Link between the Conductivity and Elastic Moduli of Composite Materials

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We derive relations linking the conductivity σ_* and elastic moduli of any two-dimensional, isotropic composite material. Specifically, upper and lower bounds are derived on the effective bulk modulus κ_* in terms of σ_* and on the effective shear modulus μ_* in terms of σ_*. In some cases the bounds are attainable by certain microgeometries and thus optimal. Knowledge of the conductivity can yield sharp estimates of the elastic moduli (and vice versa) even for infinite phase contrast.

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Can physically different properties of heterogeneous materials be *rigorously* linked to one another? Such cross-property relations become especially useful if one property is more easily measured than another property. Since effective properties of random media reflect certain morphological information about the medium, it is not surprising that one could extract useful information about one property given an accurate determination of another property [1-7]. Here we derive links between the conductivity and elastic moduli of two-phase composites.

Milton [1] showed that, for d-dimensional, isotropic, two-phase media, if the phase bulk moduli κ_i equal the phase conductivities σ_i and the phase Poisson's ratios are positive, then the effective bulk modulus κ_* is bounded from above by the effective conductivity σ_*. This result is trivially extended [5] to the more general situation in which $\kappa_2/\kappa_1 \le \sigma_2/\sigma_1$, namely,

$$\kappa_*/\kappa_1 \le \sigma_*/\sigma_1 . \tag{1}$$

Using this result, Torquato [5] was able to derive an upper bound on the effective shear modulus μ_* in terms of σ_* and the effective Poisson's ratio ν_*; for $d=2$, this expression reads

$$\frac{\mu_*}{\kappa_1} \le \frac{\sigma_*}{\sigma_1}\frac{1-\nu_*}{1+\nu_*} . \tag{2}$$

Our main results are that we have found the sharpest known bounds on the sets of pairs (σ_*,κ_*) and (σ_*,μ_*) that correspond to two-dimensional, isotropic composites of all possible microgeometries at a prescribed or unspecified volume fraction f_i. These bounds enclose certain regions in the σ_*-κ_* and σ_*-μ_* planes (Figs. 1 and 2), portions of which are realizable by certain microgeometries and thus optimal. We first introduce some necessary notation, obtain the cross-property bounds, and then apply them for special cases of interest.

Let $\langle a\rangle = a_1 f_1 + a_2 f_2$ and $\langle\tilde a\rangle = a_2 f_1 + a_1 f_2$, where a is some property, and define the following expressions:

$$\sigma_{1*} = \langle\sigma\rangle - \frac{f_1 f_2(\sigma_1-\sigma_2)^2}{\langle\tilde\sigma\rangle+\sigma_1} ,\qquad \sigma_{2*} = \langle\sigma\rangle - \frac{f_1 f_2(\sigma_1-\sigma_2)^2}{\langle\tilde\sigma\rangle+\sigma_2} , \tag{3}$$

$$\kappa_{1*} = \langle\kappa\rangle - \frac{f_1 f_2(\kappa_1-\kappa_2)^2}{\langle\tilde\kappa\rangle+\mu_1} ,\qquad \kappa_{2*} = \langle\kappa\rangle - \frac{f_1 f_2(\kappa_1-\kappa_2)^2}{\langle\tilde\kappa\rangle+\mu_2} , \tag{4}$$

$$\mu_{1*} = \langle\mu\rangle - \frac{f_1 f_2(\mu_1-\mu_2)^2}{\langle\tilde\mu\rangle+\kappa_1\mu_1/(\kappa_1+2\mu_1)} ,\qquad \mu_{2*} = \langle\mu\rangle - \frac{f_1 f_2(\mu_1-\mu_2)^2}{\langle\tilde\mu\rangle+\kappa_2\mu_2/(\kappa_2+2\mu_2)} , \tag{5}$$

$$\mu_{3*} = \langle\mu\rangle - \frac{f_1 f_2(\mu_1-\mu_2)^2}{\langle\tilde\mu\rangle+\kappa_2\mu_1/(\kappa_2+2\mu_1)} ,\qquad \mu_{4*} = \langle\mu\rangle - \frac{f_1 f_2(\mu_1-\mu_2)^2}{\langle\tilde\mu\rangle+\kappa_1\mu_2/(\kappa_1+2\mu_2)} . \tag{6}$$

