.4}$$

where the tensor of elastic moduli $L_{ijkl}(x)$ is a random function of coordinates. In the above expression ε_{kl} denotes the tensor of micro-strain which is related in the usual way to the vector of micro-displacements $u_i(x)$:

$$\varepsilon_{kl} = \frac{1}{2}\left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k}\right). \tag{1.5}$$

Let us assume that the inhomogeneity of the medium is due to the presence of micro-constituents which have various elastic properties; those could be monocrystal grains with random distribution of the crystallographic axes' orientations, or inclusions into a composite material, differing in elastic moduli from the surrounding embedment.

Consider now an elementary macro-volume $V=\Delta X_1\,\Delta X_2\,\Delta X_3$, the dimensions of which are much greater than the characteristic length of the micro-inhomogeneity scale. Integration of Eq. (1.1) over this volume leads to

$$\int_S \sigma_{ij}\,dS_j+\int_V f_i\,dV=0, \tag{1.6}$$

where S denotes the surface of the volume V, $dS_j=n_j\,dS$ represents a surface element with a normal vector n_j. Divide Eq. (1.6) by V and define in the following way the mean values over the volume and over the surface element $\Delta X_k\,\Delta X_m$:

$$\langle\ldots\rangle=\frac{1}{V}\int_V(\ldots)\,dV,\qquad \langle\ldots\rangle_j=\frac{1}{\Delta X_k\,\Delta X_m}\int_{S_j}(\ldots)\,n_j\,dS,\qquad k\neq m\neq j.$$

The surface integral in Eq. (1.6) is reduced to the sum of three subsequent differences Δ of the surface integrals taken over the elements of the surface.

As an example, consider one of these differences:

$$\frac{1}{V}\Delta\int_{S_1}\sigma_{i1}\,dS_1=\frac{1}{\Delta X_1}\left\{\langle\sigma_{i1}\rangle_1\left(X_1+\frac{\Delta X_1}{2},X_2\,X_3\right)-\langle\sigma_{i1}\rangle_1\left(X_1-\frac{\Delta X_1}{2},X_2,X_3\right)\right\}.$$

In order to derive the equations of macro-continuum, let us investigate the limit transition for the above relation when $\Delta X_1\to 0$. The result will be

$$\frac{1}{V}\Delta\int_{S_1}\sigma_{i1}\,dS_1=\frac{\partial}{\partial X_1}\langle\sigma_{i1}\rangle_1.$$

Adding in a similar way the expressions for $j=1, 2, 3$, in Eq. (1.6), and dividing by the volume V, we obtain the equation of the macro-equilibrium

$$\frac{\partial}{\partial X_j}\langle\sigma_{ij}\rangle_j+\langle f_i\rangle=0, \tag{1.7}$$

where the tensor of macro-stress $\langle\sigma_{ij}\rangle_j$ is, in general, non-symmetric.

Let X_i denote the macro-coordinates of the center of masses of the volume V. Denote with ξ_i the vector of the relative position with respect to the centre of masses for some material point within the vegion V. Averaging Eq. (1.2) over the volume V and observing that $x_i=X_i+\xi_i$, we obtain

$$\langle\sigma_{ik}\rangle=\langle\sigma_{ik}\rangle_k+\frac{\partial}{\partial X_j}\langle\sigma_{ij}\,\xi_k\rangle_j-\langle f_i\,\xi_k\rangle. \tag{1.8}$$

It follows from this relation that the mean value of the stress tensor $\langle\sigma_{ik}\rangle$, taken over the volume, constitutes only a part of the macro-stress tensor $\langle\sigma_{ik}\rangle_k$, and must not be directly substituted into the equation of equilibrium, [3]. Actually, the relation (1.8) presents an equilibrium equation corresponding to the additional degrees of freedom of the medium. In fact by multiplying the relation (1.8) with ε_{lik} we obtain a particular case of this additional motion (the balance of kinetic energy):

$$e_{lik}\langle\sigma_{ik}\rangle_k+\frac{\partial}{\partial X_i}\langle e_{1ki}\,\sigma_{ij}\,\xi_k\rangle_j-\langle e_{lki}f_i\,\xi_k\rangle=0. \tag{1.9}$$

In deriving the above relation it has been taken into account that $\varepsilon_{lik}\langle\sigma_{ik}\rangle=0$, i.e. averaging over the volume does not change the symmetry of the tensor σ_{ik}. Equation (1.9) contains, as it should have happened, the skew-symmetric part of the macro-tensor $\langle\sigma_{ik}\rangle_k$. Let us introduce the notation below:

$$\langle\sigma_{ik}\rangle_k=T_{ik}, \quad \langle\sigma_{ik}\rangle=T^V_{ik}, \quad \langle\sigma_{ij}\xi_k\rangle_j=\mu_{ijk},$$

$$\langle\epsilon_{ljk}\sigma_{ij}\xi_k\rangle_j=\mu_{il}, \quad \langle f_i\xi_k\rangle=\Phi_{ik}, \quad \langle\epsilon_{lik}f_i\xi_k\rangle=M_l.$$

Following the current terminology T_{ik} denotes the usual macro-stress (Cuachy's), μ_{ijk} — double stress, μ_{il}-couple stress, Φ_{ik}-double body forces, μ_i-body couple.

