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ON MACROSCOPIC ELASTIC AND CONDUCTIVITY PROPERTIES OF PERFECTLY RANDOM CELL COMPOSITES

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Abstract—Upper and lower bounds on the macroscopic elastic and conductivity properties of perfectly-random heterogeneous media depending on material microgeometry characteristics, particularly those composed of homogeneous cells of spherical (or platelet) form and varying sizes distributed randomly in the material space (including random cell polycrystals), are given.

1. INTRODUCTION

A random (or disordered) composite is composed of material components distributed randomly (disorderly) in space and thus it has isotropic macroscopic properties. In Pham (1994) we considered special random composites called perfectly random (or fully disordered) ones with isotropic components, where besides possible differences in the volume fractions of phases, the microgeometries of the constituent components are statistically indistinguishable [the same materials are called symmetric cell materials by Miller (1969) and infinitely-interchangeable materials by Bruno (1991)]. The upper and lower bounds on the effective properties of perfectly random multicomponent materials have been derived, which—in the case of two-component materials—reduce to Miller's shape-independent ones for symmetric cell materials given in Miller (1969). In his paper, Miller introduced the subclasses of the composites with definite microgeometrical characteristics including spherical (or platelet) cell material, which is composed entirely of homogeneous cells of spherical (platelet) form and varying sizes. He particularly obtained upper and lower bounds for the conductivity and bulk modulus of two-component cell materials. In this work we use the same idea to study the properties of multicomponent cell materials and random cell polycrystals. Based on the approach developed in Le and Pham (1991) and Pham (1993, 1994, 1995) we derive the explicit bounds for the effective properties of such materials. In some cases the bounds are shown to be optimal (i.e., to be attained by some specific models).

2. THE CONDUCTIVITY

From formulae (1) and (8) in Pham (1994) the following bounds on the effective conductivity σ_c of a perfectly random multicomponent material can be deduced:

$$P_\sigma(\sigma_*^u) \geqslant \sigma_c \geqslant P_\sigma(\sigma_*^l), \tag{1}$$

where

$$P_\sigma(\sigma_*) = \left(\sum_\alpha \frac{v_\alpha}{\sigma_\alpha + \sigma_*}\right)^{-1} - \sigma_*, \tag{2}$$

$$\sigma_*^u = 2\sigma_0^u, \quad \sigma_*^l = 2\sigma_0^l, \tag{3}$$

σ_0^u and σ_0^l are the solutions of the following equations (to make $\sigma_{**} = \hat{\sigma}_{**} = 0$):

$$f_1 \cdot \sum_\alpha v_\alpha(\sigma_\alpha - \sigma_0^u)\left(\sum_\beta \frac{v_\beta}{\sigma_\beta + \sigma_*^u} - \frac{1}{\sigma_\alpha + \sigma_*^u}\right)^2 + f_2 \cdot \sum_\alpha v_\alpha(\sigma_\alpha - \sigma_0^u) \cdot \sum_\beta v_\beta \left(\sum_\gamma \frac{v_\gamma}{\sigma_\gamma + \sigma_*^u} - \frac{1}{\sigma_\beta + \sigma_*^u}\right)^2 = 0, \tag{4}$$

$$f_1 \cdot \sum_\alpha v_\alpha \left(\frac{1}{\sigma_\alpha} - \frac{1}{\sigma_0^l}\right)\left(\sum_\beta \frac{v_\beta}{\sigma_\beta + \sigma_*^l} - \frac{1}{\sigma_\alpha + \sigma_*^l}\right)^2 + f_2 \cdot \sum_\alpha v_\alpha \left(\frac{1}{\sigma_\alpha} - \frac{1}{\sigma_0^l}\right) \cdot \sum_\beta v_\beta \left(\sum_\gamma \frac{v_\gamma}{\sigma_\gamma + \sigma_*^l} - \frac{1}{\sigma_\beta + \sigma_*^l}\right)^2 = 0, \tag{5}$$

σ_α and v_α ($\alpha = 1, \ldots, n$) denote the conductivities and volume fractions of phases; the Greek indices under the summation sign run on natural numbers from 1 to n; the geometric parameters f_1 and f_2 are the integrals of harmonic potentials taken over an infinitely small volume part $V_{\alpha m}$ (of a representative element V), which could be called a forming unit of the perfectly random multicomponent material (the significance of $V_{\alpha m}$ is that interchanges of materials between any different parts of $\{V_{\alpha m}\}$ should not affect the macroscopic property of the composite):

$$f_1 = \frac{1}{v_0} \int_{V_{\alpha m}} \varphi_{ij}^{\alpha m} \varphi_{ij}^{\alpha m} \, d\mathbf{x}, \quad f_2 = \frac{1}{v_0^2} \int_{V_{\alpha m}} \varphi_{ij}^{\beta r} \varphi_{ij}^{\beta r} \, d\mathbf{x} \quad (\beta r \not\equiv \alpha m), \tag{6}$$

v_0 is the volume of $V_{\alpha m}$ ($m = 1, \ldots, \mathrm{p}_\alpha$; $v_\alpha = \mathrm{p}_\alpha \cdot v_0$; $\alpha = 1, \ldots, n$); the conventional summation on repeating subscripts is assumed;

$$\varphi_{ij}^{\beta r}(\mathbf{x}) = \varphi_{,ij}^{\beta r} - \frac{1}{v_{\alpha m}} \int_{V_{\alpha m}} \varphi_{,ij}^{\beta r} \, d\mathbf{y} \quad (\mathbf{x} \in V_{\alpha m}),$$

$$\varphi^{\alpha m}(\mathbf{x}) = -\frac{1}{4\pi} \cdot \int_{V_{\alpha m}} |\mathbf{x} - \mathbf{y}|^{-1} \, d\mathbf{y}. \tag{7}$$