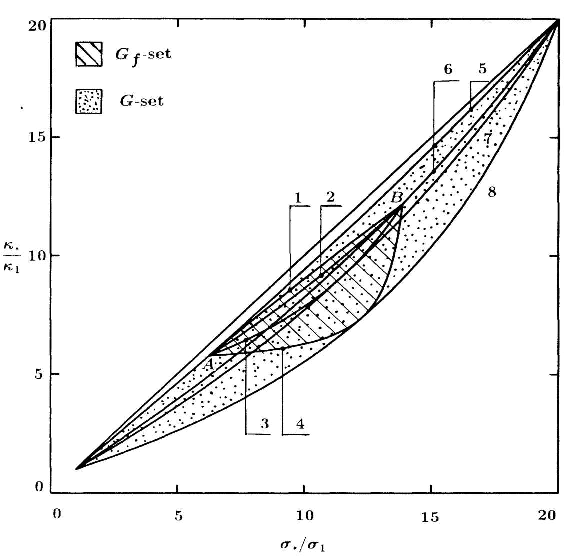

FIG. 1. Cross-property bounds in the σ_*-κ_* plane for a composite with parameters given in text. The internal lens-shaped region with cross-hatching G_f, bounded by curves 1 and 4, represents the bounds for fixed volume fraction $f_1=0.2$. The bigger set G, bounded by curves 5 and 8 and shaded with dots, is the union of the sets G_f over volume fractions.

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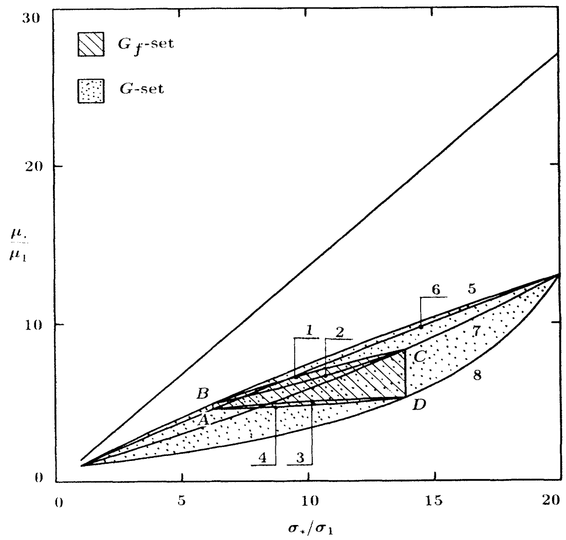

FIG. 2. Cross-property bounds in the σ_*-μ_* plane for a composite with parameters given in text. The internal trapezium with cross-hatching G_f, bounded by curves 1 and 4, represents the bounds for fixed volume fraction $f_1=0.2$. The bigger set G, bounded by curves 5 and 8 and shaded with dots, is the union of the sets G_f over volume fractions.

Formulas (3)-(5) coincide with the Hashin-Shtrikman bounds [8] on σ_*, κ_*, and μ_*, and (6) coincides with the Walpole bounds [9] on μ_*.

Our bounds are given by hyperbolas in σ_*-κ_* and σ_*-μ_* planes. Denote by $\mathrm{hyp}[(x_1,y_1),(x_2,y_2),(x_3,y_3)]$ the segment of the hyperbola that joins the points $(x_1,y_1),(x_2,y_2)$, and when extended passes through the point (x_3,y_3). It may be parametrically described in the x_*-y_* plane as

$$x_*=\langle x\rangle_\gamma-\frac{\gamma(1-\gamma)(x_1-x_2)^2}{\langle\tilde{x}\rangle_\gamma-x_3}\,,\qquad y_*=\langle y\rangle_\gamma-\frac{\gamma(1-\gamma)(y_1-y_2)^2}{\langle\tilde{y}\rangle_\gamma-y_3}\,, \tag{7}$$

where $\langle a\rangle_\gamma=\gamma a_1+(1-\gamma)a_2$, $\langle\tilde{a}\rangle_\gamma=\gamma a_2+(1-\gamma)a_1$, and $\gamma\in[0,1]$. To prove our bounds for a composite for a *fixed* volume fraction, we use the recently formulated *translation method* [10,11]. This technique is very powerful and general [6,7,10-14], and has been applied to obtain bounds on a variety of properties. We first state our results and then sketch the derivations.

