Effective Medium Theory for Elastic Composites

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Abstract

The theoretical foundations of a variant on effective medium theories for elastic constants of composites are discussed. The connection between this approach and the methods of Zeller and Dederichs, Korringa, and Gubernatis and Krumhansl is elucidated. A review of the known relationships between the various effective medium theories and rigorous bounding methods for elastic constants is also provided.

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Introduction

In a series of papers a variant on effective medium theories for elastic composites has been developed by the author. In this paper, I will review the derivation of the effective medium formulas for the elastic constants of composites and also elucidate the relationships between my results and the results of other effective medium theories. These results are also compared to known rigorous bounds on the effective elastic constants.

The general background for theories of elastic composites with special emphasis on earth sciences applications is provided in the review article by Watt, Davies, and O'Connell (1976). Another review of effective medium theories with an emphasis on connections to general applied physics applications is given by Elliott, Krumhansl, and Leath (1974).

Effective Elastic Constants

Mal and Knopoff (1967) derived an integral equation for the scattered displacement field from a single elastic scatterer. Let Ω_i be the volume of the region occupied by a single inclusion. Let the incident field be $\vec{u}^0(\vec{x})\exp(-i\omega t)$ and let $\vec{u}(\vec{x})\exp(-i\omega t)$ and $\vec{v}(\vec{x})\exp(-i\omega t)$ be the total field outside and inside the inclusion volume such that

$$\begin{aligned} \vec{u}(\vec{x}) &= \vec{u}^0(\vec{x}) + \vec{u}^s(\vec{x}) \qquad \text{for} \qquad \vec{x} \notin \Omega_i, \\ \vec{v}(\vec{x}) &= \vec{u}^0(\vec{x}) + \vec{v}^s(\vec{x}) \qquad \text{for} \qquad \vec{x} \in \Omega_i. \end{aligned} \tag{1}$$

$$\epsilon_{pq} = T_{pqrs}\epsilon^0_{rs}, \tag{2}$$

Equation (**??**) must be changed by replacing T_{pqrs} everywhere by

$$U_{pqrs} = \ell_{p\alpha}\ell_{q\beta}\ell_{r\gamma}\ell_{s\delta}T_{\alpha\beta\gamma\delta}, \tag{3}$$

where $\ell_{\alpha\beta}$ are the appropriate direction cosines. For homogeneous, isotropic composites with randomly oriented ellipsoidal inclusions, the general form of the average tensor is (Wu, 1966)

$$\bar{U}_{pqrs} = \frac{1}{3}(P-Q)\delta_{pq}\delta_{rs} + \frac{1}{2}Q(\delta_{pr}\delta_{qs} + \delta_{ps}\delta_{qr}), \tag{4}$$

where

$$P = \frac{1}{3}T_{ppqq} \qquad \text{and} \qquad Q = \frac{1}{5}\left(T_{pqpq} - T_{ppqq}\right). \tag{5}$$

Finally, suppose N inclusions are contained in a small volume of radius a centered at $\vec{\xi}_0$. Assume that the effects of multile scattering may be neglected at sufficiently low frequencies (long wavelengths) to the lowest order. Then,

To apply this thought experiment to the analytical problem of estimating elastic constants, consider replacing the true composite sphere with a sphere composed of matrix material identical to the imbedding material and of ellipsoidal inclusions of the same materials as those in the true composite, and also in the same proportions. Then, if multiple scattering effects are neglected, the theoretical expression which determines the elastic constants is

$$\langle u_\ell^s(\vec{x})\rangle^* = 0, \tag{6}$$

where the left hand side is given by Equation (**??**) with matrix-type $m = *$. Equation (6) states simply that the net scattering in the self-consistently determined medium vanishes to lowest order.

