Journal of Applied Mechanics and Technical Physics, Vol. 37, No. 4, 1996

GENERALIZED SELF-CONSISTENT-FIELD METHOD FOR DETERMINING THE ELASTIC CHARACTERISTICS OF POLYDISPERSE SYSTEMS

E. M. Lubimtseva and E. A. Mityushov

UDC 539.32

Heterogeneous materials, which are microinhomogeneous media in which the dimensions of inhomogeneities are considerably smaller than those in a specimen or an article (see [1, 2]), are finding ever-widening application in engineering (along with isotropic and homogeneous materials). Since the inhomogeneities are small and the their distribution in such a medium is of a statistical character, one can single out so-called representative volumes whose properties are uniform and correspond to the characteristics of the entire material, i.e., the microinhomogeneous medium can be considered microscopically homogeneous and characterized by a set of effective coefficients (electrical conductivity, thermal conductivity, elasticity, etc.).

The effective characteristics of microinhomogenous media are largely determined by the service properties of the material. The possibility of wide variation of the volume portions of various constituents in composite materials enables one to produce materials with a necessary set of service characteristics. There are various methods for calculation of the effective characteristics of heterogeneous materials using data on the properties and structures of phase constituents [3, 4]. All of these are based on various assumptions that facilitate solution of the equations taking into account the complex character of the interaction between the structural elements of these materials and involve primarily calculation of the effective characteristics of two-phase materials [5–7].

A promising method for determining the elastic characteristics of heterogeneous materials is the self-consistent-field method [6]. The essence of this method is that the field of the particles of a multiphase system which are placed in turn in a homogeneous medium with characteristics of a certain reference body is equated to the average field of the particles of the given phase in the heterogeneous system. We extend this method to systems with an arbitrary distribution of the elastic characteristics of structural elements and also consider solution of the problem of the competing effect of dispersed particles on the effective characteristics of microinhomogeneous materials. To this end, we first consider the Eshelby problem [8] of the deformation of an elastic inclusion placed in an infinite homogeneous matrix of a material with different elastic characteristics. Let $\boldsymbol{\varepsilon}^c$ be the restrained strain of inclusion of a larger size of the matrix material with elastic characteristics $\mathbf{c}^m$. We equate the stress in this inclusion under given uniform strain $\tilde{\varepsilon}$ to the strain in a foreign inclusion with properties $\mathbf{c}^f$ with the same uniform strain [7]:

$$\mathbf{c}^f : (\boldsymbol{\varepsilon}^c + \tilde{\varepsilon}) = \mathbf{c}^m : (\boldsymbol{\varepsilon}^c + \tilde{\varepsilon} - \boldsymbol{\varepsilon}^T). \tag{1}$$

Here $\boldsymbol{\varepsilon}^T$ is the strain incompatibility tensor; the division sign denotes the biscalar product of two tensors ($\mathbf{c}^f : \boldsymbol{\varepsilon}^c = c_{ijkl}\varepsilon^c_{kl}\mathbf{e}_i\mathbf{e}_j$); $\mathbf{e}_i$ are unit vectors of the corresponding basis; summation from 1 to 3 is performed over repetitive indices.

By virtue of the Eshelby's solution, the restrained strain tensor is related to the incompatibility tensor as follows:

$$\boldsymbol{\varepsilon}^c = \mathbf{N} : \boldsymbol{\varepsilon}^T \qquad \text{or} \qquad \boldsymbol{\varepsilon}^T = \mathbf{W} : \boldsymbol{\varepsilon}^c, \tag{2}$$

Ural'sk Polytechnical Institute, Ekaterinburg 620002. Translated from Prikladnaya Mekhanika i Tekhnicheskaya Fizika, Vol. 37, No. 4, pp. 139–144, July–August, 1996. Original article submitted December 1, 1994; revision submitted May 10, 1995.

0021-8944/96/3704-0577 $15.00

and the components of the Eshelby's tensor $\mathbf{N} = \mathbf{W}^{-1}$ are given by

$$N_{ijkl} = \frac{1}{2}\, c^m_{pqkl} \int\limits_{v_0} \left[\frac{\partial^2 G_{pi}(\mathbf{x}, \mathbf{x}')}{\partial x_i \partial x_q} + \frac{\partial^2 G_{pj}(\mathbf{x}, \mathbf{x}')}{\partial x_j \partial x_q} \right] dv,$$

where $G_{pi}(\mathbf{x}, \mathbf{x}')$ is the Green tensor for an infinite homogeneous medium; and v_0 is the region occupied by the inclusion.

