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VALERIY M. LEVIN
Doctor of Physics and Mathematics, Researcher, Mexican Oil Institute (Mexico City, Mexico)
vlevine@imp.mx
SERGUEY K. KANAUN
Doctor of Physics and Mathematics, Professor, Technological Institute of Higher Education of Monterrey (Mexico City, Mexico)
kanaoun@itesm.mx

APPLICATION OF MAXWELL METHOD IN SOLUTION OF HOMOGENIZATION PROBLEM FOR ANIZOTROPIC ELASTIC MEDIA WITH ELLIPSOIDAL INCLUSIONS

The Maxwell method is applied to calculate effective elastic constants of matrix composite materials containing a random set of anisotropic ellipsoidal inclusions. It is shown that the method allows derivation of analytical equations for effective elastic constants that coincide with the equations obtained by the Mori-Tanaka method and other self-consistent methods known in literature.

Key words: Matrix composites, homogenization problem, self-consistent schemes, Maxwell´s method, effective properties

INTRODUCTION

Intensive development of the theory of heterogeneous media in the past few decades is the result of a constantly increasing role of composite materials in the modern industry. Nowadays, composites successfully compete with traditional homogeneous materials like metals, homopolymers and ceramics. Synthesis of composite materials requires comprehensive knowledge of influence of details of their microstructure on macro properties.

One of the important problems of the mechanics of heterogeneous materials is the so-called homogenization problem. The solution of this problem allows replacing a heterogeneous material by a homogeneous one with the same response to external loading. Because exact solutions of the homogenization problem exist only for composites with very specific microstructures, various methods of approximate solution of this problem were proposed (the review of these methods may be found, e. g., in [8]). One of these methods belongs to J. C. Maxwell [9]. In application to the conductivity problem, the Maxwell method was discussed in details in [7], [8]. The method is based on the hypothesis of non-interacting inclusions. But it is shown in [7] that the equations for the effective conductivity derived by the Maxwell method coincide with the ones obtained by other methods that apparently take into account the inclusion interactions.

In his original work [9], Maxwell calculated effective conductivity of an isotropic medium with an array of isotropic spherical inclusions. In the second part of twentieth century, the Maxwell method was used for the calculation of the effective elastic constants of the composites with spherical particles. For isotropic matrix and inclusion phases, the homogenization problem was solved by this method in [6]. It turned out that the method leads to the equations for the effective elastic constants that coincide with the ones obtained by other self-consistent methods (the effective field method [4] and the Mori-Tanaka method [1], [10]).

In the present work, the Maxwell method is extended to the case of homogeneous anisotropic medium containing a random set of ellipsoidal homogeneous anisotropic inclusions. It is shown that the Maxwell method is the most simple and straightforward way of deriving the equations for the effective elastic constants that coincide with the equations obtained by other self-consistent methods.

THE MAXWELL SCHEME FOR ELASTIC COMPOSITES

The Maxwell approach is based on the solution of the so-called one-particle problem. In the case of elasticity, it is the problem for an isolated inclusions in an infinite homogeneous matrix subjected to a constant external field.

Let an infinite elastic medium with the stiffness tensor C^0 contains an inhomogeneity (inclusion) with the stiffness $C^0 + C^1$ in a finite region V with the characteristic function $V(x)$ ($V(x) = 1$ when $x \in V$, $V(x) = 0$, when $x \notin V$). The system of differential equations for the stress $\sigma_{ij}(x)$ and strain $\varepsilon_{ij}(x)$ tensors in such a medium is:

$$\nabla_j \sigma_{ij}(x) = -q_i(x), \quad \sigma_{ij}(x) = C_{ijkl}(x)\varepsilon_{kl}(x), \quad \varepsilon_{kl}(x) = \nabla_{(i}u_{j)}(x). \quad (2.1)$$

$$C_{ijkl}(x) = C^0_{ijkl} + C^1_{ijkl}V(x)$$

Here $u_i(x)$ is the displacement vector, the parenthesis in indices mean symmetrization. This problem may also be formulated in term of an integral equation for the strain field in the medium with the inclusion [5]

$$\varepsilon_{ij}(x) + \int_V K_{ijkl}(x-x')C^1_{klmn}\varepsilon_{mn}(x')dx' = \varepsilon^0_{ij}(x). \quad (2.2)$$

Here $\varepsilon^0_{ij}(x)$ is the external strain field applied to the medium,

$$C^1_{ijkl} = C_{ijkl} - C^0_{ijkl}, \quad K_{ijkl}(x) = -\left[\nabla_j \nabla_l G_{ik}(x)\right]_{(ij)(kl)}, \quad (2.3)$$

$G_{ik}(x)$ is the Green's function of the operator $\nabla_j C^0_{ijkl} \nabla_l$ for the unbounded elastic medium. This function is a vanishing at infinity solution of the equation

$$\nabla_j C^0_{ijkl} \nabla_l G_{km}(x) = -\delta_{im}\delta(x), \quad (2.4)$$

where $\delta(x)$ is Dirac's delta-function.