If the volume fraction of the i-th component is defined by $f_i = \Omega_i / \sum_{j=1}^N \Omega_j$, then Equation (6) implies the following formulas:

$$\sum_{i=1}^N f_i(\rho_i - \rho^*) = 0, \tag{7}$$

$$\sum_{i=1}^N f_i(K_i - K^*)P^{*i} = 0, \tag{8}$$

and

$$\sum_{i=1}^N f_i(\mu_i - \mu^*)Q^{*i} = 0. \tag{9}$$

Equation (7) states that the effective density ρ^* is just the volume average density. Equations (8) and (9) provide implicit formulas for K^* and μ^*. Such implicit formulas are typically solved numerically by iteration (Berryman, 1980b). This step is usually necessary because the factors P^{*i} and Q^{*i} are themselves both typically functions of the unknown quantities K^* and μ^*.

Equations (8) and (9) were obtained independently by Korringa, Brown, Thompson, and Runge (1979) using an entirely different method. In the following sectins, I will compare the results obtained from this effective medium theory to the known rigorous bounds on elastic constants and to the results of other effective medium theories.

Rigorous Bounds on Effective Moduli

In their review, Watt, Davies, and O'Connell (1976) discuss various rigorous bounds on the effective moduli of composites. For example, the well-known Voigt (arthimetic) and Reuss (harmonic) averages are respectively rigorous (Hill, 1952) upper and lower bounds for both K^* and μ^*. Generally tighter bounds have been given by Hashin and Shtrikman (1961, 1962, 1963).

Still tighter bounds have been obtained in principle by Beran and Molyneux (1966) for the bulk modulus and by McCoy (1970) for the shear modulus. However, the resulting formulas depend on three-point spatial correlation functions for the composite and are therefore considerably more difficult to evaluate than the expressions for the Hashin-Shtrikman (1961, 1962, 1963) bounds that depend only on the material constants and volume fractions. Miller (1969a,b) evaluated the bounds of Beran and Molyneux by treating an isotropic homogeneous distribution of statistically independent cells. Silnutzer (1972) use the same approach to simplify the bounds of McCoy (1970) for cell materials. Recently, Milton (1981) has shown that the bounds of Beran and Molyneux (1966) and McCoy (1970) can be simplified somewhat even if the composite is not a cell material. Nevertheless, the bounds which are most easily evaluated are still the Hashin-Shtrikman (1961, 1962, 1963) bounds, the Beran-Molyneux-Miller (BMM) bounds, and the McCoy-Silnutzer (MS) bounds. I will compare these bounds to the estimates obtained from the coherent potential approximation (CPA) effective medium theory.

To aid in our comparisons, it is convenient to introduce the following functions:

$$\Lambda(x) = \left(\sum_{i=1}^{N} \frac{f_i}{K_i + 4x/3}\right)^{-1} - \frac{4}{3}x, \tag{10}$$

$$\Gamma(y) = \left(\sum_{i=1}^{N} \frac{f_i}{\mu_i + y}\right)^{-1} - y, \tag{11}$$

and

$$F(x,z) = \frac{x}{6}\left(\frac{9z+8x}{z+2x}\right). \tag{12}$$

It has been shown previously (Berryman, 1980) that $\Lambda(x)$ and $\Gamma(y)$ are monotonically increaseing functions of their real arguments. Similarly, I find

$$\frac{\partial F}{\partial z} = \frac{5x^2}{3(z+2x)^2} \geq 0 \tag{13}$$

and

$$\frac{\partial F}{\partial x} = \frac{9z^2 + 16xz + 16x^2}{6(z+2x)^2}. \tag{14}$$

When both arguments of $F(x,z)$ are positive, it follows that F is a monotonically increasing function of both arguments.

Now, if I define the minimum and maximum moduli among all the constitutents by

$$\begin{aligned} \mu_+ &= \max(\mu_1,\ldots,\mu_N), & \mu_- &= \min(\mu_1,\ldots,\mu_N), \\ K_+ &= \max(K_1,\ldots,K_N), & K_- &= \min(K_1,\ldots,K_N), \end{aligned} \tag{15}$$

then the Hashin-Strikman bounds are given in general by

$$K_{HS}^{\pm} = \Lambda\left(\mu_{\pm}\right) \tag{16}$$

and

$$\mu_{HS}^{\pm} = \Gamma\left[F\left(\mu_{\pm}, K_{\pm}\right)\right]. \tag{17}$$

[The only combinations considered on the right hand side of (17) are those with both pluses or both minuses – no mixing of the subscripts.]

