Clausius–Mossotti-type approximation for elastic moduli of a three-dimensional, two-component composite

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A new approach to the problem of calculating the bulk elastic moduli of two-component composites with a specified microgeometry is applied to the problem of a 3-D system of circular-cylindrical inclusions with cubic symmetry. Explicit expressions, valid at least up to and including terms of order p^2 (where p is the volume fraction of the inclusions), are obtained for the bulk compressibility and the two shear moduli. The approximation used, which is the leading order in a systematic expansion of the bulk moduli, is related to the Clausius–Mossotti approximation of electrostatics.

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In a recent article, we introduced a new approach to the problem of calculating the effective elastic moduli $C^{(e)}$ of two-component composite materials with a specified microgeometry.[1,2] The approach, which was based on a calculation of the elastostatic resonances of the system, was applied to composites in the form of regular two-dimensional (2-D) arrays of circular-cylindrical inclusions of an isotropic elastic material $C^{(1)}$ embedded in an isotropic host $C^{(2)}$. For the cases of hexagonal and square arrays, we were able to obtain an explicit expansion of the 2-D effective moduli $C^{(e)}$ in powers of the volume fraction p of the $C^{(1)}$ component up to a rather high order [e.g., the 2-D compressibility $\kappa^{(e)}$ was evaluated up to and including $O(p^{11})$ terms for the hexagonal array].

In this letter, we give a preliminary discussion as well as results for an interesting two-component, three-dimensional (3-D) composite geometry. As in I (Ref. 1), we consider an array of identical circular-cylindrical, nonoverlapping inclusions of an isotropic material $C^{(1)}$ in an isotropic host $C^{(2)}$, but now the cylinders are grouped into three families x,y,z according to which of the coordinate axes they lie parallel to. In this array, which has a simple-cubic space symmetry, the axes of the x cylinders intersect the y,z plane at the square array of points $(0,mb,nb)$, where m,n are integers, and b is the "lattice parameter." Similarly, the y-cylinder axes intersect the x,z plane at the points $[nb,0,(m+\frac{1}{2})b]$, and the z-cylinder axes interesect the x,y plane at the points $[(m+\frac{1}{2})b,(n+\frac{1}{2})b,0]$. All the cylinders have the same radius a which must satisfy

$$a < b/4, \tag{1}$$

in order to ensure that the cylinders are nonoverlapping (see Fig. 1).

In this letter we describe our method of calculation and obtain explicit approximate expressions for the bulk compressibility $\kappa^{(e)}$, where

$$\kappa \equiv \tfrac{1}{3} C_{1111} + \tfrac{2}{3} C_{1122}, \tag{2}$$

and for the two bulk shear moduli $\mu^{(e)}, m^{(e)}$, where

$$\mu \equiv C_{1212}, \tag{3}$$

$$m \equiv \tfrac{1}{2}(C_{1111} - C_{1122}), \tag{4}$$

($m = 0$ in an isotropic elastic material).

Our approach begins by considering a family of composites with the same microgeometry but with different values of $C^{(1)}$ and $C^{(2)}$, depending on a parameter s. This is described by writing $C(\mathbf{r})$ in the following form:

$$C(\mathbf{r}) = C^{(2)} + [\theta_1(\mathbf{r})/s](C^{(1)} - C^{(2)}), \tag{5}$$

where θ_1 is a step function that takes the value 1 when $\mathbf{r}$ is inside the $C^{(1)}$ component, and zero otherwise. The actual composite under consideration is retrieved if we set $s = 1$; but, in general, we will consider $C^{(e)}$ to be a function of s. Moreover, we will allow s to take "unphysical values," i.e., either real values that lead to a nonpositive definite $C(\mathbf{r})$, or even complex values.

In I we showed that any elastic coefficient of the com-

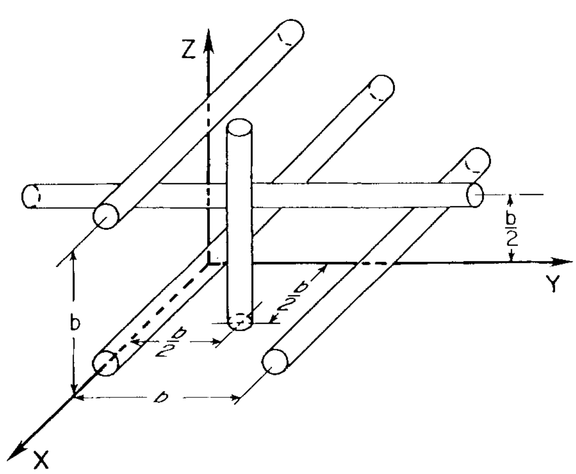

FIG. 1. Schematic drawing of some of the circular-cylindrical inclusions that form the cubic array. Depicted are three x, one y, and one z cylinder. The configuration avoids overlap so long as the radius of the cylinders a and the lattice constant b satisfy $a < \frac{1}{4}b$. The maximum filling fraction of the inclusions, attained when $a = \frac{1}{4}b$, is $\pi/16 \simeq 0.20$.