Let the region V be ellipsoid with the semi-axes a_1, a_2, a_3. If the external field ε^0_{ij} is constant, then, according to Eshelby's theorem [3], the strain field ε^+_{ij} inside V is also constant and determined by the equation

$$\varepsilon^+_{ij} = \Lambda^\varepsilon_{ijkl}\varepsilon^0_{kl}, \quad \Lambda^\varepsilon_{ijkl} = \left(I_{ijkl} + A_{ijmn}(a)C^1_{mnkl}\right)^{-1}. \quad (2.5)$$

Here $I_{ijkl} = \delta_{i(k}\delta_{l)j}$ is the unit rank four tensor, $A_{ijkl}(a)$ is the constant tensor that is presented as integral over the unit sphere Ω in the 3D-space

$$A_{ijkl}(a) = \frac{1}{4\pi}\int_\Omega K^*_{ijkl}(a^{-1}k)d\Omega, \quad K^*_{ijkl}(k) = \left[k_j k_l G^*_{ik}(k)\right]_{(ij)(kl)}. (2.6)$$

In these equations, $K^*_{ijkl}(k)$ is the Fourier transform of the function $K_{ijkl}(x)$ in equation (2.3), k is the Fourier transform parameter, and $a = (a_{ij})$ is a linear transformation that converts an ellipsoidal domain V into a unit sphere. For an isotropic medium, the function $K^*_{ijkl}(k)$ has the form

$$K^*_{ijkl}(k) = \frac{1}{\mu_0}\left[m_{(i}\delta_{j)(k}m_{l)} - \kappa_0 m_i m_j m_k m_l\right], \quad m_i = \frac{k_i}{|k|}, \quad \kappa_0 = \frac{\lambda_0 + \mu_0}{\lambda_0 + 2\mu_0}, (2.7)$$

Where λ_0 and μ_0 are the Lame constants of the medium. The tensor $A_{ijkl}(a)$ in equations (2.5) has the symmetry of ellipsoid (orthorhombic symmetry) and is defined by 9 essential components. Explicit expressions for $A_{ijkl}(a)$ in the case of an arbitrary ellipsoid and its limit forms (oblate and prolate ellipsoids) for some special symmetries of the tensor C^0_{ijkl} can be found in [5].

Note that the integral equation similar to (2.2) can be derived for the stress tensor $\sigma_{ij}(x)$ in a homogeneous medium with an isolated inclusion. Multiplying the both sides of equation (2.2) by the tensor C^0_{ijkl} and taking into account the equivalences

$$\varepsilon_{ij} = B_{ijkl}(x)\sigma_{kl}(x), \quad B_{ijkl}(x) = \left(C_{ijkl}(x)\right)^{-1}, \quad (2.8)$$

we obtain

$$C^0_{ijkl}B_{klmn}\sigma_{mn}(x) + \int_V C^0_{ijkl}K_{klmn}(x-x')C^1_{mnpq}B_{pqrs}\sigma_{rs}(x')dx' = C^0_{ijkl}\varepsilon^0_{kl}(x). \quad (2.9)$$

For the following obvious relations

$$\begin{aligned} &C^0_{ijkl}B_{klmn} = C^0_{ijkl}\left(B^0_{klmn} + B^1_{klmn}\right) = I_{ijmn} + C^0_{ijkl}B^1_{klmn}, \\ &C^0_{ijkl}B_{klmn} = \left(C_{ijkl} - C^0_{ijkl}\right)B_{klmn} = I_{ijmn} - C^0_{ijkl}B_{klmn} = -C^0_{ijkl}B^1_{klmn}, \\ &B^1_{ijkl} = B_{ijkl} - B^0_{ijkl}, \quad B^0_{ijkl} = \left(C^0_{ijkl}\right)^{-1}, \end{aligned} \quad (2.10)$$

we finally yield the equation for the tensor $\sigma_{ij}(x)$ in the form

$$\begin{aligned} &\sigma_{ij}(x) + \int_V S_{ijkl}(x-x')B^1_{klmn}\sigma_{mn}(x')dx' = \sigma^0_{ij}(x), \\ &S_{ijkl}(x) = C^0_{ijmn}K_{mnrs}(x)C^0_{rskl} - C^0_{ijkl}\delta(x), \quad \sigma^0_{ij}(x) = C^0_{ijkl}\varepsilon^0_{kl}(x). \end{aligned} \quad (2.11)$$