The Beran-Molyneux-Miller bounds and the McCoy-Silnutzer bounds are known for two-phase composites (*i.e.*, $N = 2$). These bounds can be written in concise form using the notation of Milton (1981). Defining two geometric parameters $\zeta_1 = 1 - \zeta_2$ and $\eta_1 = 1 - \eta_2$, and two related averages (analogous to the volume fraction weighted average $\langle M\rangle = f_1M_1 + f_2M_2$) of any modulus M by $\langle M\rangle_\zeta = \zeta_1M_1 + \zeta_2M_2$, and $\langle M\rangle_\eta = \eta_1M_1 + \eta_2M_2$, then the bounds can be written as:

$$K_{BMM}^{+} = \Lambda\left(\langle\mu\rangle_\zeta\right), \tag{18}$$

$$K_{BMM}^{-} = \Lambda\left(\left\langle\frac{1}{\mu}\right\rangle_\zeta^{-1}\right), \tag{19}$$

$$\mu_{MS}^{+} = \Gamma(\Theta/6), \tag{20}$$

and

$$\mu_{MS}^{-} = \Gamma(\Xi^{-1}/6), \tag{21}$$

where

$$\Theta = \left[10\langle\mu\rangle^2\langle K\rangle_\zeta + 5\langle\mu\rangle\langle 2K+3\mu\rangle\langle\mu\rangle_\zeta + \langle 3K+\mu\rangle^2\langle\mu\rangle_\eta\right] / \langle K+2\mu\rangle^2 \tag{22}$$

and

$$\Xi = \left[10 \langle K \rangle^2 \left\langle \frac{1}{K} \right\rangle_\zeta + 5 \langle \mu \rangle \langle 2K + 3\mu \rangle \left\langle \frac{1}{\mu} \right\rangle_\zeta + \langle 3K + \mu \rangle^2 \left\langle \frac{1}{\mu} \right\rangle_\eta \right] / \langle 9K + 8\mu \rangle^2 . \quad (23)$$

For symmetric cell materials, it is known that $\zeta_1 = \eta_1 = f_1$ for spherical cells, $\zeta_1 = \eta_1 = f_2$ for disks, and $\zeta_1 = (3f_1 + f_2)/4$, while $\eta_1 = (5f_1 + f_2)/6$ for needles.

It is particularly simple to compare these bounds with the results of effective medium theory when the inclusions are assumed to be spherical in shape. Then, the estimates of the moduli are given by

$$K^* = \Lambda(\mu^*) \quad (24)$$

and

$$\mu^* = \Gamma \left[F \left(\mu^*, K^* \right) \right] . \quad (25)$$

Furthermore, the bounds (18–20) simplify in this case and are given by

$$K^+_{BMM} = \Lambda \left(\langle \mu \rangle \right) , \quad (26)$$

$$K^+_{BMM} = \Lambda \left(\left\langle \frac{1}{\mu} \right\rangle^{-1} \right) , \quad (27)$$

and

$$\mu^+_{MS} = \Gamma \left[F \left(< \mu >, < K > \right) \right] . \quad (28)$$

From the monotonicity properties of the functionns (10–12) and from elementary arguments relating the estimates to the Voigt and Reuss averages, I find for the bulk modulus that

$$\Lambda(\mu_-) \leq \Lambda \left(\left\langle \frac{1}{\mu} \right\rangle^{-1} \right) \leq \Lambda(\mu^*) = K^* \leq \Lambda \left(\langle \mu \rangle \right) \leq \Lambda(\mu_+), \quad (29)$$

or equivalently

$$K^-_{HS} \leq K^-_{BMM} \leq K^* \leq K^+_{BMM} \leq K^+_{HS}. \quad (30)$$

Similarly, by making use of $\Gamma(y)$ from (11), it follows for the shear modulus that

$$\mu^-_{HS} \leq \mu^* \leq \mu^+_{MS} \leq \mu^+_{HS} \quad (31)$$

The arguments just given are valid *only* for the case of spherical inclusions. The author knows of no general argument relating the effective medium results to the rigorous bounds for arbitrary inclusion shapes. However, as we shall see, numerical examples show that the effective medium estimates always lie between the bounds.