Statement 1.—To find bounds on a set of the pairs (σ_*,κ_*) in the σ_*-κ_* plane for *fixed* volume fraction f_i, we need to enscribe in this plane the following four curves:

$$\mathrm{hyp}[(\sigma_{1*},\kappa_{1*}),(\sigma_{2*},\kappa_{2*}),(\sigma_1,\kappa_h)]\,,$$
$$\mathrm{hyp}[(\sigma_{1*},\kappa_{1*}),(\sigma_{2*},\kappa_{2*}),(\sigma_2,\kappa_h)]\,,$$
$$\mathrm{hyp}[(\sigma_{1*},\kappa_{1*}),(\sigma_{2*},\kappa_{2*}),(\sigma_1,\kappa_1)]\,,$$
$$\mathrm{hyp}[(\sigma_{1*},\kappa_{1*}),(\sigma_{2*},\kappa_{2*}),(\sigma_2,\kappa_2)]\,,$$

where $\kappa_h=[f_1/\kappa_1+f_2/\kappa_2]^{-1}$ is the harmonic average. The outermost curves give the desired bounds (see Fig. 1).

Statement 2.—To find bounds on a set of the pairs (σ_*,μ_*) in the σ_*-μ_* plane for fixed f_i, we need to enscribe in this plane segments of four hyperbolas:

$$\mathrm{hyp}[(\sigma_{1*},\mu_{1*}),(\sigma_{2*},\mu_{3*}),(\sigma_1,\mu_1)]\,,$$
$$\mathrm{hyp}[(\sigma_{1*},\mu_{1*}),(\sigma_{2*},\mu_{3*}),(\sigma_2,\mu_2)]\,,$$
$$\mathrm{hyp}[(\sigma_{1*},\mu_{4*}),(\sigma_{2*},\mu_{2*}),(\sigma_1,\mu_1)]\,,$$
$$\mathrm{hyp}[(\sigma_{1*},\mu_{4*}),(\sigma_{2*},\mu_{2*}),(\sigma_2,\mu_2)]\,,$$

and segments of two straight lines, $\sigma_*=\sigma_{1*},\mu_*\in[\mu_{1*},\mu_{3*}]$ and $\sigma_*=\sigma_{2*},\mu_*\in[\mu_{2*},\mu_{4*}]$. The outermost of these curves give the desired bounds (see Fig. 2).

The cross-property bounds for a composite with *arbitrary* f_i can be found as the union of the aforementioned bounds for a fixed f_i. The bounds are again defined by hyperbolas in the conductivity-elastic moduli planes. We shall give these details elsewhere.

We now discuss the basic idea behind the translation method used to obtain statements 1 and 2, while at the same time stressing its applicability to a general class of problems. Consider a two-phase composite with a local constitutive relation $\mathbf{J}(\mathbf{x})=\mathbf{D}(\mathbf{x})\mathbf{E}(\mathbf{x})$ at a point $\mathbf{x}$. Here $\mathbf{J}$ is a generalized "flux," $\mathbf{E}$ is a generalized "gradient," and $\mathbf{D}$ is some local property, generally a tensor, equal to $\mathbf{D}_1$ in phase 1 and $\mathbf{D}_2$ in phase 2. For example, in the *pure* conduction (elasticity) problem, $\mathbf{J}$, $\mathbf{E}$, and $\mathbf{D}$ represent the current (stress), electric field (strain), and conductivity tensor (stiffness tensor), respectively. In the present problem, $\mathbf{D}$ is actually a "supertensor" discussed below. The effective property $\mathbf{D}_*$ is defined by relation $\langle\mathbf{J}\rangle=\mathbf{D}_*\langle\mathbf{E}\rangle$ or equivalently by the averaged energy expression $\langle\mathbf{E}\cdot\mathbf{D}\cdot\mathbf{E}\rangle=\langle\mathbf{E}\rangle\cdot\mathbf{D}_*\cdot\langle\mathbf{E}\rangle$, where angular brackets denote a volume average. Now consider a "comparison" medium with local property tensor $\mathbf{D}'(\mathbf{x})=\mathbf{D}(\mathbf{x})-\mathbf{T}$, where $\mathbf{T}$ is a constant *translation* tensor chosen such that $\mathbf{D}'$ is positive semidefinite and the quadratic form associated with $\mathbf{T}$ is *quasiconvex* [10-13]. Given such a $\mathbf{T}$ one can easily show, using classical energy minimization principles, that the effective properties of the comparison and original media are related by $\mathbf{D}_*-\mathbf{T}\geq\mathbf{D}'_*$, implying