If the external field σ^0_{ij} is constant and the region V is ellipsoidal, the stress field σ^+_{ij} inside the inclusion is also constant and defined by the expressions

$$\begin{aligned} &\sigma^+_{ij} = \Lambda^\sigma_{ijkl}\sigma^0_{kl}, \quad \Lambda^\sigma_{ijkl} = \left(I_{ijkl} + D_{ijmn}(a)B^1_{mnkl}\right)^{-1}, \\ &D_{ijkl}(a) = C^0_{ijmn}A_{mnpq}(a)C^0_{pqkl} - C^0_{ijkl}. \end{aligned} \quad (2.12)$$

Let us apply now the Maxwell scheme for the calculation of the effective elastic stiffness tensor of the composite material with a random set of ellipsoidal inclusions with arbitrary anisotropy of the inclusion and matrix phases.

As in [7], we consider a large sphere V^A of the radius R_A that contains N "small" ellipsoidal inclusions subjected to a constant external field ε^0_{ij} applied to the heterogeneous medium. If this field acts on every inclusion (inclusions don't interact!), the field inside the inclusions is defined by the expressions

$$\varepsilon^{(k)}_{ij} = \Lambda^\varepsilon_{ijkl}(a_k)\varepsilon^0_{kl}, \quad \Lambda^\varepsilon_{ijkl}(a_k) = \left(I_{ijkl} + A_{ijmn}(a_k)C^1_{mnkl}\right)^{-1}, (2.13)$$

where the tensor $A_{ijkl}(a_k)$ (k = 1, 2, ..., N) is given in equation (2.6) and the linear transformation a_k depends on the shape and orientation of the k-th ellipsoidal inclusion.

The strain field ε^A_{ij} inside the homogeneous sphere V^A with the effective stiffness tensor C^*_{ijkl} of the composite is

$$\varepsilon^A_{ij} = \Lambda^*_{ijkl}\varepsilon^0_{kl}, \quad \Lambda^*_{ijkl} = \left(I_{ijkl} + A_{ijmn}C^{1*}_{mnkl}\right)^{-1}, \quad C^{1*}_{mnkl} = C^*_{mnkl} - C^0_{mnkl}, (2.14)$$

where A_{ijkl} is defined by the same formula (2.6), in which transformation a_{ij} is a unit tensor ($a_{ij}=\delta_{ij}$).

Far from the center of the large sphere, the disturbances of the strain field induced by N small inclusions and by the homogeneous large sphere are

$$\begin{aligned} &\varepsilon'_{ij}(x) = \frac{1}{4\pi\mu_0 R^3_A}F_{ijkl}(n^A)C^1_{klmn}\sum_{k=1}^N v_k\Lambda^\varepsilon_{mnrs}(a_k)\varepsilon^0_{rs}, \\ &\varepsilon''_{ij}(x) = \frac{1}{4\pi\mu_0 R^3_A}F_{ijkl}(n^A)C^{1*}_{klmn}\Lambda^*_{mnrs}\varepsilon^0_{rs}, \end{aligned} \quad (2.15)$$

where $F_{ijkl}(n^A)$ is a tensor function on a unit sphere (its explicit expression is insignificant), v_k is a volume of the k-th inclusion. Equating the fields $\varepsilon'_{ij}(x)$ and $\varepsilon''_{ij}(x)$ we obtain the equation

$$C^1_{ijkl}\sum_{k=1}^N \frac{v_k}{V}\Lambda^\varepsilon_{klmn}(a_k) = C^{1*}_{ijkl}\Lambda^*_{klmn}. \quad (2.16)$$

This equation may be rewritten in the form

$$pP_{ijkl} = C^{1*}_{ijmn}\left(I_{mnkl} + A_{mnrs}C^{1*}_{rskl}\right)^{-1}. \quad (2.17)$$

Here p is the volume fraction of the inclusions, and it is denoted

$$P_{ijkl} = \frac{1}{\langle v(a)\rangle}\left\langle C^1_{ijmn}\left(I_{mnkl} + A_{mnrs}(a)C^1_{rskl}\right)^{-1}v(a)\right\rangle, \quad v(a) = \frac{4}{3}\pi a_1 a_2 a_3, (2.18)$$

where averaging is performed over the ensemble distribution of the ellipsoid semi-axes and orientations.