Typical results are presented in Figures 1–3. The values of the constituents' moduli were chosen to be: $K_1 = 44.0$ GPa, $\mu_1 = 37.0$ GPa, $K_2 = 14.0$ GPa, and $\mu_2 = 10.0$ GPa. The values of K_2 and μ_2 were chosen as a compromise between two extremes: (a) If K_2 and μ_2 are too close to K_1 and μ_1, then the bounds are too close toether to be distinguishable on the plots. (b) If K_2 and μ_2 are both chosen to be zero, the iteration to the effective medium theory results does not converge for the case of disk-like inclusions (Berryman, 1980), although all the other cases are fine. I find in all cases considered that the effective medium theory result lie between the rigorous bounds.

Other Effective Medium Theories

Various effective medium theories of the elastic properties of composites exist. Of these theories, the scattering theory presented by Zeller and Dederichs (1973), Korringa (1973), and Gubernatis and Krumhansl (1975) has the most in common with the scattering-theory approach presented here. However, this approach appears to be unique among the self-consistent scattering-theory variety, being dynamic while all the others are based on static or quasi-static derivations. This difference becomes a very useful advantage if we want to generalize the approach to finite (nonzero) frequencies.

Another class of effective medium theories studied by Hill (1965), Budiansky (1965), Wu (1966), Walpole (1969), and Boucher (1974) does *not* yield the same results as the present one, except for the case of spherical inclusions. It has been shown elsewhere (Berryman, 1980) how the derivation of the approach of Hill, Budiansky, and others can be symmetrized to yield the symmetrical results that I prefer. Since this class of effective medium theories gives results equivalent to the Hashin-Shtrikman (1961, 1962, 1963) bounds when the the inclusions are disk-shaped, I conclude that these results are preferred – since they do satisfy these bounding constraints while the alternatives do not.

To elucidate the relationship between the static and dynamic derivations of the effective medium results further, I will outline the static derivation next. The integral equations for the static strain field is given by

$$\epsilon_{ij}(\vec{x}) = \epsilon^0_{ij}(\vec{x}) + \int d^3x' G_{ijkl}(\vec{x}, \vec{x}') \Delta c_{klmn}(\vec{x}') \epsilon_{mn}(\vec{x}'), \tag{32}$$

where Green's function is

$$G_{ijkl}(\vec{x},\vec{x}') = \frac{1}{2}\left(g^0_{ik,jl} + g^0_{jk,il}\right), \tag{33}$$

with the Kelvin solution given by

$$g_{pq}(\vec{x},\vec{x}') = \frac{1}{4\pi\mu_m}\left[\frac{\delta_{pq}}{r} - \frac{1}{4(1-\nu_m)}\frac{\partial^2 r}{\partial x_p \partial x_q}\right], \tag{34}$$

where $r = |\vec{x} - \vec{x}'|$ and μ_m and ν_m are respectively the shear modulus and Poisson's ratio of the matrix material. Equation (32) may be rewritten formally as

$$\epsilon = \epsilon^0 + G\Delta c\epsilon, \tag{35}$$

where G is now an integral operator defined by

$$Gf = \int d^3x' G(\vec{x},\vec{x}')f(\vec{x}'). \tag{36}$$

Iterating Equation (35), I obtain the Born series

$$\epsilon = \epsilon^0 + G\Delta c\epsilon^0 + G\Delta c\epsilon^0\Delta c\epsilon^0 + \ldots, \tag{37}$$

and then summing the Born series formally yields

$$\epsilon = (I + Gt)\,\epsilon^0 = (I - G\Delta c)^{-1}\,\epsilon^0, \tag{38}$$

where the t matrix is defined by

$$t = \Delta c\,(I - G\Delta c)^{-1} = \Delta c\,(I + Gt)\,. \tag{39}$$

Taking the ensemble average of Equation (38), I have

$$\langle\epsilon\rangle = (I + G\,\langle t\rangle)\,\epsilon^0 = \left\langle (I - G\Delta c)^{-1}\right\rangle \epsilon^0. \tag{40}$$