Taking into account that the strain in the foreign inclusion is the sum of the restrained and uniform strains ($\varepsilon^f = \varepsilon^c + \tilde{\varepsilon}$), from equality (1) with allowance for (2), we have

$$\mathbf{c}^f : \varepsilon^f = \mathbf{c}^m : [\varepsilon^f - \mathbf{W} : (\varepsilon^f - \tilde{\varepsilon})]. \tag{3}$$

Solving matrix Eq. (3), we obtain

$$[(\mathbf{c}^m)^{-1} : \mathbf{c}^f - \mathbf{I}] : \varepsilon^f = \mathbf{W} : (\tilde{\varepsilon} - \varepsilon^f)$$

($\mathbf{I}$ is a unit tensor of rank four). Then,

$$\tilde{\varepsilon} - \varepsilon^f = \mathbf{N} : [(\mathbf{c}^m)^{-1} : \mathbf{c}^f - \mathbf{I}] : \varepsilon^f.$$

As a result, for the strain tensor of the foreign inclusion we find that

$$\varepsilon^f = \{\mathbf{I} + \mathbf{N} : [(\mathbf{c}^m)^{-1} : \mathbf{c}^f - \mathbf{I}]\}^{-1} : \tilde{\varepsilon}. \tag{4}$$

When the matrix and inclusion materials are isotropic, the tensors $(\mathbf{c}^m)^{-1}$, $\mathbf{c}^f$, and $\mathbf{N}$ can be written as [7]

$$(\mathbf{c}^m)^{-1} = \frac{1}{3k^m}\mathbf{V} + \frac{1}{2\mu^m}\mathbf{D}, \quad \mathbf{c}^f = 3K^f\mathbf{V} + 2\mu^f\mathbf{D}, \quad \mathbf{N} = \frac{3K^m}{3K^m + 2\mu^m}\mathbf{V} + \frac{6(K^m + 2\mu^m)}{5(K^m + 4\mu^m)}\mathbf{D},$$

where $K^{m(f)}$ and $\mu^{m(f)}$ are the volume and shear moduli of the matrix and the inclusion; $\mathbf{V}$ and $\mathbf{D}$ are the volume and deviator component of the unit tensor $\mathbf{I}$.

With allowance for this decomposition, it is easy to obtain from equality (4) a formula for the strain of a spherical inclusion placed in an infinite medium and subjected to uniform deformation:

$$\varepsilon^f = \left[\frac{\mathbf{V}}{1 + a(K^f - K^m)} + \frac{\mathbf{D}}{1 + b(\mu^f - \mu^m)} \right] : \tilde{\varepsilon}. \tag{5}$$

Here $a = 3/(3K^m + 4\mu^m)$ and $b = 6(K^m + 2\mu^m)/[5\mu^m(3K^m + 4\mu^m)]$.

We use these formulas to determine the effective characteristics of a polydisperse system whose shear and volume moduli take the values μ_i and K_i, respectively.

Considering a homogeneous reference body with elastic characteristics μ_r and K_r and placing in it by turn single spherical inclusions with elastic characteristics μ_i and K_i, we require that, upon application of an external field $\langle\varepsilon\rangle$ which is equal to the volume-averaged field of the polydisperse system, the field in the inclusion coincides with the average field in the corresponding phase ε_i. Then, according to (5), the average values of the strain tensors of the ith phase can be written as

$$\varepsilon_i = \left[\frac{\mathbf{V}}{1 + a_r(K_i - K_r)} + \frac{\mathbf{D}}{1 + b_c(\mu_i - \mu_r)} \right] : \langle\varepsilon\rangle, \tag{6}$$

where $a_r = 3/(3K_r + 4\mu_r)$ and $b_r = 6(K_r + 2\mu_r)/[5\mu_r(3K_r + 4\mu_r)]$.

Substituting these values into the following expression for the tensor of average stresses in a heterogeneous system:

$$\langle\sigma\rangle = \sum_{i=1}^{n} c_i \sigma_i$$

and taking into account the generalized Hooke's law for macro- and microvolumes of a polydisperse medium

$\langle \boldsymbol{\sigma} \rangle = \mathbf{c}^* : \langle \boldsymbol{\varepsilon} \rangle$, $\boldsymbol{\sigma}_i = \mathbf{c}^{(i)} : \boldsymbol{\varepsilon}_i$ we obtain for the effective characteristics:

$$K^* = \sum_{i=1}^{n} \frac{c_i K_i}{1 + a_r(K_i - K_r)}, \qquad \mu^* = \sum_{i=1}^{n} \frac{c_i \mu_i}{1 + b_r(\mu_i - \mu_r)}. \tag{7}$$

Here c_i is the relative volume portion of the ith phase constituent.