The solution of equation (2.17) with respect to the effective moduli tensor C^*_{ijkl} yields

$$C^*_{ijkl} = C^0_{ijkl} + pP_{ijmn}\left(I_{mnkl} - pA_{mnrs}P_{rskl}\right)^{-1}. \tag{2.19}$$

Note that in the case of multi-phase composites the tensor C^*_{ijkl} is defined by the same formula (2.19), in which the averaging is performed over the ensemble realizations of elastic property tensor C^1_{ijkl} in equation (2.18).

The same method allows deriving expression for the tensor of the effective elastic compliances B^*_{ijkl} of the medium with a random set of ellipsoidal inclusions

$$B^*_{ijkl} = B^0_{ijkl} + pQ_{ijmn}\left(I_{mnkl} - pD_{mnrs}Q_{rskl}\right)^{-1}, \tag{2.20}$$

$$D_{ijkl} = C^0_{ijmn}A_{mnrs}C_{rskl} - C^0_{ijkl},$$
$$Q_{ijkl} = \frac{1}{\langle v(a)\rangle}\left\langle B^1_{ijmn}\left(I_{mnkl} + D_{mnrs}(a)B^1_{rskl}\right)^{-1}v(a)\right\rangle \tag{2.21}$$

and $D_{ijkl}(a)$ is defined in (2.12).

Let the inclusions be spheres of a random radius a isotropically distributed in space. In this case

$$A_{ijkl}(a)=A_{ijkl} \tag{2.22}$$

and equation (2.19) is simplified as follows

$$C^*_{ijkl} = C^0_{ijkl} + pC^1_{ijmn}\left[I_{mnkl} + (1-p)A_{mnrs}C^1_{rskl}\right]^{-1}. \tag{2.23}$$

Suppose that the materials of the inclusions and the matrix are isotropic with the bulk K, K_0 and shear μ, μ_0 elastic moduli. Then, the equation (2.23) leads to the following expressions for the effective elastic moduli K^* and μ^*

$$K^* = K_0 + p(K-K_0)\left[1+(1-p)\frac{3(K-K_0)}{3K_0+4\mu_0}\right]^{-1} \tag{2.24}$$

$$\mu^* = \mu_0 + p(\mu-\mu_0)\left[1+(1-p)\frac{6(K_0+2\mu_0)(\mu-\mu_0)}{5\mu_0(3K_0+4\mu_0)}\right]^{-1}. \tag{2.25}$$

The formulas for the effective compliances $1/K^*$ and $1/\mu^*$ may be obtained from (2.24), (2.25) or from the general formula (2.20).

As was mentioned above, in [6] (this work is often cited in geophysical community) a generalization of the Maxwell scheme was proposed for the calculation of the effective dynamic properties of the matrix composites with isotropic host material and isotropic spherical and spheroidal inclusions. In the long-wave approximation, for the static bulk and shear effective elastic moduli of such materials, the authors obtained the expressions coincided with (2.24) and (2.25). By derivation of these equations a spherical form of the large region V^A containing a set of small spheres was adopted.

Note that in [6], the authors started with the solution of a plane elastic wave scattering problem on small and large spheres. Thus, the reader could suppose that in [6], the solution of the dynamic homogenization problem would be presented at least in the long wave limit. But in result, the authors obtained only static effective bulk and shear moduli defined in equations (2.24) and (2.25), when frequency ω is equal to zero. As a matter of fact, when ω is not zero, the solution of the one-particle problems depends on new undimensional parameters: the ratio of the external wave length and the radius of small and large spheres. But the radius of the large sphere cannot be reasonably defined. Meanwhile in statics, the solution of the one-particle problem does not depend on the sphere radius. Hence, application of the Maxwell scheme for the solution of the dynamic homogenization problem is impossible in principle.

In the considered examples, a spherical form of the large region V^A was accepted. It was mentioned in [2] that taking an ellipsoidal form of the region V^A it is possible to describe the properties of a broader class of the composite materials. Naturally, the choice of the large ellipsoid is not unique. In the other words, possibility to vary the form of the region V^A demonstrates ambiguity of the Maxwell scheme. But for some cases, this choice of a certain form of the large region may be justified.