For a single scatterer, Equation (38) is equivalent to Equation (2). Therefore, it is worth noting that Wu's tensor T is formally related to the t-matrix by

$$T = I + Gt = (I - G\Delta c)^{-1}\,. \tag{41}$$

Equation (40) is now in a convenient form for use in determining the effective elastic tensor c^* of a composite defined by

$$\langle\sigma\rangle = \langle c\,\epsilon\rangle \equiv c^*\,\langle\epsilon\rangle\,, \tag{42}$$

where the averages in Equation (42) are again ensemble averages. Using the standard definition $c = c^m + \Delta c$, I find that

$$\langle c\,\epsilon \rangle = c^m \langle \epsilon \rangle + \langle \Delta c\,\epsilon \rangle = c^m \langle \epsilon \rangle + \langle t \rangle \epsilon^0. \tag{43}$$

From Equation (43), it follows earily taht the effective elastic tensor is given by

$$c^* = c^m + \langle t \rangle \left(I + G \langle t \rangle \right)^{-1}. \tag{44}$$

The choice of matrix elastic tensor c^m is still completely free since the decomposition $c = c^m + \Delta c$ is not unique. Thus, we are free to choose, for example, $c^m = c^*$, which implies:

$$\langle t \rangle \equiv 0. \tag{45}$$

Equation (45) is an implicit formula determining the effective elastic tensor c^*.

In principle, Equation (45) provides an exact solution for the effective moduli. However, the total t matrix is generally too difficult to calculate. It turns out to be more reasonable and more effective (Velicky, Kirkpatrick, and Ehrenriech, 1968) to rearrange the terms of the total t matrix into a series of terms of repeated scattering from individual scatterers (t_i). Then, by setting the ensemble avrage of the individual t matrices to zero

$$\langle t_i \rangle = \sum_{i=1}^{N} f_i \Delta c_i \left(I - G \Delta c_i \right)^{-1} = 0, \tag{46}$$

and neglecting terms correspoinding to fluctuations in the scattered wave (Velicky, Kirkpatrick, and Ehrenriech, 1968), a tractable approximation for the estimate of the elastic moduli is obtained.

When the constituents and the composite as a whole are all homogeneous and isotropic, the tensor Equation (46) reduces to two coupled equations:

$$\sum_{i=1}^{N} f_i (K_i - K^*) P^{*i} = 0, \tag{47}$$

and

$$\sum_{i=1}^{N} f_i (\mu_i - \mu^*) Q^{*i} = 0, \tag{48}$$

where Equations (4), (5), and (41) were used to simplify Equation (46). Note that Equations (47) and (48) are identifical to Equations (8) and (9), thereby establishing the equivalence of the two approaches in the isotropic case.

Conclusions

I conclude that my effective medium theory satisfies all the known constraints on a viable theory: (a) it gives correct values and slopes for both large and small volume fractions of inclusions. (b) Numerical evidence indicates that the results always satisfy the Hashin-Shtrikman bounds, the Beran-Molyneux-Miller bounds, and the McCoy-Silnutzer bounds. (c) The theory is known (Berryman, 1980b) to reproduce Hill's exact result (Hill, 1963) for composites with uniform shear modulus.

The single-scatterer theory is designed to minimize multiple scattering effects while yielding formulas which are relatively easy to use. Nevertheless, the theory is not exact, and some potentially significant effects have been neglected. The neglected terms become more important for propagation of higher frequency elastic waves. Future efforts should therefore be directed toward extending the effective medium theory to scattering from clusters of inclusions at finite frequency.