Assume that the considered medium is a homogeneous continuum at the macro-level. If the elementary volume is reducible to a point ($\xi_i\to 0$), i.e. if the medium is additionally homogeneous at the micro-level, then the following relations are valid: $\mu_{ijk}=0$, $T_{ik}=T^v_{ik}$, and it is sufficient to take into consideration only the first, „classical", equilibrium equation

$$\frac{\partial}{\partial X_j}T_{ij}+\langle f_i\rangle=0. \tag{1.10}$$

Due to the fact that in the limit transition of a macro-volume down to a point the macro- and micro-coordinates actually coincide, Eq. (1.10) obviously does not differ from Eq. (1.1). If the considered medium was micro-inhomogeneous, the characteristic dimension of an elementary volume should fulfil additionally the following requirement: it should contain a sufficiently large number of microelements so as to make it possible to treat the material as a macro-homogeneous one. In consequence, the diemensions of V have a lower limit which is at least of one order higher than the characteristic scale of the micro-inhomogeneity. In this case $T_{ik}\neq T^v_{ik}$, the macro-element can be subjected to a rigid rotation independently of the field of displacements. This means that the limiting volume V is no more a point but rather a „rigid particle". Therefore, Eq. (1.10) has to be completed with Eq. (1.9)

$$T_{[ik]}+\frac{\partial}{\partial X_j}\mu_{[ki]jk}+\Phi_{[ik]}=0, \qquad T_{ik}\neq T^V_{ik}, \tag{1.11}$$

where the square brackets denote antisymmetrization with respect to the corresponding indices. The obtained equation is typical of couple-stress elasticity, [11].

In a more general case of deformation of a particle one should consider Eq. (1.8)

$$T_{ik}-T^V_{ik}+\frac{\partial}{\partial X_j}\mu_{ijk}+\Phi_{ik}=0. \tag{1.12}$$

However, when the characteristic length for the gradient of macro-displacement is comparable with the dimensions of the macro-volume, the stress field within the latter will be inhomogeneous, and the limiting macro-volume will possess the ability of performing more complex „elementary" motions. To describe the latter some more detailed equations of equilibrium might be needed. These new independent equations which contain couple stresses of increasing order can be derived in the following way. Let us multiply Eqs. (1.1) with the diadic product $x_k x_m$:

$$\sigma_{ik} x_m + \sigma_{im} x_k - \frac{\partial}{\partial X_j} (\sigma_{ij} x_k x_m) + f_i x_k x_m = 0 .$$

Averaging this relation over the volume brings

$$\langle \sigma_{ik} x_m \rangle + \langle \sigma_{im} x_k \rangle - \frac{\partial}{\partial X_j} \langle \sigma_{ij} x_k x_m \rangle_j + \langle f_i x_k x_m \rangle = 0 .$$

After substituting the equality $x_k = X_k + \xi_k$ and applying the above notation, we get

(1.13) $$\mu_{i(mk)} - \mu^V_{i(mk)} + \frac{1}{2} \frac{\partial}{\partial X_j} \mu_{ijkm} + \frac{1}{2} \Phi_{ikm} = 0 .$$

The paranthesis denotes here symmetrization with respect to corresponding indices,

$$\mu_{ijkm} = \langle \sigma_{ij} \xi_k \xi_m \rangle , \qquad \Phi_{ikm} = \langle f_i \xi_k \xi_m \rangle ;$$

and the upper index V indicates, as it did before, the mean value of the same quantity taken over the volume, with exception of its surface. By means of a similar procedure we can derive the S-th equation of equilibrium:

$$\sigma_{i(k_1 \dots k_S)} - \mu^V_{i(k_1 \dots k_S)} + \frac{1}{S} \frac{\partial}{\partial X_j} \mu_{ijk_1 \dots k_S} + \frac{1}{S} \Phi_{ik_1 \dots k_S} = 0 .$$

It can be seen that Eqs. (1.10) and (1.14) form with $S=1, 2, \dots$, a chain set of coupled equations of increasing orders. It isn't difficult to observe as well that in the case when the mean values over the volume and over the surface coincide for all orders of couple-stresses, the equations of the set separate and become a chain of consequences.

In the paper [12] flow of a Stokesian fluid was considered and the characteristic macro-volume was chosen with dimensions comparable to the characteristic length velocity field gradient. The stress tensor in an arbitrary point of the macro-volume was expanded in Taylor series

$$\sigma_{ij}(X+\xi) = \sigma_{ij}(X) + \frac{\partial \sigma_{ij}(X)}{\partial X_k} \xi_k + \frac{1}{2} \frac{\partial^2 \sigma_{ij}(X)}{\partial X_k \partial X_m} \xi_k \xi_m + \dots .$$

Within such a definition the macro-stress tensor $\sigma_{ij}(X)$ was obviously a symmetric one, while the first non-vanishing components of the Taylor expansion of the kinetic moment of the particle led to the equation of diffusion of vorticity, as a consequence of the balance of momentum equation. A similar situation arises in the case of Eqs. (1.10) and (1.14) when the micro-inhomogeneities of the medium vanish.

2.

Let us introduce the vector of macro-displacement $U_i(X)$, defining it as a mean value over the volume V for the field of local displacements $u_i(x)$:

(2.1) $$U_i = \langle u_i \rangle .$$

We shall present the field of micro-displacements $u_i(x)$ as the sum of a regular component and an irregular one:

(2.2)
$$u_i(\xi)=U_i+\frac{\partial U_i}{\partial X_j}\xi_j+u_i^*.$$

Here $u_i^*(x)$ denotes the pulsation of the displacement caused by the inhomogeneities of the medium. The representation (2.2) is compatible with the definition (2.1) if the following condition is fulfilled: $\langle u_i^*\rangle=0$.