It is clear that f_1 and f_2 do not depend on the number of phases forming the composite, the volume fractions and the material properties of phases, but the particular configuration of the infinitely small volume parts $\{V_{\alpha m}\}$. Once the configuration of the parts $\{V_{\alpha m}\}$ is given, one can form a whole subclass of perfectly random composites by assigning different sets of material properties to $\{V_{\alpha m}\}$. All the composites of that subclass share the common values of geometric parameters f_1, f_2. So to determine f_1, f_2 it is sufficient to consider a representative element of that subclass—a two-component material with small volume fraction of one component. In the two-component case, (4) and (5) reduce to:

$$f_1(v_1\sigma_2 + v_2\sigma_1 - \sigma_0^u) + f_2(v_1\sigma_1 + v_2\sigma_2 - \sigma_0^u) = 0, \tag{8}$$

$$f_1(v_1/\sigma_2 + v_2/\sigma_1 - 1/\sigma_0^l) + f_2(v_1/\sigma_1 + v_2/\sigma_2 - 1/\sigma_0^l) = 0. \tag{9}$$

Denote $f_{12} = f_1/f_2$ ($0 \leqslant f_{12} < \infty$ as f_1 and f_2 are positive), the solution σ_0^u and σ_0^l of (8) and (9) can be given as

$$\sigma_0^u = \frac{(f_{12}v_2+v_1)\sigma_1+(f_{12}v_1+v_2)\sigma_2}{f_{12}+1}, \tag{10}$$

$$\sigma_0^l = \frac{(f_{12}v_2+v_1)/\sigma_1+(f_{12}v_1+v_2)/\sigma_2}{f_{12}+1}. \tag{11}$$

Following Miller (1969), we consider a subclass of perfectly random materials called the spherical cell one, which are composed of spherical cells of varying diameters (each cell is made from only one material). The effective property of the two-component spherical cell material with small volume fraction of one component ($v_1 \ll 1$) coincides with the property of the composite with dilute dispersion of spherical inclusions in a continuous matrix (Miller, 1969; Christensen, 1979; Bruno, 1991):

$$\sigma_c = \sigma_2+v_1(\sigma_1-\sigma_2)\frac{3\sigma_2}{\sigma_1+2\sigma_2}. \tag{12}$$

At $v_1 \ll 1$, the bounds (1), (10), (11) become asymptotic and coincide with (12) when $f_{12} = 0$. This suggests but still does not prove that $f_{12} = 0$ is the geometrical characteristic of spherical cell materials. We should show that at other values of f_{12} the bounds (1), (10), (11) would not keep (12) inside. At $v_1 \ll 1$, the upper bound (1), (10) has the value:

$$\sigma^u = \sigma_2+v_1(\sigma_1-\sigma_2)\frac{\sigma_1 2f_{12}+\sigma_2(3+f_{12})}{\sigma_1(1+3f_{12})+2\sigma_2}. \tag{13}$$

The upper bound σ^u in (13) is a monotone function of f_{12} on $[0,\infty)$; at $\sigma_2 > \sigma_1$ it is a decreasing function and attains absolute maximum equal to (12) at $f_{12} = 0$; other $f_{12} > 0$ could not bound (12) from above. Thus $f_{12} = f_1/f_2 = 0$ is really the geometrical characteristic of spherical cell materials. For them (look at (4), (5)) one has the bounds (1) with

$$\sigma_0^u = \sum_\alpha v_\alpha\sigma_\alpha, \quad \sigma_0^l = \left(\sum_\alpha v_\alpha\sigma_\alpha^{-1}\right)^{-1}. \tag{14}$$

Now we consider another subclass—the platelet cell materials composed of the cells of platelet forms. The effective property of the two-component platelet cell material with small volume fraction of one component ($v_1 \ll 1$) is (Miller, 1969; Christensen, 1979; Bruno, 1991):

$$\sigma_c = \sigma_2+v_1(\sigma_1-\sigma_2)\frac{2\sigma_1+\sigma_2}{3\sigma_1}. \tag{15}$$