Acknowledgments

Work performed under the auspices of the U.S. Department of Energy, at the Lawrence Berkeley National Laboratory under Contract No. DE-AC03-76SF00098. Support was provided specifically by the Geosciences Research Program of the DOE Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences.

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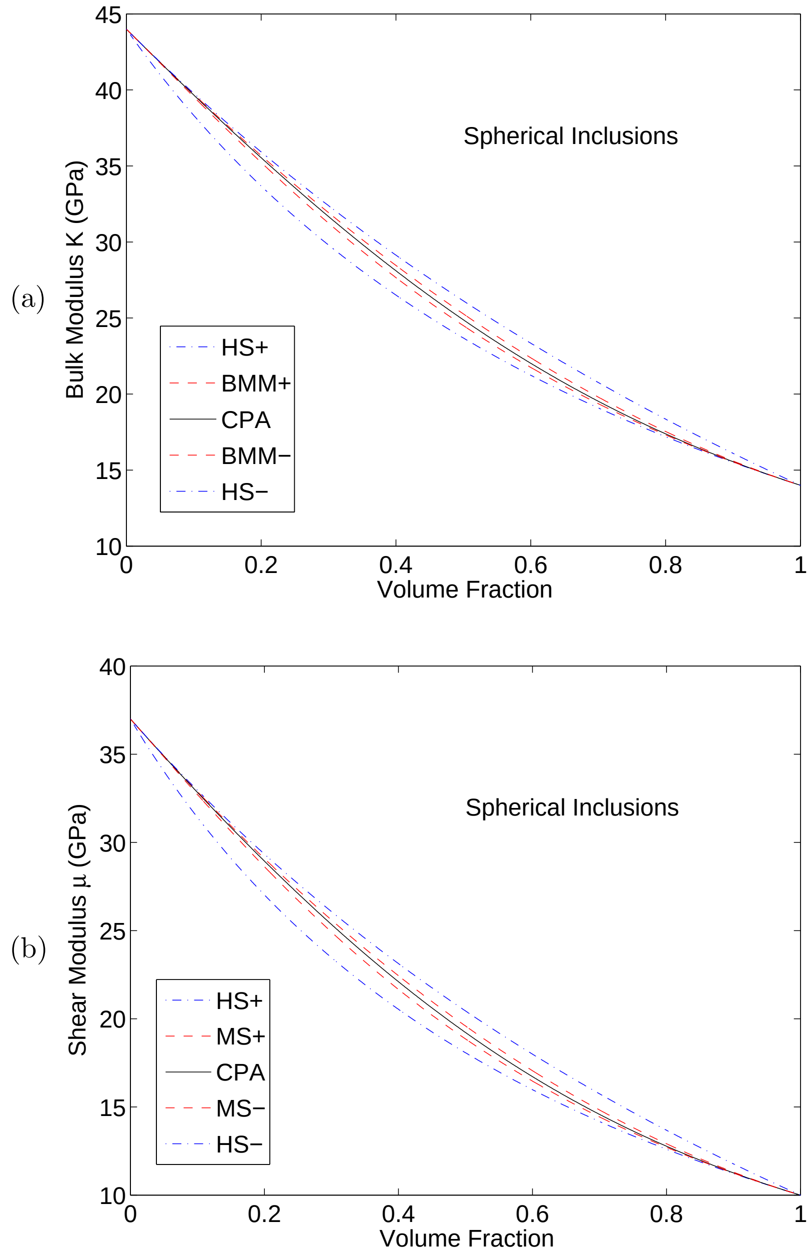

FIG. 1: Estimates of the effective bulk (a) and shear (b) moduli of elastic composites with constituents $K_1 = 44.0$ GPa, $\mu_1 = 37.0$ GPa, $K_2 = 14.0$ GPa, and $\mu_2 = 10.0$ GPa as the volume fraction of type-2 increases. The curves are respectively the CPA (or coherent potential approximation: a self-consistent estimator) — which is the black solid line, the Beran-Molyneux-Miller bounds for the bulk modulus and the McCoy-Silnutzer bounds for the shear modulus — which are the red dashed lines, and the Hashin-Shtrikman bounds — which are the blue dot-dashed lines. Inclusions are treated as having spherical shape.