$$(\mathbf{D}_*-\mathbf{T})\geq[f_1(\mathbf{D}_1-\mathbf{T})^{-1}+f_2(\mathbf{D}_2-\mathbf{T})^{-1}]^{-1}\,. \tag{8}$$

Equation (8) is the basic inequality of the translation method. We now show how to obtain the best possible bound on the effective bulk modulus κ_* for fixed volume fraction. For an isotropic d-dimensional composite,

$$(D_*)_{ijkl}=\kappa_*\delta_{ij}\delta_{kl}+\mu_*[\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-(2/d)\delta_{ij}\delta_{kl}]\,, \tag{9}$$

where δ_{ij} is the Kronecker delta function. Let us select an isotropic translation tensor $T_{ijkl}=\kappa_0\delta_{ij}\delta_{kl}+\mu_0[\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-(2/d)\delta_{ij}\delta_{kl}]$. Here κ_0 and μ_0 are free parameters. It follows [13] that $\mathbf{T}$ will be quasiconvex if $\mu_0\geq 0$

and $\kappa_0 \geq -2(d-1)\mu_0/d$. Setting $\mu_0 = \min(\mu_1,\mu_2)$ and $\kappa_0 = -2(d-1)\mu_0/d$ ensures both quasiconvexity and that $\mathbf{D}' \geq 0$, and yields $(\kappa_* - \kappa_0) \geq [f_1(\kappa_1-\kappa_0)^{-1} + f_2(\kappa_2-\kappa_0)^{-1}]^{-1}$, which is the well-known *optimal* Hashin-Shtrikman lower bound on κ_*. (The corresponding upper bound can be similarly derived.) For our problem, we must study several "supertensors" composed of the stiffness tensor $\mathbf{C}$ and the conductivity tensor $\mathbf{\Sigma}$ [15]. Using the procedure outlined above for the supertensors, we obtain statements 1 and 2.

Figures 1 and 2 depict our results for the case $\sigma_2/\sigma_1 = 20$, $\kappa_2/\kappa_1 = 20$, $\nu_1 = 0.15$, $\nu_2 = 0.35$, where $\nu_i = (\kappa_i - \mu_i)/(\kappa_i + \mu_i)$ is the Poisson's ratio of phase i. Figure 1 shows that the conductivity–bulk-modulus bounds for any such composite with fixed ($f_1 = 0.2$) and arbitrary volume fraction are defined by *lens-shaped regions.* The points $A = (\sigma_{1*},\kappa_{1*})$ and $B = (\sigma_{2*},\kappa_{2*})$ and the curves 5 and 6 are *optimal* because they are attainable by Hashin-Shtrikman assemblages of singly coated circles [8,16] as well as isotropic matrix laminate composites [17]. The curves 1 and 2 correspond to assemblages of doubly coated circles [18] or to doubly coated matrix laminate composites [6,7,19]. Presently, we do not know any structures that correspond to curves 3,4 and 7,8 in Fig. 1. The unmarked straight line in Fig. 1 is the upper bound of (1) and is optimal and coincides with our new bound when $\sigma_2/\sigma_1 = \kappa_2/\kappa_1$ and $\mu_1 = \kappa_1$ or $\mu_2 = \kappa_2$. In general the new upper bound is more restrictive than (1).