Note that the condition of additivity of the strain tensor average over the volume of the polydisperse system

$$\langle \varepsilon \rangle = \sum_{i=1}^{n} c_i \varepsilon_i$$

and formulas (6) for the average strains over the volumes occupied by the corresponding phase components lead to relations for the characteristics of the reference body:

$$\begin{gathered} \prod_{i=1}^{n} (a_r^{-1} - K_r + K_i) = \sum_{j=1}^{n} c_j \frac{\prod\limits_{i=1}^{n} (a_r^{-1} - K_r + K_i)}{a_r^{-1} - K_r + K_j}, \\ \prod_{i=1}^{n} (b_r^{-1} - \mu_r + \mu_i) = \sum_{j=1}^{n} c_j \frac{\prod\limits_{i=1}^{n} (b_r^{-1} - \mu_r + \mu_i)}{b_r^{-1} - \mu_r + \mu_j}. \end{gathered} \tag{8}$$

After identical transformations in equalities (7) and taking into account formulas (8), we find

$$K^* = \left[\sum_{i=1}^{n} \frac{c_i}{a_r^{-1} - K_r + K_i} \right]^{-1} - (a_r^{-1} - K_r), \quad \mu^* = \left[\sum_{i=1}^{n} \frac{c_i}{b_r^{-1} - \mu_r + \mu_i} \right]^{-1} - (b_r^{-1} - \mu_r). \tag{9}$$

For the microinhomogeneous media satisfying the ergodicity condition [7], averaging over volume in equalities (9) can be replaced by statistical averaging over an ensemble of the corresponding bodies. Then the volume and shear moduli of the polydisperse system are written as

$$K^* = \left\langle \left(\frac{4}{3} \mu_r + K \right)^{-1} \right\rangle^{-1} - \frac{4}{3} \mu_r, \quad \mu^* = \left\langle \left(\frac{\mu_r(9K_r + 8\mu_r)}{6(K_r + 2\mu_r)} + \mu \right)^{-1} \right\rangle^{-1} - \frac{\mu_r(9K_r + 8\mu_r)}{6(K_r + 2\mu_r)}, \tag{10}$$

where K and μ are random moduli that takes the values K_i and μ_i with probability c_i.

The proposed method for calculation of the effective elastic characteristics of polydisperse and multiphase systems can be used for materials with discrete and continuous distribution of the properties of the structural elements. Formulas (9) and (10) contain the variable parameters μ_r and K_r which allows one to describe the effective characteristics of microinhomogeneous materials of arbitrary type. Thus setting in equalities (9) $n = 2$, $\mu_r = \mu_1 = \mu^m$, $K_r = K_1 = K^m$ and also $\mu_2 = \mu^f$ and $K_2 = K^f$ we determine the effective characteristics of a two-phase matrix system. If we let in these equalities $\mu_r = \mu^*$ and $K_r = K^*$, formulas (9) become formulas for the effective characteristics of a statistical system of equivalent phases, which correspond to the well-known method of a self-consistent field.

As an illustration Fig. 1 gives the calculated and experimental values of Young's modulus for WC–Co composite produced by a powder technology $[E^* = 9K^*\mu^*/(3K^* + \mu^*)]$. In this case, the following elastic constants were used: $K_1 = 1.87 \cdot 10^{11}$ Pa and $\mu_1 = 0.81 \cdot 10^{11}$ Pa for cobalt and $K_2 = 3.92 \cdot 10^{11}$ Pa and $\mu_2 = 3.04 \cdot 10^{11}$ Pa for tungsten carbide. As can be seen from the figure, the experimental values of Young's modulus [9, 10], shown by points, correspond to the solution obtained by the consistent model. At low and high concentrations, at which cobalt is a matrix and dispersed phase, these values are close to the corresponding solutions of matrix systems.