The macro-strain tensor $\langle\varepsilon_{ij}\rangle$ can also be introduced as a mean value over the volume V for the tensor ε_{ij}, defined by Eq. (1.5):

(2.3)
$$\langle\varepsilon_{ij}\rangle=\frac{1}{2}\left(\left\langle\frac{\partial u_i}{\partial X_j}\right\rangle+\left\langle\frac{\partial u_j}{\partial X_i}\right\rangle\right)=\frac{1}{2}\left(\frac{\partial\langle u_i\rangle_j}{\partial X_j}+\frac{\partial\langle u_j\rangle_i}{\partial X_i}\right).$$

The above expression contains mean values over the surface for a vector quantity. In the papers [2, 3] it was assumed that there is an equivalence between the mean values of a vector when taken over a volume or over a surface. This assumption can be justified on the basis of the following consideration.

A mean value over a volume for a quantity $\varphi_{ij\ldots}(x)$, denoted $\langle\varphi_{ij\ldots}\rangle$, can be reduced to an integral from mean values over the surface. For example, with the normal vector n_1:

$$\langle\varphi_{ij\ldots}\rangle=\frac{1}{V}\int_V\varphi_{ij}(x_1,x_2,x_3)\,dV=\frac{1}{\Delta X_1}\int\langle\varphi_{ij\ldots}\rangle_1\,dx_1\,.$$

Since the calculations are performed within the elementary volume $V=\Delta X_1\,\Delta X_2\,\Delta X_3$, the quantity $\langle\varphi_{ij\ldots}\rangle$ becomes a function of the point $x_1=X_1+\xi_1$, X_2, X_3. We shall consider further the situations for which this function is a deterministic one only. The necessary condtion for that is a sufficient "stirring" of the micro-inhomogeneities, and $V\gg\Delta^3$, where Δ denotes the characteristic length or micro-inhomogeneities. Only in the case when $\langle\varphi_{ij\ldots}\rangle_j=\text{const}$, which means equal mean values over the limiting planes, are the mean values over the volume and over planes of different orientations identical. The differences in averaging over various planes as well as over the volume involve automatically some additional geometric characteristics, like normal vectors to the planes. Consequently, averaging over the surfaces might put a macro-vector $\langle\varphi\rangle_j$ in correspondence to the micro-scalar φ, as well as a macro-tensor $\langle\varphi_i\rangle_j$ in correspondence to the micro-vector φ_i. This possibility must be excluded for physical reasons since we demand the macro-characteristic of the density to remain a scalar, and the macro-displacement a vector. Beginning with tensors of the second order, e.g. the stress tensor, the introduction of the vector of the averaging plane orientation can change the quantitative relations between the components and can disturb even the symmetry of the tensor but, at the same time, must not change its order.

Therefore if

$$\langle u_i(x)\rangle_j=\langle u_i(x)\rangle=U_i(X),$$

we have

$$\langle \varepsilon_{ij} \rangle = \frac{1}{2}\left(\frac{\partial U_i(X)}{\partial X_j} + \frac{\partial U_j(X)}{\partial X_i}\right). \tag{2.4}$$

In accordance with the expression (2.2) the field ε_{ij} can be presented in the following form:

$$\varepsilon_{ij}(\xi) = \frac{1}{2}\left(\frac{\partial U_i}{\partial X_j} + \frac{\partial U_j}{\partial X_i}\right) + \varepsilon^*_{ij}(\xi). \tag{2.5}$$

It is assumed here that the field of fluctuations $\varepsilon^*_{ij}(\xi)$ obeys the condition

$$\langle \varepsilon^*_{ij} \rangle = 0. \tag{2.6}$$

Suppose that the fluctuations of the strain tensor ε^*_{ij}, due to the micro-inhomogeneities of the elastic properties of the material are caused by the macro-strain $\langle \varepsilon_{ij} \rangle$. This corresponds to the case when the only kinematic variable is the displacement vector of the centre of masses of the region V.

3.

In order to establish the dependence of the fluctuations ε^*_{ij} on the mean strain $\langle \varepsilon_{ij} \rangle$, let us investigate the micro-equation of equilibrium (1.1). Assume that the body forces vanish ($f_i = 0$) and denote by σ_{ij} the difference

$$\sigma'_{ij} = \sigma_{ij}(x) - \langle \sigma_{ij} \rangle. \tag{3.1}$$

This yields the equation

$$\frac{\partial}{\partial x_j}\sigma'_{ij} = 0. \tag{3.2}$$

In deriving this equation the fact that the tensor $\langle \sigma_{ij} \rangle$ does not depend on micro--coordinates was taken into account. The tensor of elastic moduli $L_{ijkl}(x)$ for the volume V can be expressed in the form

$$L_{ijkl}(x) = L^V_{ijkl} + \delta L_{ijkl}(x), \tag{3.3}$$

where $L^V_{ijkl} = \langle L_{ijkl} \rangle$ is a deterministic quantity independent of coordinates, while $\langle \delta L_{ijkl} \rangle = 0$. Taking into account the representation (2.5), we get

$$\sigma'_{ij} = L^V_{ijkl}\varepsilon^*_{kl} + \delta L_{ijkl}(\langle \varepsilon_{kl} \rangle + \varepsilon^*_{kl}) - \langle \delta L_{ijk}\varepsilon^*_{kl} \rangle. \tag{3.4}$$

Substituting this expression into Eq. (3.2), we find

$$\frac{\partial}{\partial x_j} L^V_{ijkl}\varepsilon^*_{kl} = F_i \tag{3.5}$$

where

$$F_i = -\frac{\partial}{\partial x_j}\left[\delta L_{ijkl}(\langle \varepsilon_{kl} \rangle + \varepsilon^*_{kl}) - \langle \delta L_{ijkl}\varepsilon^*_{kl} \rangle\right].$$