At $\sigma_1 > \sigma_2$, σ^u in (13) is an increasing function of f_{12} on $[0,\infty)$ and it attains absolute maximum equal to (15) at $f_{12} = \infty$. Other positive f_{12} could not bound (15) from above. Thus $f_{12} = f_1/f_2 = \infty$ is really the geometrical characteristic of platelet cell materials. For them the equations (4), (5) become

$$\sum_\alpha v_\alpha(\sigma_\alpha-\sigma_0^u)\left(\sum_\beta\frac{v_\beta}{\sigma_\beta+\sigma_*^u}-\frac{1}{\sigma_\alpha+\sigma_*^u}\right)^2 = 0, \tag{16}$$

$$\sum_\alpha v_\alpha\left(\frac{1}{\sigma_\alpha}-\frac{1}{\sigma_0^l}\right)\left(\sum_\beta\frac{v_\beta}{\sigma_\beta+\sigma_*^l}-\frac{1}{\sigma_\alpha+\sigma_*^l}\right)^2 = 0. \tag{17}$$

Thus (1), (16), (17) are the bounds on the effective conductivity of platelet cell materials. In the case of two-component platelet cell materials, (16) and (17) are resolved explicitly:

$$\sigma_0^u = v_1\sigma_2+v_2\sigma_1, \quad \sigma_0^l = (v_1/\sigma_2+v_2/\sigma_1)^{-1}. \tag{18}$$

The laminate model constructed in Pham (1994) also serves to prove the optimality of the upper bound (1), (18) on the conductivity of two-component platelet cell materials. The lower bound—as has been shown in that paper—at least is not the optimal one at $v_1 = v_2 = 1/2$. There is a simple correspondence between our f_{12} and Miller's G:

$$G = \frac{1+3f_{12}}{9(1+f_{12})}, \quad f_{12} = \frac{9G-1}{3-9G}, \quad (1/9 \leqslant G \leqslant 1/3, \quad 0 \leqslant f_{12} \leqslant \infty). \tag{19}$$

Our results are more general than those of Miller in that they apply not only to two-component but also to multicomponent materials.

3. THE BULK MODULUS

The general bounds on the elastic moduli k_c, μ_c of isotropic composites have been derived in Pham (1993), which depend on the geometric parameters $A_\alpha^{\beta\gamma}$ and $B_\alpha^{\beta\gamma}$. For perfectly-random composites—because of the geometric restrictions imposed—the parameters $A_\alpha^{\beta\gamma}$ are reduced to depend only on two positive coefficients f_1, f_2 ($\alpha \neq \beta \neq \gamma \neq \alpha$):

$$\begin{aligned} A_\alpha^{\beta\gamma} &= v_\alpha v_\beta v_\gamma(f_1-f_2), \quad A_\alpha^{\alpha\alpha} = v_\alpha(1-v_\alpha)[(1-v_\alpha)f_1+v_\alpha f_2], \\ A_\alpha^{\alpha\beta} &= v_\alpha v_\beta[(v_\alpha-1)f_1-v_\alpha f_2], \quad A_\alpha^{\beta\beta} = v_\alpha v_\beta[(1-v_\beta)f_2+v_\beta f_1] \end{aligned} \tag{20}$$

[see (6) and Pham (1994)]. Similarly, $B_\alpha^{\beta\gamma}$ depend only on two positive coefficients g_1, g_2 ($\alpha \neq \beta \neq \gamma \neq \alpha$):

$$\begin{aligned} B_\alpha^{\beta\gamma} &= v_\alpha v_\beta v_\gamma(g_1-g_2), \quad B_\alpha^{\alpha\alpha} = v_\alpha(1-v_\alpha)[(1-v_\alpha)g_1+v_\alpha g_2], \\ B_\alpha^{\alpha\beta} &= v_\alpha v_\beta[(v_\alpha-1)g_1-v_\alpha g_2], \quad B_\alpha^{\beta\beta} = v_\alpha v_\beta[(1-v_\beta)g_2+v_\beta g_1], \end{aligned} \tag{21}$$

where g_1 and g_2 are defined as f_1, f_2 in (6), (7):

$$g_1 = \frac{1}{v_0}\int_{V_{\alpha m}} \psi_{ijkl}^{\alpha m}\psi_{ijkl}^{\alpha m}\,\mathrm{d}\mathbf{x}, \quad g_2 = \frac{1}{v_0^2}\int_{V_{\alpha m}} \psi_{ijkl}^{\beta r}\psi_{ijkl}^{\beta r}\,\mathrm{d}\mathbf{x} \quad (\beta r \not\equiv \alpha m), \tag{22}$$

$$\begin{aligned} \psi_{ijkl}^{\beta r}(\mathbf{x}) &= \psi_{,ijkl}^{\beta r} - \frac{1}{v_{\alpha m}}\int_{V_{\alpha m}} \psi_{,ijkl}^{\beta r}\,\mathrm{d}\mathbf{y} \quad (\mathbf{x} \in V_{\alpha m}), \\ \psi^{\alpha m}(\mathbf{x}) &= -\frac{1}{8\pi}\cdot\int_{V_{\alpha m}} |\mathbf{x}-\mathbf{y}|\,\mathrm{d}\mathbf{y}. \end{aligned} \tag{23}$$