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posite can be written as a sum of simple poles in the following form:

$$\epsilon^0 C^{(e)}(s)\epsilon^0 - \epsilon^0 C^{(2)}\epsilon^0 = \sum_n \frac{F_n}{s - s_n}, \tag{6}$$

where summation over tensorial indices is implied on the left-hand side, and where the poles s_n and the weights F_n on the right-hand side are all real. Each pole is obtained as an eigenvalue or resonance of the elastostatic problem in the specified microgeometry, while the weight is obtained from a knowledge of the eigenfunction $\epsilon_n(\mathbf{r})$ (i.e., the strain field of the resonance) and of the constant strain field ϵ^0 that describes a uniform boundary condition on the composite:

$$F_n = \frac{1}{V}\left[\int dV_1(\mathbf{r})\epsilon^0 \delta C \epsilon_n(r)\right]^2 \Big/ \left[\int dV \theta_1 \epsilon_n \delta C \epsilon_n\right],$$
$$\delta C \equiv C^{(1)} - C^{(2)}. \tag{7}$$

Confining ourselves at first to the 3-D eigenstates of an isolated cylindrical inclusion, we find that although they comprise an infinite set, only a small number of them have a nonzero weight F_n in the expansion of Eq. (6), no matter what boundary conditions ϵ^0 we choose. For example, if we take $\epsilon^0_{ij} = \delta_{ij}/3$ (in this case $\epsilon^0 C \epsilon^0 = \kappa$), we find that the only contributing states for a z cylinder through the origin are

$$\epsilon_1 = \begin{cases} \begin{pmatrix} 1 & & \\ & 1 & \\ & & 0 \end{pmatrix} & \text{for } \rho < a \\ \begin{pmatrix} -1 & & \\ & +1 & \\ & & 0 \end{pmatrix} \dfrac{a^2}{\rho^2}\cos 2\phi + \begin{pmatrix} 0 & -1 & 0 \\ & 0 & 0 \\ & & 0 \end{pmatrix} \dfrac{a^2}{\rho^2}\sin 2\phi & \text{for } \rho > a \end{cases}, \tag{8}$$

$$s_1 = -\frac{\delta\lambda + \delta\mu}{\lambda_2 + 2\mu_2},$$

and

$$\epsilon_0 = \begin{pmatrix} \delta\lambda & & \\ & \delta\lambda & \\ & & -2(\delta\lambda + \delta\mu) \end{pmatrix} \quad \text{for } \rho \leqslant a, \tag{9}$$
$$s_0 = 0,$$

where we have used cylindrical coordinates (ρ,ϕ,z) around the z axis, and introduced the 3-D Lamé constant $\lambda = \kappa - 2\mu/3$. We note that the state ϵ_1 already appeared as a 2-D eigenstate of the cylinder in I, where it was called "2-D compression dipole." The state ϵ_0 did not appear before—it is a 3-D state which could be called a "longitudinal compression diople." It is a special state for many reasons, not least of which is the fact that it does not interact with any other state.

Consequently, the only interactions between eigenstates of different cylinders that must be considered in leading order are interactions between the states ϵ_1. These can be calculated in the form of overlap integrals between the eigenfunctions, as described in I. For states of parallel cylinders, this was already done in I, so that we only need to add a calculation of the overlap integral for ϵ_1 states of perpendicular cylinders. The two body interactions must now be summed over all the cylinder pairs in the system, and in the case of summation over dipole-dipole interactions special care must be taken in doing this since the sums do not converge absolutely. We have evaluated these sums by using a Clausius–Mossotti-type procedure,[1] in which a sum is broken up into near terms (evaluated exactly for a square-symmetric array of cylindrical shape that is far from the boundaries) and faraway terms (evaluated by replacing the discrete dipole array by a uniform continuous strain polarization, and taking into account the correct boundary conditions). The resulting matrix of interactions between ϵ_1 states, summed over all cylinder pairs, is found to be

$$s_1 \times \begin{pmatrix} 1-p & -p & -p \\ -p & 1-p & -p \\ -p & -p & 1-p \end{pmatrix},$$

where each row or column represents the ϵ_1 states on cylinders along one of the coordinate axes. The eigenvalues and eigenvectors of this matrix are easily found, and we get the following result for the bulk compressibility $\kappa_e = \epsilon^0 C^{(e)} \epsilon^0$:

$$\kappa_e = \kappa_2 + \frac{p\delta\kappa\delta\mu}{3(\delta\lambda + \delta\mu)} + \frac{p\delta\kappa^2/(\delta\lambda + \delta\mu)}{1 + (1-p)(\delta\lambda + \delta\mu)/(\lambda_2 + 2\mu_2)} + O(p^3). \tag{10}$$

This result is valid at least up to and including terms of order $O(p^2)$ (in order to decide whether the next correction is $O(p^3)$ or higher, we have to calculate the next order in the perturbation series—this will be done in a forthcoming article).