One can consider the vector $F_i(x)$ as a distribution of body forces in the homogeneous medium, characterized by the tensor of elastic moduli L^V_{ijkl}. It follows here that the particular solution of Eq. (3.5) can be expressed with the Green's tensor $U_{lm}(x, x')$ which is defined as such a solution to the equation

$$L^V_{ijkl} \frac{\partial^2 U_{lm}(x,x')}{\partial x_j \partial x_k} + \delta(x-x')\delta_{im} = 0\,, \tag{3.6}$$

which has the property of vanishing on the surface of the characteristic volume. Instead of demanding an exact satisfaction of the unknown boundary conditions for the function $\varepsilon^*_{ij}(x)$, we will apply rather the condition (2.6), that is satisfy the boundary conditions integrally. One can show that this condition is fulfilled by the following solution:

$$u^*_i(x) = \int_V U_{ik}(x,x') \frac{\partial}{\partial x'_j} [\delta L_{kjmn}(x)(\langle\varepsilon_{mn}\rangle + \varepsilon^*_{mn}(x')) - \langle\delta L_{kjmn}\varepsilon^*_{mn}\rangle]\,dx\,.$$

After differentiation of both sides and partial integration, we get

$$\varepsilon^*_{ij}(x) = \int_V G_{ijkl}(x,x')[\delta L_{klmn}(x')(\langle\varepsilon^*_{mn}(x')) - \langle\delta L_{klmn}\varepsilon^*_{mn}\rangle]\,dx\,, \tag{3.7}$$

where

$$G_{ijkl} = \left[\frac{\partial^2 U_{ik}}{\partial x_j \partial x'_l}\right]_{(ij)(kl)}.$$

Under the assumption that the dimensions of the characteristic length of the micro-inhomogeneities, we substitute for the Green's function U_{ik} the function U^∞_{ik} for an unbounded medium. For a polycrystal, for example, this leads to an error of the order d/Δ, where d is the characteristic lenght of a grain, Δ denotes the characteristic dimension of the macro-volume. Being translationally — invariant, the tensor U^∞_{ik}, and hence the tensor G^∞_{ijkl}, depends on the difference $x-x'$ only, except for the vicinity of the surface. Therefore, the integral in Eq. (3.7) turns to a convolution. Bearing in mind the commutative properties of convolutions and performing averaging over the characteristic volume on both sides of Eq. (3.7), we come to the conclusion that $\langle\varepsilon^*_{ij}\rangle = 0$. The integral equation (3.7) gives a relation between the fluctuations ε^*_{ij} and the regular part of the strain tensor $\langle\varepsilon_{ij}\rangle$, as well as fluctuations of the elastic moduli of the material. We shall give an approximate solution to this equation, assuming the micro-inhomogeneous material to be a polycrystal.

The tensor $L_{ijkl}(x)$ becomes a step function for a polycrystal. It can be presented therefore in the following form:

$$L_{ijkl}(x) = \sum_r \delta_r(x) L^r_{ijkl}\,. \tag{3.8}$$

Here L^r_{ijkl} denotes the constant value of the field $L_{ijkl}(x)$ within the region v_r occupied by the r-th crystal, $\delta_r(x)$ is the characteristic function of this region equal to unity within the region and vanishin everywhere beyond it. In a similar fashion we can present the quantity δL_{ijl} where $\delta L^r_{ijkl} = L^r_{ijkl} - L_{ijkl}$.

Averaging on both sides of Eq. (3.8) over the volume V, we get

$$L^V_{ijkl}=\frac{1}{V}\sum_r L^r_{ijkl}v_r, \tag{3.9}$$

where the summation is extended over all crystals contained in the region V. The differences in values of the tensor L^r_{ijkl} for neighbouring grains are due to variations in the orientation of the crystallographic axes of monocrystals. Denoting by ω_r the orientation of the r-th grains axis with respect to ths laboratory system of coordinates, we can transform the expression (3.9) and obtain

$$L^V_{ijkl}=\sum_r C_r L_{ijkl}(\omega_r), \tag{3.10}$$

where $c_r=v_r/V$. Taking into account a large number of crystals in the region V, we shall make a limit transition from the discret to the continuous distribution of the orientations of crystals, substituting an integral for the sum in Eq. (3.10):

$$L^V_{ijkl}=\int L_{ijkl}(\omega)C(\omega)d\omega=\langle L_{ijkl}\rangle_\omega. \tag{3.11}$$

Here $c(\omega)$ denotes the continuous density of distribution over orientations, and $\langle\delta L_{ijkl}\rangle_\omega=0$. Thus averaging over the volume for the field of elastic moduli has been reduced to the calculation of the ensemble average over the set of realizations. When the polycrystal is macroscopically isotropic, we get

$$L^V_{ijkl}=k^V\delta_{ij}\delta_{kl}+2\mu^V\left(I_{ijkl}-\frac{1}{3}\delta_{ij}\delta_{kl}\right),$$

where the mean elastic moduli, the bulk modulus k^v and the shear modulus μ^v, are expressed by linear invariants of the tensor L_{ijkl} according to the well-known relations

$$k^V=\frac{1}{9}L_{iijj},\qquad \mu^V=\frac{1}{10}(L_{ijij}-3k^V). \tag{3.12}$$

Taking into account these results and introducing for a while symbolic notation, we obtain

$$\langle\delta L:\varepsilon^*\rangle=\sum_r C_r\,\delta L^r:\varepsilon^*_v(\omega_r)=\langle\delta L:\varepsilon^*_v\rangle_\omega, \tag{3.13}$$

where $\varepsilon^*_v(\omega_r)$ denotes the mean field of $\varepsilon^*(x)$ for the volume v_r.