Similar to the bounds on the conductivity in (1)–(5), the bounds on the effective bulk modulus k_c (and the bounds on the shear modulus considered in the next section) of a perfectly random composite composed of n components with elastic moduli k_α, μ_α can be derived using the general bounds constructed in Pham (1993) and the relations (20), (21):

$$P_k(k_*^u) \geqslant k_c \geqslant P_k(k_*^l), \tag{24}$$

where

$$P_k(k_*) = \left(\sum_\alpha \frac{v_\alpha}{k_\alpha + k_*}\right)^{-1} - k_*, \quad k_*^u = 4/3\mu_0^{ku}, \quad k_*^l = 4/3\mu_0^{kl},$$

μ_0^{ku} and μ_0^{kl} are the solutions of the following equations:

$$f_1 \cdot \sum_\alpha v_\alpha(\mu_\alpha - \mu_0^{ku})\left(\sum_\beta \frac{v_\beta}{k_\beta + k_*^u} - \frac{1}{k_\alpha + k_*^u}\right)^2 + f_2 \cdot \sum_\alpha v_\alpha(\mu_\alpha - \mu_0^{ku}) \cdot \sum_\beta v_\beta \left(\sum_\gamma \frac{v_\gamma}{k_\gamma + k_*^u} - \frac{1}{k_\beta + k_*^u}\right)^2 = 0, \quad (25)$$

$$f_1 \cdot \sum_\alpha v_\alpha \left(\frac{1}{\mu_\alpha} - \frac{1}{\mu_0^{kl}}\right)\left(\sum_\beta \frac{v_\beta}{k_\beta + k_*^l} - \frac{1}{k_\alpha + k_*^l}\right)^2 + f_2 \cdot \sum_\alpha v_\alpha \left(\frac{1}{\mu_\alpha} - \frac{1}{\mu_0^{kl}}\right) \cdot \sum_\beta v_\beta \left(\sum_\gamma \frac{v_\gamma}{k_\gamma + k_*^l} - \frac{1}{k_\beta + k_*^l}\right)^2 = 0. \quad (26)$$

The bounds (24), (25), (26) depend on the same geometric parameters $f_{12} = f_1/f_2$ discussed in the previous section. At $f_{12} = 0$, (25) and (26) are resolved explicitly:

$$\mu_0^{ku} = \sum_\alpha v_\alpha \mu_\alpha, \quad \mu_0^{kl} = \left(\sum_\alpha v_\alpha/\mu_\alpha\right)^{-1}. \quad (27)$$

At $f_{12} = \infty$, (25) and (26) reduce to:

$$\sum_\alpha v_\alpha(\mu_\alpha - \mu_0^{ku})\left(\sum_\beta \frac{v_\beta}{k_\beta + k_*^u} - \frac{1}{k_\alpha + k_*^u}\right)^2 = 0, \quad (28)$$

$$\sum_\alpha v_\alpha \left(\frac{1}{\mu_\alpha} - \frac{1}{\mu_0^{kl}}\right)\left(\sum_\beta \frac{v_\beta}{k_\beta + k_*^l} - \frac{1}{k_\alpha + k_*^l}\right)^2 = 0. \quad (29)$$

(24), (27) bound the bulk modulus of spherical cell materials, while (24), (28), (29) bound that of platelet cell materials. In the case of two-component platelet cell material (28), (29) yield:

$$\mu_0^{ku} = v_1\mu_2 + v_2\mu_1, \quad \mu_0^{kl} = (v_1/\mu_2 + v_2/\mu_1)^{-1}. \quad (30)$$

We construct a laminate composed of a great many thin laminae and assign properties k_1, k_2, μ_1, μ_2 to these laminae randomly with frequencies according to the volume fractions v_1, v_2 of phases. The laminate is transverse-isotropic and its five elastic constants are calculated readily [see e.g. Christensen (1979)]. Now viewing the laminate as the base crystal and following Avallaneda and Milton (1989) one can construct aggregates with maximal and minimal effective bulk moduli. One can verify that the moduli of the aggregates coincide with the bounds (24), (30). Thus the bounds (24), (30) for two-component platelet cell materials are optimal. So the derived bounds for the whole class of two-component perfectly random composites are optimal over half the ranges of parameters. In particular, the upper bound

$$P_k(4/3\mu_0^{ku}) \geqslant k_c, \quad \mu_0^{ku} = \max\{v_1\mu_1 + v_2\mu_2, v_2\mu_1 + v_1\mu_2\} \quad (31)$$

is optimal over $v_1\mu_1 + v_2\mu_2 \leqslant v_2\mu_1 + v_1\mu_2$, and the lower bound

$$P_k(4/3\mu_0^{kl}) \leqslant k_c, \quad \mu_0^{kl} = \max\{(v_1/\mu_1+v_2/\mu_2)^{-1},(v_2/\mu_1+v_1/\mu_2)^{-1}\} \tag{32}$$

is optimal over $v_1/\mu_1+v_2/\mu_2 \geqslant v_2/\mu_1+v_1/\mu_2$.