Relations (10) can be used to solve problems of the mutual compensating effect of soft and rigid inclusions distributed randomly in a uniform matrix. Modeling such a material by a three-phase matrix system and assuming in equalities (7) that c_1 and c_2 are the volume concentrations of the soft and rigid inclusions, and $\mu_3 = \mu^m = \mu_r$ and $K_3 = K^m = K_r$, we equate the effective elastic characteristics to those of

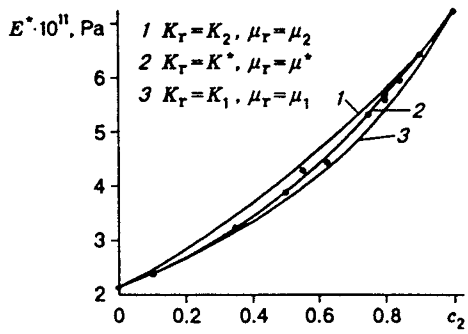

Fig. 1

the matrix material. As a result, we find that the compensating effect of dispersed particles on the volume modulus is ensured if their volume concentrations are in the ratio

$$\frac{c_2}{c_1} = -\frac{(K_1 - K^m)(3K_2 + 4\mu^m)}{(K_2 - K^m)(3K_1 + 4\mu^m)}. \tag{11}$$

If compensation of the pores is performed by the addition of absolutely rigid particles, passing to the limits $K_1 \to 0$ and $K_2 \to \infty$ in equality (11) we have

$$\frac{c_2}{c_1} = \frac{3}{4}\frac{K^m}{\mu^m}. \tag{12}$$

Then, by virtue of relations (7), the effective shear modulus is found from the equality

$$\mu^* = \mu^m(1 - c_1 - c_2) + c_2\left[\frac{5\mu^m(3K^m + 4\mu^m)}{6(K^m + 2\mu^m)}\right].$$

The dispersed particles in a three-phase matrix system have a compensating effect on the shear modulus provided that

$$\frac{c_2}{c_1} = -\frac{(\mu^m - \mu_1)}{(\mu^m - \mu_2)}\frac{[\mu^m(9K^m + 8\mu^m) + 6\mu_2(K^m + 2\mu^m)]}{[\mu^m(9K^m + 8\mu^m) + 6\mu_1(K^m + 2\mu^m)]}.$$

For $\mu_1 \to 0$ and $\mu_2 \to \infty$ we obtain

$$c_2/c_1 = 6(K^m + 2\mu^m)/(9K^m + 8\mu^m). \tag{13}$$

In this case, for the effective modulus it follows from equality (7) that $K^* = K^m(1 - c_1) + (4/3)\,\mu^m c_2$.

From relations (12) and (13) it follows in particular that the total compensating effect of the rigid inclusions on the elastic characteristics of a porous material is possible only for the following ratio of the elastic properties of the matrix:

$$K^m = (4/3)\,\mu^m, \tag{14}$$

when the relative volume portions of pores and inclusions are similar. Condition (14) corresponds to Poisson's ratio $\nu = 1/3$ which holds for many pure metals.

In particular, this is easily seen for lead and zinc from Table 1, which gives compensating ratios of the volume concentrations of some metals [11]. In addition, Table 1 shows that the concentration ratio that ensures the mutual compensation of the pores and rigid inclusions can vary over a wide range.

The relative changes in the concentration ratios with allowance for the compliance of the dispersed particles is easily estimated from the formula

$$\delta = \left|\frac{(c_2/c_1)^2 - 1}{(c_2/c_1)^2 + nc_2/c_1}\right| \cdot 100\,\%,$$

where $n = K^m/K_2 = K_1/K^m$ or $n = \mu^m/\mu_2 = \mu_1/\mu^m$; and c_2/c_1 is the ratio of the volume concentrations

TABLE 1

Material	μ^m	K^m	c_2/c_1 ($K^m = K^*$)	μ^*	c_2/c_1 ($\mu^m = \mu^*$)	K^*
Diamond	47.22	41.70	0.662	41.704	1.085	48.941
Corundum	19.98	24.00	0.901	19.279	1.021	22.994
Lead	0.70	0.99	1.061	0.715	0.979	0.861
Zinc	4.82	6.88	1.071	4.943	0.986	5.955
Copper	4.40	8.72	1.486	5.202	0.943	6.386
Aluminum	2.55	7.78	2.288	3.833	0.855	4.814
Gold	2.75	6.91	4.612	6.854	0.772	8.853

ignoring the compliance of the dispersed particles. If the elastic characteristics of the dispersed particles differ by an order of magnitude from those of the matrix, the changes in the concentration ratios in compensation of, e.g., the volume moduli of lead and gold are 1 and 30%, respectively.

Thus, using the self-consistent-field method, we obtained formulas for the effective elastic characteristics of polydisperse systems with an arbitrary distribution of the local elastic characteristics and also solved the problem of the competing effect of disperse particles on the elastic characteristics of matrix three-phase systems. Relations are determined for volume concentrations that ensure complete or partial compensation of pores and rigid inclusions in such materials.

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