Observing that $\varepsilon(x)=\langle\varepsilon\rangle+\varepsilon^*(x)$, $\langle\delta L:\varepsilon^*_v\rangle_\omega=\langle\delta L:\varepsilon_v\rangle_\omega$, we can present Eq. (3.7) in the following form:

$$\varepsilon(x)=\langle\varepsilon\rangle+\int_V G(x-x'):[\delta L(x'):\varepsilon(x')-\langle\delta L:\varepsilon_v\rangle_\omega]\,dx'. \tag{3.14}$$

Let us fix the point of observation x in the region v_α of an arbitrary grain. Separating the integral over region, we can write

$$\varepsilon(x)=\langle\varepsilon\rangle+\int_{v_\alpha}G(x-x'):[\delta L^\alpha:\varepsilon(x')-\langle\delta L:\varepsilon_v\rangle_\omega]\,dx'+ \tag{3.15}$$
$$+\sum_r{}'\int_{v_r}G(x-x'):\delta L^r:\varepsilon(x')\,dx'-\int_{V-v_\alpha}G(x-x'):\langle\delta L:\varepsilon_v\rangle_\omega\,dx',$$

where the apostrophe at the sum denotes lack of summation over the region v_α. Let us present the sum in the form

$$\sum_r{}' \int_{v_r} G(x-x'): \delta L^r: \varepsilon(x')\, dx = \sum_r{}' \int_{v_r} G(x-\xi^r-\zeta): \delta L^r: \varepsilon(\xi^r+\zeta)\, d\zeta ,$$

where ζ denotes the vector connecting the centre of masses ξ^r of the r-th crystallite with an arbitrary inner point of the volume. Since the integrals are non-singular, we can expand them in Taylor's series in the neighbourhood of points ξ^r, retaining only the first term of the expansion

$$\sum_r{}' \int_{v_r} G(x-x'): \delta L^r: \varepsilon(x')\, dx' \approx \sum_r{}' G(x-\xi^r): \delta L^r: \varepsilon_v(\omega_r) v_r .$$

The idea of the expansion, with the following rejection of all but the first term, consists in substituting dipoles located at the points ξ^r, instead of taking into account the influence of the whole crystalline structure on the field ε. The next step towards the calculation of the sum will be made when the discreet distribution of the dipoles in the region $V-v_\alpha$ is replaced by a continuous one. To this end, the density $C(x,\omega)$ will be introduced; this in turn under the assumption of the macroscopic homogeneity in the neighbourhood of the considered grain can be expressed in an approximate way by the relation $C(x,\omega)\approx\frac{1}{V}C(\omega)$. Finally, assuming that the absolute and relative (for fixed ω_α) mean values coincide for a large number of crystals in the region V, we get

$$\sum_r{}' G(x-\xi^r): \delta L^r: \varepsilon_v(\omega_r) v_r = \int_{V-v_\alpha} G(x-\xi): \langle \delta L: \varepsilon_v \rangle_\omega\, d\xi .$$

In this case, the sum and the last addend on the right hand side of Eq. (3.15) are equal. As a result the equation takes the following form:

$$\varepsilon(x) = \langle \varepsilon \rangle + \int_{v_\alpha} G(x-x'): [\delta L^\alpha: \varepsilon(x') - \langle \delta L: \varepsilon_v \rangle_\omega]\, dx' . \tag{3.16}$$

In order to proceed with calculations further, we need to know the shape of the region v_α. If the geometry of the grain can be approximated by a sphere, we may use the expression for the Green's function which corresponds to the isotropic tensor L^V_{ijkl}

$$U^\infty_{ik}(x-x') = \frac{1}{8\pi\mu^V}\left[\frac{\delta_{ik}}{|x-x'|} - \frac{3k^V+\mu^V}{3k^V+4\mu^V}\cdot\frac{\partial^2 |x-x'|}{\partial x_i \partial x_k}\right].$$

In this case

$$\int_{v_\alpha} G(x-x')\, dx' = -P ,$$

where P denotes a constant isotropic tensor. It can be expressed by the components of the tensor L^V_{ijkl} in the following way (*):

$$P = (P_{ijkl}) = \frac{1}{3(3k^V+4\mu^V)}\delta_{ij}\delta_{kl} + \frac{2(3k^V+6\mu^V)}{5\mu^V(3k^V+4\mu^V)}\left(I_{ijkl} - \frac{1}{3}\delta_{ij}\delta_{kl}\right).$$

(*) Note that in the case of an ellipsoidal shape of the v_α region the tensor P is also a constant one which possess an orthorhomboidal symmetry.

Consequently, we obtain

$$\varepsilon(x)=\langle\varepsilon\rangle+P:\langle\delta L:\varepsilon_v\rangle_\omega+\int_{v_\alpha} G(x-x'):\delta L^\alpha:\varepsilon(x')\,dx'. \tag{3.17}$$

On account of the polynomial conservativeness of the operator $(I-G)^{-1}$, [13], the solution of the integral equation (3.17) is given by the function $\varepsilon(\omega_\alpha)$ which depends solely on the orientation of the considered grain and does not depend on the micro-coordinates:

$$\varepsilon(\omega_\alpha)=A_\alpha:(\langle\varepsilon\rangle+P:\langle\delta L:\varepsilon_v\rangle_\omega). \tag{3.18}$$

Here A_α denotes

$$A_\alpha=A(\omega_\alpha)=(I+P:\delta L^\alpha)^{-1}.$$

Thus, $\varepsilon_v(\omega_\alpha)=\varepsilon(\omega_\alpha)$ and $\langle\delta L:\varepsilon_v\rangle_\omega=\langle\delta L:\varepsilon\rangle_\omega$. Multiplication of both sides of Eq. (3.18) with $\delta L(\omega_\alpha)$ and calculation of the ensemble average over orientations brings the expression of the ensemble average over orientations brings the expression for $\langle\delta L:\varepsilon\rangle_\omega$

$$\langle\delta L:\varepsilon\rangle_\omega=\langle\delta L:A\rangle_\omega:\langle A\rangle_\omega^{-1}:\langle\varepsilon\rangle. \tag{3.19}$$