4. THE SHEAR MODULUS

For the effective shear modulus μ_c of a perfectly random multicomponent material we have the bounds:

$$P_\mu(\mu_*^u) \geqslant \mu_c \geqslant P_\mu(\mu_*^l), \tag{33}$$

where

$$P_\mu(\mu_*) = \left(\sum_\alpha \frac{v_\alpha}{\mu_\alpha+\mu_*}\right)^{-1} - \mu_*,$$

$$\mu_*^u = \mu_0^u \frac{9k_0^u+8\mu_0^u}{6k_0^u+12\mu_0^u}, \quad \mu_*^l = \mu_0^l \frac{9k_0^l+8\mu_0^l}{6k_0^l+12\mu_0^l},$$

k_0^u, k_0^l, μ_0^u and μ_0^l can be taken as the solutions of the following equations:

$$g_1 \cdot \sum_\alpha v_\alpha(\mu_\alpha-\mu_0^u)\left(\sum_\beta \frac{v_\beta}{\mu_\beta+\mu_*^u} - \frac{1}{\mu_\alpha+\mu_*^u}\right)^2 + g_2 \cdot \sum_\alpha v_\alpha(\mu_\alpha-\mu_0^u)\cdot\sum_\beta v_\beta\left(\sum_\gamma \frac{v_\gamma}{\mu_\gamma+\mu_*^u} - \frac{1}{\mu_\beta+\mu_*^u}\right)^2 = 0, \tag{34}$$

$$f_1 \cdot \sum_\alpha v_\alpha\left[3(k_\alpha-k_0^u) + \frac{8(\mu_0^u)^2-9(k_0^u)^2}{2(\mu_0^u)^2}(\mu_\alpha-\mu_0^u)\right]\cdot\left(\sum_\beta \frac{v_\beta}{\mu_\beta+\mu_*^u} - \frac{1}{\mu_\alpha+\mu_*^u}\right)^2 + f_2 \cdot \sum_\alpha v_\alpha\left[3(k_\alpha-k_0^u) + \frac{8(\mu_0^u)^2-9(k_0^u)^2}{2(\mu_0^u)^2}(\mu_\alpha-\mu_0^u)\right]\cdot\sum_\beta v_\beta\left(\sum_\gamma \frac{v_\gamma}{\mu_\gamma+\mu_*^u} - \frac{1}{\mu_\beta+\mu_*^u}\right)^2 = 0, \tag{35}$$

$$g_1 \cdot \sum_\alpha v_\alpha(1/\mu_\alpha-1/\mu_0^l)\left(\sum_\beta \frac{v_\beta}{\mu_\beta+\mu_*^l} - \frac{1}{\mu_\alpha+\mu_*^l}\right)^2 + g_2 \cdot \sum_\alpha v_\alpha(1/\mu_\alpha-1/\mu_0^l)\cdot\sum_\beta v_\beta\left(\sum_\gamma \frac{v_\gamma}{\mu_\gamma+\mu_*^l} - \frac{1}{\mu_\beta+\mu_*^l}\right)^2 = 0, \tag{36}$$

$$f_1 \cdot \sum_\alpha v_\alpha\left[3(1/k_\alpha-1/k_0^l) + \frac{8(\mu_0^l)^2-9(k_0^l)^2}{2(k_0^l)^2}(1/\mu_\alpha-1/\mu_0^l)\right]\cdot\left(\sum_\beta \frac{v_\beta}{\mu_\beta+\mu_*^l} - \frac{1}{\mu_\alpha+\mu_*^l}\right)^2 + f_2 \cdot \sum_\alpha v_\alpha\left[3(1/k_\alpha-1/k_0^l) + \frac{8(\mu_0^l)^2-9(k_0^l)^2}{2(k_0^l)^2}(1/\mu_\alpha-1/\mu_0^l)\right]\cdot\sum_\beta v_\beta\left(\sum_\gamma \frac{v_\gamma}{\mu_\gamma+\mu_*^l} - \frac{1}{\mu_\beta+\mu_*^l}\right)^2 = 0. \tag{37}$$

Once the geometric parameters f_1, f_2, g_1, g_2 for a particular subclass of perfectly random materials are given, one can obtain from (33), (34), (35) the upper bound and from (33), (36), (37) the lower bound for the shear modulus of such materials.

Further we are interested in the subclasses of spherical and platelet cell materials. For two-component materials (34), (35) reduce to:

$$g_1(v_1\mu_2+v_2\mu_1-\mu_0^u)+g_2(v_1\mu_1+v_2\mu_2-\mu_0^u) = 0, \tag{38}$$

$$f_1\left[3(v_1k_2+v_2k_1-k_0^u)+\frac{8(\mu_0^u)^2-9(k_0^u)^2}{2(\mu_0^u)^2}(v_1\mu_2+v_2\mu_1-\mu_0^u)\right]$$
$$+f_2\left[3(v_1k_1+v_2k_2-k_0^u)+\frac{8(\mu_0^u)^2-9(k_0^u)^2}{2(\mu_0^u)^2}(v_1\mu_1+v_2\mu_2-\mu_0^u)\right] = 0. \tag{39}$$