In order to calculate analogous expressions for the bulk shear moduli, we must choose an appropriate uniform boundary condition ϵ^0, and then determine the individual-cylinder eigenstates that have a nonzero weight, as well as any states that are degenerate with those. We then use degenerate state perturbation theory, as before. Choosing

$$\epsilon^0_{ij} = \begin{pmatrix} 0 & 1 & 0 \\ & 0 & 0 \\ & & 0 \end{pmatrix}, \tag{11a}$$

we find

$$\mu_e \equiv \epsilon^0 C^{(e)} \epsilon^0 = \mu_2 + p\delta\mu \times \left(\frac{\mu_2 + \frac{8}{3}p(\lambda_2 + 2\mu_2)}{3\mu_2 + \frac{1}{2}(3-p)\delta\mu(\lambda_2 + 3\mu_2)/(\lambda_2 + 2\mu_2) + 0.80p\delta\mu(\lambda_2 + \mu_2)/(\lambda_2 + 2\mu_2)} + \frac{2\mu_2 + \frac{8}{3}p(\lambda_2 + 2\mu_2)}{3\mu_2 + \frac{1}{2}(3-p)\delta\mu} \right) + O(p^3), \tag{11b}$$

while choosing

$$\epsilon_{ij}^0 = \frac{1}{2} \begin{pmatrix} 1 & & \\ & -1 & \\ & & 0 \end{pmatrix}, \tag{12a}$$

we find[3]

$$m_e \equiv \epsilon^0 C^{(e)} \epsilon^0 = \mu_2 + \frac{1}{2}\frac{\delta\mu\delta\kappa}{\delta\lambda + \delta\mu} + \frac{\frac{1}{2}p\delta\mu\{1 + \frac{4}{3}p\delta\mu\mu_2/[2\delta\lambda\mu_2 - \delta\mu(\lambda_2 + \mu_2)]\}}{1 + \frac{1}{6}(3-p)(\delta\mu/\mu_2)(\lambda_2 + 3\mu_2)/(\lambda_2 + 2\mu_2) - 0.27p(\delta\mu/\mu_2)(\lambda_2 + \mu_2)/(\lambda_2 + 2\mu_2) - \frac{1}{3}p[\delta\mu/(\lambda_2 + 2\mu_2)]} + \frac{\frac{1}{6}p[\delta\mu^2/(\delta\lambda + \delta\mu)]\{1 - 4p(\delta\lambda + \delta\mu)\mu_2/[2\delta\lambda\mu_2 - \delta\mu(\lambda_2 + \mu_2)]\}}{1 + (\delta\lambda + \delta\mu)/(\lambda_2 + 2\mu_2)} + O(p^3). \tag{12b}$$

In these cases, we know that the next correction terms are $O(p^3)$. We would also like to point out that the numerical factors 0.80 and 0.27 that appear in Eqs. (11b) and (12b) are not exact; they were evaluated to the indicated accuracy by series summation.

We note that Eq. (10) coincides with one of the Hashin–Shtrikman bounds,[4] but that we have obtained it here as an approximation that is valid to $O(p^2)$ for the cubic array of cylinders. Equations (11b) and (12b) are, however, completely new. Moreover, all three expressions are not only known to be correct up to a specific order in p, but can be extended to higher orders as well by continuing the perturbation expansion for $C^{(e)}$. These extensions, as well as a detailed exposition of the theory leading to our results, will be given elsewhere.

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[1] Y. Kantor and D. J. Bergman, J. Mech. Phys. Solids (to be published); this is referred to as I in the text.
[2] A review of the traditional approaches to this problem, as well as an exhaustive list of references, can be found in J. P. Watt, G. F. Davies, and R. J. O'Connell, Rev. Geophys. Space Phys. **14**, 541 (1976).
[3] This equation ceases to be valid when a quotient inside one of the square brackets becomes large due to a nearly vanishing denominator. This corresponds to an accidental degeneracy of two isolated-cylinder eigenstates, in which case their interaction cannot be treated by perturbation theory as we have done here.
[4] Z. Hashin and S. Shtrikman, J. Mech. Phys. Solids **11**, 127 (1963).