Substituting back into Eq. (3.18) gives

$$\varepsilon(\omega_\alpha)=A_\alpha:\langle A\rangle_\omega^{-1}:\langle\varepsilon\rangle. \tag{3.20}$$

Finally, making use of th relation $\varepsilon^*(\omega_\alpha)=\varepsilon(\omega_\alpha)-\langle\varepsilon\rangle$, we come to the expression

$$\varepsilon^*(\omega_\alpha)=-B_\alpha:\langle\varepsilon\rangle, \quad B_\alpha=I-A_\alpha:\langle A\rangle_\omega^{-1}. \tag{3.21}$$

This is the solution to the problem of the relationship between the fluctuations of the strain tensor and its regular part, obtained within the assumptions given above. The flucutations' field ε^* turns out to be piece-wise constant, with $B_\alpha=B(\omega_\alpha)$ being a fourth-order positive determined tensor.

4.

In order to find the only kinematic variable, the macro-displacement vector $U_i(X)$, we need one macro-equation of equilibrium. It might be obtained from Eqs. (1.10) to (1.14) by reducing the set of equations into a single equation of some higher order. In fact, substituting into Eq. (1.10) the expression for T_{ik} from Eq. (1.12) and assuming vanishing body forces, we get

$$\frac{\partial}{\partial X_k}T^V_{ik}-\frac{\partial^2}{\partial X_k\partial X_j}\mu_{i(jk)}=0. \tag{4.1}$$

Subsequently, the quantity $\mu_{i(jk)}$ can be expressed from Eq. (1.13) and substituted into Eq. (4.1). As a result we obtain

$$\frac{\partial}{\partial X_k}T^V_{ik}-\frac{\partial^2}{\partial X_k\partial X_j}\mu^V_{i(jk)}+\frac{1}{2}\frac{\partial^3}{\partial X_k\partial X_j\partial X_m}\mu_{i(jkm)}=0 \tag{4.2}$$

Continuation of this procedure yields the following equation:

$$(4.3)\qquad \frac{\partial}{\partial X_k}\left[T^V_{ik}+\sum_{S=2}^{n}\frac{(-1)^{S-1}}{(S-1)!}\cdot\frac{\partial^S}{\partial X_{m_2}\ldots\partial X_{m_S}}\mu^V_{i\,(m_2\cdots m_S k)}+\right.$$
$$\left.+\frac{(-1)^n}{n!}\cdot\frac{\partial^n}{\partial X_{m_1}\ldots\partial X_{m_n}}\mu_{i\,(m_1\ldots m_n k)}\right]=0$$

for an arbitrary value of n. The presented procedure means in fact the reduction of the macro-stress tensor T_{ik} to a sum of gradients of moments of increasing orders for the micro-stress tensor σ_{ij} distribution. Consequently, we get the equation of equilibrium which contains mean values over the volume only, except for the last addend, which presents the mean value over the surface of the region. Assuming some particular order of the exactness of the theory, we can neglect the differential terms of the higher order so that the truncated equation of equilibrium will not contain any more the mean value over the surface. For example, when the members of order $(\Delta/l)^2$ are kept, where l denotes the characteristic length for the gradient of macro-displacement, the macro-equation of equilibrium takes the form

$$(4.3)\qquad \frac{\partial}{\partial X_k}T^V_{ik}-\frac{\partial^2}{\partial X_k\partial X_j}\mu^V_{i\,(jk)}+\frac{1}{2}\,\frac{\partial^3}{\partial X_k\partial X_j\partial X_m}\mu^V_{i\,(jkm)}=0\,.$$

Substituting into this equation the relation (3.1), one gets

$$(4.4)\qquad \frac{\partial}{\partial X_k}\langle\sigma_{ik}\rangle-\frac{\partial^2}{\partial X_k\partial X_j}\langle\sigma'_{ij}\xi_k\rangle+\frac{1}{2}\,\frac{\partial^3}{\partial X_k\partial X_j\partial X_m}\langle\sigma'_{ij}\xi_k\xi_m\rangle+$$
$$+\frac{1}{2}\,\frac{\partial^3}{\partial X_k\partial X_j\partial X_m}J_{jm}\langle\sigma_{ik}\rangle=0\,,$$

where $J_{jm}=\langle\xi_j\,\xi_m\rangle$ denotes the specific moment of inertia of the macro-region V. If there is no micro-inhomogeneity ($\sigma'_{ik}=0$), we get $\langle\sigma_{ik}\rangle_k=\langle\sigma_{ik}\rangle$ and $\frac{\partial}{\partial X_k}\langle\sigma_{ik}\rangle=0$, according to Eq. (1.10) for $f_i=0$. In this case the last member of Eq. (4.4) also vanishes as a consequence of Eq. (1.10). In order to retain in the equation of macro-equilibrium only the moments of the stress tensor distribution σ'_{ij}, let us multiply Eq. (4.3) by $\frac{\partial^2}{\partial X_j\partial X_m}J_{jm}$ and deduct subsequently the result from Eq. (4.4), neglecting the higher order terms. In effect we will obtain

$$(4.5)\qquad \frac{\partial}{\partial X_k}\left[\langle\sigma_{ik}\rangle-\frac{\partial}{\partial X_j}\langle\sigma'_{ij}\xi_k\rangle+\frac{1}{2}\,\frac{\partial^2}{\partial X_j\partial X_m}\langle\sigma'_{ij}\xi_k\xi_m\rangle\right]=0\,.$$