The effective shear modulus of two-component spherical cell material with small volume fraction of one component ($v_1 \ll 1$) asymptotically equals the modulus of the composite with dilute dispersion of spherical inclusions in a continuous matrix:

$$\mu_c = \mu_2+v_1\cdot\frac{\mu_1-\mu_2}{1+(\mu_1-\mu_2)/(\mu_2+\mu_{*2})}, \quad \mu_{*2} = \mu_2\frac{9k_2+8\mu_2}{6k_2+12\mu_2}. \tag{40}$$

For spherical cell materials we have $f_{12} = f_1/f_2 = 0$ and (39) reduces to

$$3(v_1k_1+v_2k_2-k_0^u)+\frac{8(\mu_0^u)^2-9(k_0^u)^2}{2(\mu_0^u)^2}(v_1\mu_1+v_2\mu_2-\mu_0^u) = 0. \tag{41}$$

If $g_{12} = g_1/g_2 = 0$, we have $\mu_0^u = v_1\mu_1+v_2\mu_2$ and $k_0^u = v_1k_1+v_2k_2$ be the results of (38), (41), then the upper bound (33) asymptotically equals μ_c in (40) at $v_1 \ll 1$. This suggests that $g_{12} = g_1/g_2 = 0$ might be the geometric characteristic of spherical cell materials. Keeping in mind that g_{12} is independent of the moduli of phases, we should show that with $g_{12} > 0$ the upper bound (33), (38), (41) does not always bound (40) from above.

Suppose $g_{12} > 0$. Take $k_1 = k_2 = \mu_2 = 1$. At $v_1 \ll 1$, from (38) we have

$$\mu_0^u = \frac{g_{12}\mu_1+1}{g_{12}+1}.$$

Because $g_{12} > 0$, it is possible to choose a positive μ_1 such that

$$\mu_0^u = \frac{g_{12}\mu_1+1}{g_{12}+1} = 1-\varepsilon \quad (\mu_1 = 1-\varepsilon-\varepsilon/g_{12}),$$

$\varepsilon > 0$ is some infinitesimal number.

From (41) we obtain the equation determining positive k_0^u:

$$-\tfrac{3}{2}\varepsilon(1+2\varepsilon)(k_0^u)^2-k_0^u+1+\tfrac{4}{3}\varepsilon = 0 \quad \text{or} \quad k_0^u = 1-\tfrac{1}{6}\varepsilon+o(\varepsilon^2).$$

Subsequently

$$\mu_*^u = \mu_0^u\frac{9k_0^u+8\mu_0^u}{6k_0^u+12\mu_0^u} = \tfrac{17}{18}(1-\tfrac{128}{153}\varepsilon+o(\varepsilon^2)).$$

On the other hand, from (40) we have

$$\mu_{*2} = \mu_2 \frac{9k_2+8\mu_2}{6k_2+12\mu_2} = \tfrac{17}{18} > \mu_*^u.$$

The upper bound (33), (38), (41) at $v_1 \ll 1$ reduces to a form similar to that of μ_c in (40) with the only difference in that μ_*^u takes the place of μ_{*2}. As μ_c in (40) is an increasing function of μ_{*2}, the inequality $\mu_{*2} > \mu_*^u$ implies that μ_c is greater than the upper bound, which is unacceptable. Thus we conclude $g_{12} = g_1/g_2 = 0$ for spherical cell materials.

A similar trick would enable us to confirm that $g_{12} = g_1/g_2 = \infty$ is the geometrical characteristic of platelet cell materials.

Finally from (34)–(37) we obtain the following simple expressions of $\mu_0^u, k_0^u, \mu_0^l, k_0^l$ for the bounds (33) for multicomponent spherical cell materials:

$$\mu_0^u = \sum_\alpha v_\alpha \mu_\alpha, \quad k_0^u = \sum_\alpha v_\alpha k_\alpha,$$

$$\mu_0^l = \left(\sum_\alpha v_\alpha/\mu_\alpha\right)^{-1}, \quad k_0^l = \left(\sum_\alpha v_\alpha/k_\alpha\right)^{-1}.$$

The bounds (33) for platelet cell materials require $\mu_0^u, k_0^u, \mu_0^l, k_0^l$ satisfying the equations:

$$\sum_\alpha v_\alpha(\mu_\alpha - \mu_0^u)\left(\sum_\beta \frac{v_\beta}{\mu_\beta+\mu_*^u} - \frac{1}{\mu_\alpha+\mu_*^u}\right)^2 = 0,$$

$$\sum_\alpha v_\alpha(k_\alpha - k_0^u)\left(\sum_\beta \frac{v_\beta}{\mu_\beta+\mu_*^u} - \frac{1}{\mu_\alpha+\mu_*^u}\right)^2 = 0,$$

$$\sum_\alpha v_\alpha(1/\mu_\alpha - 1/\mu_0^l)\left(\sum_\beta \frac{v_\beta}{\mu_\beta+\mu_*^l} - \frac{1}{\mu_\alpha+\mu_*^l}\right)^2 = 0,$$

$$\sum_\alpha v_\alpha(1/k_\alpha - 1/k_0^l)\left(\sum_\beta \frac{v_\beta}{\mu_\beta+\mu_*^l} - \frac{1}{\mu_\alpha+\mu_*^l}\right)^2 = 0.$$