For fixed f_i the shear modulus bounds are represented by a *curvilinear trapezium* (cf. Fig. 2). The sides AB and CD are given by the Hashin-Shtrikman bounds on σ_*. The other two curvilinear sides (new bounds denoted as $B1C$ and $A4D$) are the hyperbola segments. The two corner points $A = (\sigma_{1*},\mu_{1*})$, and $C = (\sigma_{2*},\mu_{2*})$ correspond to the matrix laminate composites that realize the Hashin-Shtrikman bounds for elasticity and conductivity [19]. The other two points $B = (\sigma_{1*},\mu_{4*})$ and $D = (\sigma_{2*},\mu_{3*})$ correspond to the Walpole shear modulus bounds but their realizability is presently unknown. The hyperbolas that join the points of the original materials and pass through the corner points of the trapezium are those for arbitrary volume fractions. The ones that pass through points A and C are attainable by matrix laminate composites. The unmarked straight line in Fig. 2 corresponds to the upper bound (2) with $\nu_* = 0$, i.e., a weaker form of Eq. (2). The new upper bound is more restrictive than the weak form of (2).

Let us apply our previous results to four particular cases. (i) The case of *equal shear moduli* $\mu_1 = \mu_2 = \mu$ is trivial because both effective elastic moduli do not depend on the microstructure [16] and thus are not connected with the effective conductivity. (ii) In the instance of *equal bulk moduli* $\kappa_1 = \kappa_2 = \kappa$, all composites possess the same bulk modulus $\kappa_* = \kappa$ independent of the structure [16]. In the σ_*-μ_* plane, the straight sides of the trapezium degenerate into points. (iii) Following Ref. [5] let us assume that *one of the phases is superrigid and superconducting,* i.e., $\kappa_2/\kappa_1 = \infty$, $\mu_2/\mu_1 = \infty$, and $\sigma_2/\sigma_1 = \infty$. The boundary hyperbolas degenerate into straight lines and the bounds for fixed f_i simplify as

$$\sigma_* \geq \sigma_{1*}^{\infty}, \quad \kappa_{1*}^{\infty} \leq \kappa_* \leq \kappa_{1*}^{\infty} + \max\left[\frac{\kappa_1+\mu_1}{2\sigma_1}, \frac{2\kappa_2\mu_2}{(\kappa_2+\mu_2)\sigma_2}\right](\sigma_* - \sigma_{1*}^{\infty}), \tag{10}$$

$$\sigma_* \geq \sigma_{1*}^{\infty}, \quad \mu_{1*}^{\infty} \leq \mu_* \leq \mu_{4*}^{\infty} + \max\left[\frac{\kappa_1+2\mu_1}{4\sigma_1}, \frac{\kappa_2\mu_2}{(\kappa_2+\mu_2)\sigma_2}\right](\sigma_* - \sigma_{1*}^{\infty}), \tag{11}$$

where

$$\sigma_{1*}^{\infty} = \frac{1+f_2}{f_1}\sigma_1, \quad \kappa_{1*}^{\infty} = \frac{\kappa_1+f_2\mu_1}{f_1}, \quad \mu_{1*}^{\infty} = \frac{(1+f_2)\kappa_1\mu_1+2\mu_1^2}{f_1(\kappa_1+2\mu_1)}, \quad \mu_{4*}^{\infty} = \frac{f_2\kappa_1+2\mu_1}{2f_1}. \tag{12}$$

The bounds depend on the ratio of the infinite moduli since a very small amount (volume fraction of order κ_2^{-1} or σ_2^{-1}) of a very rigid, conducting material can yield finite effective properties. (iv) Assume that *one of the phases is composed of voids,* i.e., $\kappa_2/\kappa_1 = 0$, $\mu_2/\mu_1 = 0$, $\sigma_2/\sigma_1 = 0$. For fixed volume fraction, the bounds on inverse properties become

$$1/\sigma_* \geq 1/\sigma_{1*}^{0}, \quad 1/\kappa_* \geq 1/\kappa_{1*}^{0} + \min\left[\frac{(\kappa_1+\mu_1)\sigma_1}{2\kappa_1\mu_1}, \frac{2\sigma_2}{\kappa_2+\mu_2}\right](1/\sigma_* - 1/\sigma_{1*}^{0}), \tag{13}$$