Let us now express the quantities entering Eq. (4.5) by the kinematic variable $U_i(X)$. We have

$$\langle\sigma_{ik}\rangle=\langle L_{ikmn}\,\varepsilon_{mn}\rangle=L^V_{ikmn}\frac{\partial U_m}{\partial X_n}+\langle\delta L_{ikmn}\,\varepsilon_{mn}\rangle_\omega\,.$$

Substitution of Eq. (3.19) into this relation gives

$$\langle\sigma_{ik}\rangle = L^{\ni}_{ikmn}\frac{\partial U_m}{\partial X_n}, \tag{4.6}$$

where

$$L^{\ni} = L^V + \langle\delta L\colon A\rangle_\omega\colon\langle A\rangle_\omega^{-1} \tag{4.7}$$

denotes the effective elasticity moduli tensor of the polycrystal. Note that Eq. (4.7) coincides with the expressions for this quantity derived in the papers [4, 5] using the methods of the theory of random functions. Besides, as it has been stated elsewhere, [14], the expression (4.7) for the tensor $L^{\ni}$ can be obtained as a result of the best approximation procedure of the T-matrix theory when the numerical properties are taken into account.

Let us consider now the second addend in Eq. (4.5). Using the formula (3.4) and expressing the coordinates ξ in the form $\xi=\xi^r+\zeta^r$, where ξ^r denotes the radius-vector of the centre of masses of the r-th grain ($\langle\zeta\rangle_v=0$), we get

$$\langle\sigma'\xi\rangle = \sum_r C_r[L^r\colon\varepsilon^*(\omega_r)\xi^r + \delta L^r\colon\langle\varepsilon\rangle\xi^r].$$

We shall assume that the sums in this relation can be replaced by integrals and, accordingly, the radius-vector ξ^r changes continuously. Introducing as above the density $\frac{1}{V}C(\omega)$, we obtain

$$\langle\sigma'\xi\rangle = (\langle L\colon\varepsilon^*\rangle_\omega + \langle\delta L\rangle_\omega\colon\langle\varepsilon\rangle)\langle\xi\rangle = 0 \tag{4.8}$$

since, by definition, $\langle\xi\rangle=0$. Similarly, taking into account the relation $\langle\delta L\xi\xi\rangle = \langle\delta L\rangle_\omega J=0$, we get

$$\langle\sigma'\xi\xi\rangle = \sum_r C_r[L'\colon\varepsilon^*(\omega_r)\xi^r\xi^r + L^r\colon\varepsilon^*(\omega_r)i^r] - J\langle\delta L\colon\varepsilon^*\rangle_\omega,$$

where $i^r=(i^r_{km})=\frac{1}{v_r}\int_{v_r}\zeta_k\zeta_m\,dv$. The limit transition from sums to integrals leads to

$$\sum_r C^r L^r\colon\varepsilon^*(\omega_r)\xi^r\xi^r = J\langle\delta L\colon\varepsilon^*\rangle_\omega,\quad \frac{1}{V}L^r\colon\varepsilon^*(\omega_r)i^r = \langle\delta L\colon\varepsilon^*\rangle_\omega i,$$

where $i=(i_{km})=\langle i_{km}\rangle$ denotes the mean specific moment of inertia of the crystallite ($i=0\,(d^2)$). Consequently,

$$\langle\sigma'_{ij}\xi_k\xi_m\rangle = -i_{km}\langle\delta L_{ij\alpha\beta}B_{\alpha\beta rS}\rangle_\omega\frac{\partial U_r}{\partial X_S}. \tag{4.9}$$

Since the shape of the grain has been assumed to be spherical, we have $i_{km}=i\delta_{km}$. Substitution of the formulae (4.6) to (4.9) into Eq. (4.5) leads to the following differential equation with respect to the vector of macro-displacement $U_i(X)$:

$$\left(L^{\ni}_{ikmn} - \frac{1}{2}i\Delta^2 M_{ikmn}\right)\frac{\partial^2 U_m}{\partial X_k\partial X_n} = 0, \tag{4.10}$$

where $M_{ikmn}=\langle \delta L_{ik\alpha\beta} B_{\alpha\beta mn}\rangle_\omega$ and $\nabla^2 \equiv \frac{\partial^2}{\partial X_k \partial X_k}$ denotes the Laplace operator. Equation (4.10) has the same form as in the "gradient" theory of elasticity when the considered kinematics is based on the classical theory; while the elastic potential is assumed to depend not only on the strain tensor but also on its gradient [8, 9]., The same form of the equation is obtained in the theory of elasticity with micro--structure [10] in the case of a long wave approximation, when Eq. (9.31) does not contain inertia terms. All these theories are constructed axiomatically by introducing potential energy as a function of governing parameters, and by applying subsequently the minimum principle to this function. The coefficients of the equation of equilibrium become constant tensors in such theories, and their connection with micro-structure is not clear. On the contrary, in the present approach the coefficients of Eq. (4.10) are expressed explicitly by the characteristics of the inhomogeneity. In particular, for an isotropic aggregate of cubic crystallites we obtain

$$(4.11)\qquad (\lambda^{э}+\mu^{э})(1-d_1\nabla^2)\frac{\partial^2 U_k(X)}{\partial X_1 \partial X_k}+\mu^{э}(1-d_2\nabla^2)\nabla^2 U_i(X)=0.$$