The bounds (33) on the effective shear modulus of platelet cell materials are also simple in the case of two-component materials, for them:

$$\mu_0^u = v_1\mu_2 + v_2\mu_1, \quad k_0^u = v_1 k_2 + v_2 k_1,$$

$$\mu_0^l = (v_1/\mu_2 + v_2/\mu_1)^{-1}, \quad k_0^l = (v_1/k_2 + v_2/k_1)^{-1}.$$

5. THE RANDOM CELL POLYCRYSTALS

Following Pham (1995) we consider a representative element of a polycrystal that occupies spherical region V of Euclidean three space R^3. The center of the sphere V is also the origin of the Cartesian system of coordinates $\{x_1, x_2, x_3\}$. The representative element consists of n components occupying regions $V_\alpha \subset V$ of equal volumes $v_\alpha = v_0$ (the volume of V is assumed to be the unity), each component is composed of crystals of the same crystal orientation, $\alpha = 1, \ldots, n$. The principal conductivities of the crystals are $\sigma_1^p, \sigma_2^p, \sigma_3^p$. A random polycrystal is supposed to be represented by such n-component configuration when $n \to \infty$, $v_\alpha = v_0 = 1/n \to 0$ and the crystal orientations are distributed randomly in all directions in the space. To determine the effective conductivity σ_c of the random polycrystalline aggregate, the following mathematical hypotheses have been admitted (Pham (1995)), as has been done for those with isotropic components in Pham (1994, 1993):

$$\frac{1}{v_\beta}\int_{V_\beta}\varphi^{\alpha}_{,ij}\,d\mathbf{x} = \tfrac{1}{3}\delta_{\alpha\beta}\delta_{ij},$$

$$\frac{1}{2}\int_{V_\alpha}(\varphi^{\beta}_{ij}\varphi^{\gamma}_{kl}+\varphi^{\gamma}_{ij}\varphi^{\beta}_{kl})\,d\mathbf{x} = A^{\beta\gamma}_{\alpha}\tfrac{1}{10}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\tfrac{2}{3}\delta_{ij}\delta_{kl}),$$

and for all $\alpha \neq \beta \neq \gamma \neq \alpha$:

$$\frac{1}{v_0}\int_{V_\alpha}\varphi^{\alpha}_{ij}\varphi^{\alpha}_{ij}\,d\mathbf{x} = f_1,\quad \frac{1}{v_0^2}\int_{V_\alpha}\varphi^{\beta}_{ij}\varphi^{\beta}_{ij}\,d\mathbf{x} = f_2,$$

$$\frac{1}{v_0^2}\int_{V_\alpha}\varphi^{\alpha}_{ij}\varphi^{\beta}_{ij}\,d\mathbf{x} = f_3 = -f_1,\quad \frac{1}{v_0^3}\int_{V_\alpha}\varphi^{\beta}_{ij}\varphi^{\gamma}_{ij}\,d\mathbf{x} = f_4 = f_1-f_2,$$

where

$$\varphi^{\alpha}(\mathbf{x}) = -\frac{1}{4\pi}\cdot\int_{V_\alpha}|\mathbf{x}-\mathbf{y}|^{-1}\,d\mathbf{y},$$

$$\varphi^{\beta}_{ij}(\mathbf{x}) = \varphi^{\beta}_{,ij}-\frac{1}{v_\alpha}\int_{V_\alpha}\varphi^{\beta}_{,ij}\,d\mathbf{x}\quad (\mathbf{x}\in V_\alpha),\quad A^{\beta\gamma}_{\alpha} = \int_{V_\alpha}\varphi^{\beta}_{ij}\varphi^{\gamma}_{ij}\,d\mathbf{x}.$$

For such polycrystals, the bounds on the effective conductivity can be deduced (Pham (1995)) following the same line of Pham (1994):

$$P^{p}_{\sigma}(\sigma^{pu}_{*}) \geqslant \sigma_c \geqslant P^{p}_{\sigma}(\sigma^{pl}_{*}),$$
$$P^{p}_{\sigma}(\sigma_{*}) = \langle(\sigma+\sigma_{*})^{-1}\rangle^{-1}-\sigma_{*},$$
$$\sigma^{pu}_{*} = 2\sigma^{pu}_{0},\quad \sigma^{pl}_{*} = 2\sigma^{pl}_{0}, \tag{42}$$