$$1/\sigma_* \geq 1/\sigma_{1*}^{0}, \quad 1/\mu_* \geq 1/\mu_{1*}^{0} + \min\left[\frac{(\kappa_1+\mu_1)\sigma_1}{\kappa_1\mu_1}, \frac{4\sigma_2}{\kappa_2+2\mu_2}\right](1/\sigma_* - 1/\sigma_{1*}^{0}), \tag{14}$$

where

$$1/\sigma_{1*}^{0} = \frac{1+f_2}{f_1\sigma_1}, \quad 1/\kappa_{1*}^{0} = \frac{\mu_1+f_2\kappa_1}{f_1\kappa_1\mu_1}, \quad 1/\mu_{1*}^{0} = \frac{(1+f_2)\kappa_1+2f_2\mu_1}{f_1\kappa_1\mu_1}. \tag{15}$$

Torquato [5] used (1) and (2) to show that *critical exponents* for elasticity must always be greater than or equal to the conductivity exponent near the connectivity threshold of a composite with a *perfectly insulating void phase.*

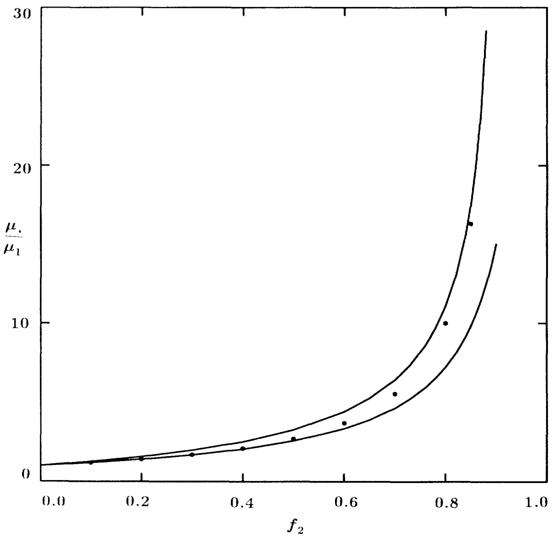

FIG. 3. Comparison of the shear modulus-conductivity bounds (11) with exact shear modulus data [21] (circles) for a superrigid, superconducting hexagonal array of circular inclusions. Curves are the bounds using exact conductivity data [20].

Our bounds cannot improve upon these results.

How sharp are our cross-property estimates given an exact determination of one of the effective properties? To examine this question we employ exact results for the effective conductivity [20] and effective elastic moduli [21] of hexagonal arrays of superconducting, superrigid inclusions (phase 2) in a matrix such that $\kappa_2/\kappa_1=\infty$, $\mu_1/\kappa_1=\mu_2/\kappa_2=0.4$, and $\sigma_2/\sigma_1=\infty$. We assume that phase 1 determines the behavior in (10) and (11). The elastic moduli bounds (10) and (11) are calculated using the σ_* values of Ref. [20]. The agreement between the bounds and the elastic-moduli data [21] is quite good. This is seen in Fig. 3 for the shear modulus. *The agreement between the bounds (10) and bulk modulus data (not shown) is even better than in the case of the shear modulus [e.g., bounds (10) provide virtually exact results up to $f_2=0.6$].* It is noteworthy that *standard variational upper bounds* on the effective properties (such as Hashin-Shtrikman) here diverge to infinity as they do not incorporate information that the superrigid phase is in fact disconnected. In contrast, our cross-property upper bound uses the fact that the infinite-contrast phase is disconnected via conductivity information.

Finally, we emphasize that the translation method is quite general under the aforementioned conditions for the local and effective properties. Thus, for example, the procedure can be applied to study piezoelectric, ferroelectric, thermoelectric, and magnetostrictive properties of composites, as well as the viscosity of suspensions. Neither is the method limited to two-dimensional composites. The basic task involved in being able to extend the present conductivity/elastic moduli results to $d=3$ is to choose the proper translation matrix $\mathbf{T}$.

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