Here $\lambda^{э}$, $\mu^{э}$ denote the effective Lamé constants:

$$d_1=\frac{1}{3}i\frac{D}{\lambda^{э}+\mu^{э}},\qquad d_2=\frac{1}{2}i\frac{D}{\mu^{э}}.$$

The quantities appearing in these relations can be expressed by the moduli of elasticity of a cubic monocrystal C_{11}, C_{12}, C_{44}:

$$\lambda^{э}=\frac{1}{3}(C_{11}+2C_{12})-\frac{2}{3}\mu^{э},\quad \mu^{э}=\mu^V-D,\quad \mu^V=C_{44}+\frac{1}{5}C,$$

$$C=C_{11}-C_{12}-2C_{44},\quad D=\frac{\delta C_{44}}{1+2v\delta C_{44}},\quad C_{12}^V=C_{12}+\frac{1}{5}C,$$

$$\delta C_{44}=25\frac{3c^2 v}{\left(1-\frac{2}{5}Cv\right)\left(1+\frac{3}{5}Cv\right)},\qquad v=\frac{1}{15\mu^V}\,\frac{3C_{12}^V+8\mu^V}{C_{12}^V+2\mu^V}.$$

Note, that averaging Eq. (1.1) over the ensemble of realizations leads to another result. In the paper [6], for example a random inhomogeneous deformation of a polycrystal was considered. It was proposed to derive the relation between the mean stress and mean strain by expanding in series the flucutation $\overset{*}{\varepsilon}_{ij}$

$$\overset{*}{\varepsilon}_{ij}(x)=\sum_{k=0}^{\infty} a_{ij}\, mn_{\lambda_1 \dots \lambda_k}(x)\frac{\partial^k\langle\varepsilon_{mn}(x)\rangle}{\partial x_{\alpha_1}\dots\partial x_{\lambda_k}},$$

where the coefficients are homogeneous random functions. Calculations have shown that such an approach leads to nonlocal constitutive relations of the following form:

$$(4.12)\qquad \langle\sigma_{ij}(x)\rangle=\int L_{ijkl}(x-x')\langle\varepsilon_{kl}(x')\rangle\,dx',$$

The nonlocality is caused on one hand by the inhomogeneity of the field $\langle \varepsilon(x) \rangle$, and on the other one, by a non-vanishing radius of correlation of the fluctuation field of elastic moduli which is of the order of the mean grain diameter.

The "gradient" theory of elasticity for a small inhomogeneity ($\delta L \ll L^v$) was proposed in the paper [15]. The following representation was assumed:

$$u_i^*(x) = \varphi_{imn}(x) \langle \varepsilon_{mn}(x) \rangle,$$

where the tensor $\varphi(x)$ is determined by the Green's tensor of the theory of homogeneous elasticity as well as by the tensor δL. Then the potential energy $W = \langle \sigma_{ij} \varepsilon_{ij}$ was calculated and the Lagrange's variational principle applied. The latter leads to an equilibrium equation of the (4.10)-type, where the coefficients have the same order as in Eq. (4.10); however, their values are nevertheless different from those in Eq. (4.10).

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Streszczenie

O PEWNEJ OGÓLNEJ TEORII KOMPOZYTÓW ORAZ SPRĘŻYSTYCH OŚRODKÓW MIKRO-NIEJEDNORODNYCH

Opracowana jest metoda uśrednienia względem objętości różniczkowych równań równowagi niejednorodnych ośrodków sprężystych, składających się ze składników o znacznie różniących się modułach sprężystości. Otrzymano układ równań równowagi w wielkościach „makro", w których pojawiają się makro-tensory naprężeń, naprężeń momentowych i innych naprężeń, wszystkie rosnącego rzędu. Tensory te są w ogólnym przypadku niesymteryczne, ponieważ wprowadzone zostały jako średnie ze względu na zorientowane elementy powierzchni. Układ równań sprowadza się do jednego równania, zawierającego szereg z pochodnych naprężeń rosnącego rzędu, uśrednionych jedynie względem objętości oraz pozostały wyraz, będący pochodną naprężenia uśrednionego względem powierzchni. Obcinając szereg dla danej dokładności otrzymuje się równanie równowagi, które okazuje się wystarczające w przypadku, kiedy jedną zmienną kinematyczną jest wektor makro-przemieszczenia. Przedstawiona jest konstrukcja równania typowa dla „gradientowej" lub „nielokalnej" teorii sprężystości. Przeprowadzono obliczenia dla polikryształu przy założeniu równoważności uśrednienia względem objętości i względem liczbiy możliwych realizacji.

Резюме

ОБ НЕКОТОРОЙ ОБЩЕЙ ТЕОРИИ КОМПОЗИТНЫХ МАТЕРИАЛОВ И МИКРО НЕОДНОРОДНЫХ УПРУГИХ СРЕД

Развивается метод осреднения по обьему дифференциальных уравнений равновесия неоднородных упругих сред, состоящих из компонентов, различающихся значениями упругих модулей. Получена цепочка макроуравнений равновесия, в которых фигурируют макротензоры напряжений, двойных напряжений и других напряжений все возрастающего ранга. В общем случае эти тензора несимметричны из-за правила введения их как средних по ориентированным площадкам. Цепочка уравнений сводится к одному уравнению, в которое входит ряд из производных от напряжений повышающихся рангов, осредненных только по обьему, и остаточный член — производная от напряжения среднего по поверхности. Обрыв ряда с заданной точностью приводит к уравнению равновесия, которое оказывается достаточным, если единственной кинематической переменной является вектор макро-мещения. Получаемая конструкция уравнения характерна для „градиентальной" или „нелокальной". теории упругости. Вычисления проведены для поликристалла в предположении об эквивалентности осреднения по об'ему и по множеству реализаций.

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