Let us consider a composite with isotropic ellipsoidal inclusions of the same orientation. In spite of isotropy of the matrix phase the macro properties of the composite will be anisotropic. It seems reasonable to take for the region V^A not a sphere but an ellipsoid which aspect ratio and orientation coincide with those of the inclusions. In this case the Maxwell scheme leads to the following expression for the effective elastic stiffness tensor

$$C^*_{ijkl} = C^0_{ijkl} + pC^1_{ijmn}\left[I_{mnkl} + (1-p)A_{mnrs}(a)C^1_{rskl}\right]^{-1}. \tag{2.26}$$

DISCUSSION AND CONCLUSION

In [4], the self-consistent effective field method was used for the construction of the tensor of the effective elastic moduli of the matrix composites containing a random set of ellipsoidal inclusions. An explicit expression for this tensor was obtained in the following form

$$C^*_{ijkl} = C^0_{ijkl} + pP_{ijmn}\left[I_{mnkl} - pA^{\Phi}_{ijrs}P_{rskl}\right]^{-1}. \tag{3.1}$$

Here A^{Φ}_{ijkl} is a constant tensor that is the following integral

$$A^{\Phi}_{ijkl} = \int K_{ijkl}(x)\Phi(x)dx. \tag{3.2}$$

Where $\Phi(x)$ is a specific correlation function that characterizes geometrical structure of the inclusion array (it determines the region in the vicinity of each inclusion where the probability of the presence of other inclusions is small). If this region has the symmetry of an ellipsoid, the integral (3.2) is calculated explicitly. For a spherical region, when the centers of the inclusions are distributed homogeneously, $A^{\Phi}_{ijkl} = A_{ijkl}$, and expression (2.19) coincides with (3.1) obtained in the frame of the simplest variant of the effective field method that takes into account interactions between the inclusions (the term in the square brackets in (3.1) is responsible for such interactions). For isotropic matrix and isotropic spherical inclusions, formula (3.1) gives the expressions (2.24) and (2.25) of the Maxwell method for the bulk and shear effective elastic moduli.

When all the inclusions are identical ellipsoids and their semi-axes are parallel (have the same orientations), the equation (3.1) takes the form

$$C^*_{ijkl} = C^0_{ijkl} + p\left[\left(C^1_{ijkl}\right)^{-1} + A_{ijkl}(a) - pA^{\Phi}_{ijkl}\right]^{-1}. \quad (3.3)$$

If the symmetry of the function $\Phi(x)$coincides with the symmetry of a typical ellipsoid with the same aspect ratios the expression (3.3) is transformed to

$$C^*_{ijkl} = C^0_{ijkl} + p\left[\left(C^1_{ijkl}\right)^{-1} + (1-p)A_{ijkl}(a)\right]^{-1}. \quad (3.4)$$

This equation again coincides with (2.26) obtained by the Maxwell approach.

Let us address now to the Mori-Tanaka method (MTM). In this method, the field acting on every inclusion in the composite is assumed to be equal to the field averaged over the matrix phase. This field is different from the external field applied to the composite material. Thus, in the MTM, interactions between the inclusions are taken into account. In the adopted notations, the MTM leads to the following expression for the tensor of the effective elastic stiffness of the two-phase composite material with the ellipsoidal inclusions [4]

$$C^*_{ijkl} = C^0_{ijkl} + n_0\langle vP_{ijmn}(x)\rangle\left[I_{mnkl} - n_0\langle vA_{mnrs}(x)P_{rskl}(x)\rangle\right]^{-1}, \quad (3.5)$$

where n_0 is the numerical concentration of the inclusions, v is the volume of the typical inclusions,

$$P_{ijkl}(x) = C^1_{ijmn}\left[I_{mnkl} + A_{mnrs}(x)C^1_{rskl}\right]^{-1}. \quad (3.6)$$

And $A_{ijkl}(x)$ is the constant tensor $A_{ijkl}(a_k)$ when $x \in v_k$ Generally speaking, the equation (3.5) differs from (3.1) and (2.26), but for the composite with the aligned ellipsoidal inclusions formula (3.5) gives the same result as (3.1) and (2.26). For the isotropic phase materials and spherical inclusions, equation (3.5) leads to the expressions (2.24) and (2.25) of the Maxwell method for the bulk and shear effective moduli.

It is necessary to emphasize that the Maxwell method allows deriving equations for the effective elastic moduli of the composite materials in the most economic fashion. The advantage of the effective field method [4] is in the possibility to take into account the peculiarities of spatial distribution of the inclusions by introducing a specific correlation function of a random field of the inclusions. It is equivalent to justification of the choice of the form of the large region in the Maxwell method. But inside the original Maxwell scheme, the form of this region cannot be defined uniquely.

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