(a)
(b)

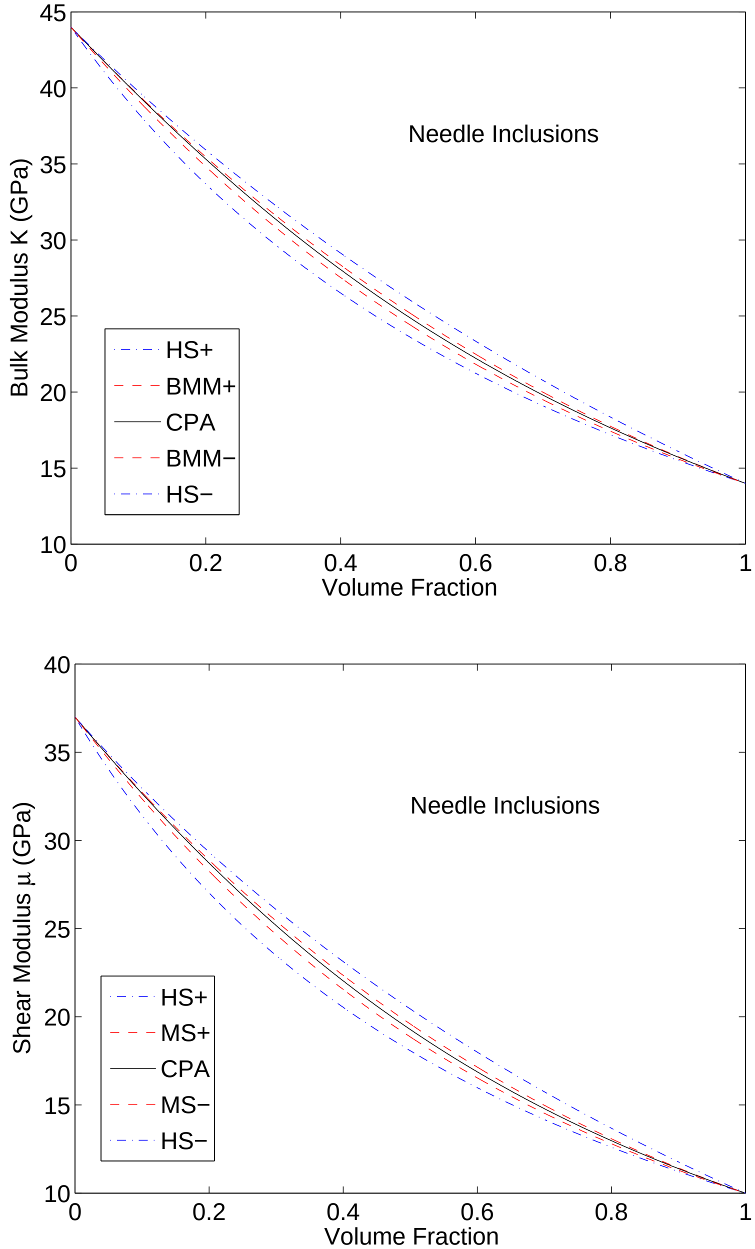

FIG. 2: Estimates of the effective bulk (a) and shear (b) moduli of elastic composites with constituents $K_1 = 44.0$ GPa, $\mu_1 = 37.0$ GPa, $K_2 = 14.0$ GPa, and $\mu_2 = 10.0$ GPa as the volume fraction of type-2 increases. The curves are respectively the CPA (or coherent potential approximation: a self-consistent estimator) — which is the black solid line, the Beran-Molyneux-Miller bounds for the bulk modulus and the McCoy-Silnutzer bounds for the shear modulus — which are the red dashed lines, and the Hashin-Shtrikman bounds — which are the blue dot-dashed lines. Inclusions are treated as having needle-like shape.

(a)

(b)

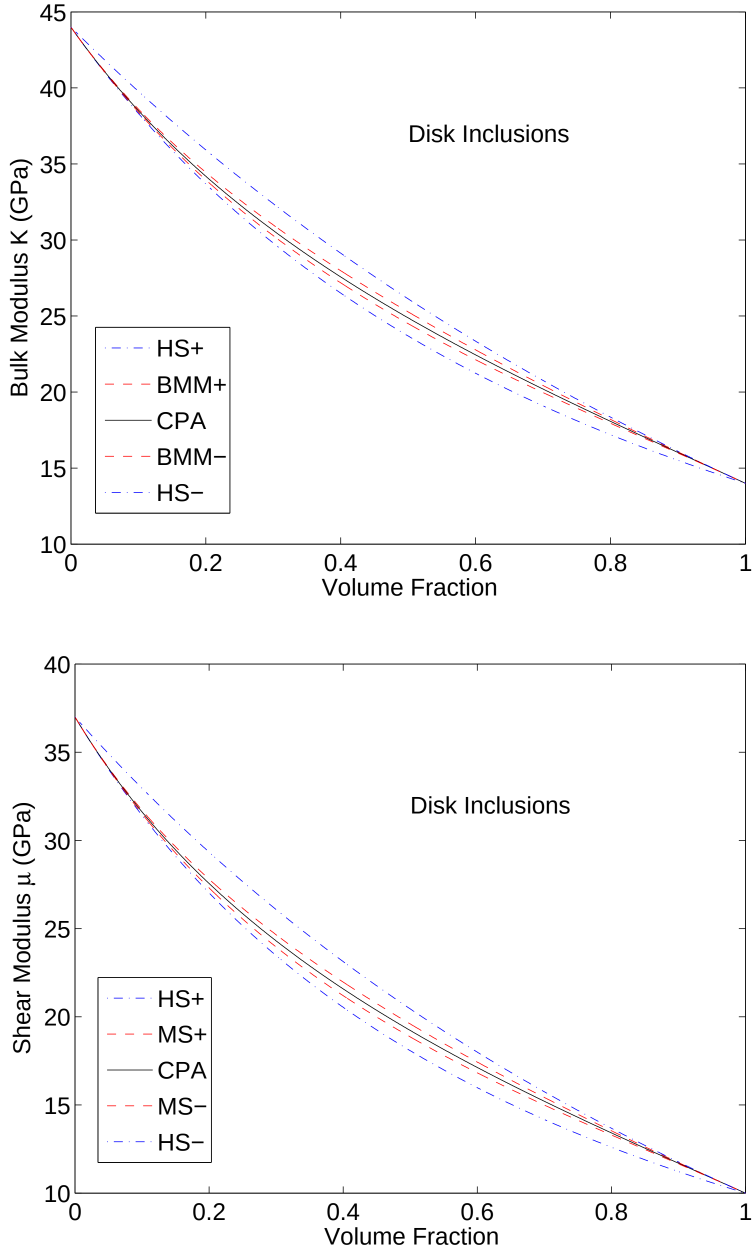

FIG. 3: Estimates of the effective bulk (a) and shear (b) moduli of elastic composites with constituents $K_1 = 44.0$ GPa, $\mu_1 = 37.0$ GPa, $K_2 = 14.0$ GPa, and $\mu_2 = 10.0$ GPa as the volume fraction of type-2 increases. The curves are respectively the CPA (or coherent potential approximation: a self-consistent estimator) — which is the black solid line, the Beran-Molyneux-Miller bounds for the bulk modulus and the McCoy-Silnutzer bounds for the shear modulus — which are the red dashed lines, and the Hashin-Shtrikman bounds — which are the blue dot-dashed lines. Inclusions are treated as having disk-like shape.