σ^{pu}_0 and σ^{pl}_0 are the solutions of the following equations:

$$f_1\cdot\{\langle(\sigma-\sigma^{pu}_0)[1-\langle(\sigma+2\sigma^{pu}_0)^{-1}\rangle^{-1}(\sigma+2\sigma^{pu}_0)^{-1}]^2\rangle$$
$$+9\langle\sigma-\sigma^{pu}_0\rangle\langle[1-\langle(\sigma+2\sigma^{pu}_0)^{-1}\rangle^{-1}(\sigma+2\sigma^{pu}_0)^{-1}]^2\rangle\}$$
$$+10f_2\cdot\langle\sigma-\sigma^{pu}_0\rangle\langle[1-\langle(\sigma+2\sigma^{pu}_0)^{-1}\rangle^{-1}(\sigma+2\sigma^{pu}_0)^{-1}]^2\rangle = 0, \tag{43}$$

$$f_1\cdot\{\langle(1/\sigma-1/\sigma^{pl}_0)[1-\langle(1/\sigma+1/2\sigma^{pl}_0)^{-1}\rangle^{-1}(1/\sigma+1/2\sigma^{pl}_0)^{-1}]^2\rangle$$
$$+9\langle 1/\sigma-1/\sigma^{pl}_0\rangle\langle[1-\langle(1/\sigma+1/2\sigma^{pl}_0)^{-1}\rangle^{-1}(1/\sigma+1/2\sigma^{pl}_0)^{-1}]^2\rangle\}$$
$$+10f_2\cdot\langle 1/\sigma-1/\sigma^{pl}_0\rangle\langle[1-\langle(1/\sigma+1/2\sigma^{pl}_0)^{-1}\rangle^{-1}(1/\sigma+1/2\sigma^{pl}_0)^{-1}]^2\rangle = 0, \tag{44}$$

where the notation $\langle S(\sigma)\rangle$ means "the average value" of the scalar function $S(\sigma)$:

$$\langle S(\sigma)\rangle = \tfrac{1}{3}[S(\sigma^{p}_1)+S(\sigma^{p}_2)+S(\sigma^{p}_3)].$$

We have shown that $f_{12} = f_1/f_2 = 0$ for spherical cell materials and $f_{12} = \infty$ for platelet cell materials. Then from (42), (43), (44) one can derive the bounds for the respective polycrystals. The bounds for the effective conductivity of spherical cell polycrystals, which are formed entirely from crystals of spherical form (and certainly of varying diameters to fill all the space of the material) are especially simple as (43) and (44) yield:

$$\sigma_0^{pu} = (\sigma_1^p + \sigma_2^p + \sigma_3^p)/3, \quad \sigma_0^{pl} = 3(1/\sigma_1^p + 1/\sigma_2^p + 1/\sigma_3^p)^{-1}. \tag{45}$$

For perfectly-random multiphase spherical cell polycrystals (when the phases are fully disordered), we get the bounds (42) with:

$$\sigma_0^{pu} = \sum_{\alpha=1}^{m} v_\alpha(\sigma_1^{p\alpha} + \sigma_2^{p\alpha} + \sigma_3^{p\alpha})/3, \quad \sigma_0^{pl} = 3\left[\sum_{\alpha=1}^{m} v_\alpha\left(\frac{1}{\sigma_1^{p\alpha}} + \frac{1}{\sigma_2^{p\alpha}} + \frac{1}{\sigma_3^{p\alpha}}\right)\right]^{-1}, \tag{46}$$

where $\sigma_1^{p\alpha}, \sigma_2^{p\alpha}, \sigma_3^{p\alpha}$ are the principal conductivities of the phase α ($\alpha = 1, \ldots, m$) having volume fraction v_α.

In Pham (1995) we have suggested (42), (45) as simple approximations for the effective properties of practical polycrystals. As many practical equiaxed crystal aggregates are better described by the spherical cell model, for which (42), (45) are exact, than by the platelet cell model in the other extreme, we get additional support for the practical value of the simple bounds (42), (45).

6. TWO-DIMENSIONAL PERFECTLY-RANDOM MEDIA

Similarly one can derive respective bounds for two-dimensional perfectly-random media. The final formulae also are similar with a few modifications given below.

The bounds for the effective conductivity (1), (2), (4), (5) are valid with $\bar{f}_1$ and $\bar{f}_2$ taking the places of f_1 and f_2 ($\bar{f}_1$ and $\bar{f}_2$ are the counterparts of f_1 and f_2 from (6), (7) in the two-dimensional space) and instead of (3) one has:

$$\sigma_*^u = \sigma_0^u, \quad \sigma_*^l = \sigma_0^l;$$

$\bar{f}_{12} = \bar{f}_1/\bar{f}_2 = 0$ for circular cell materials and $\bar{f}_{12} = \infty$ for striped cell materials.

In the two-dimensional space we deal with the two-dimensional bulk modulus K, which is related to the bulk modulus k and shear modulus μ by:

$$K = k + \mu/3 \quad \text{(for plane strain state)},$$

$$K = (1/k + 1/(4\mu))^{-1} \quad \text{(for plane stress state)}.$$

The bounds for the effective modulus K_e have the forms similar to those of k_e in (24), (25), (26) with $K_\alpha, \bar{f}_1, \bar{f}_2, K_*^u, K_*^l$ taking the places of $k_\alpha, f_1, f_2, k_*^u, k_*^l$ and

$$K_*^u = \mu_0^{ku}, \quad K_*^l = \mu_0^{kl}.$$

The bounds for the effective shear modulus keep the forms (33), (34), (36) with $\bar{g}_1, \bar{g}_2$ taking the places of g_1, g_2 ($\bar{g}_1$, $\bar{g}_2$ are the counterparts of g_1, g_2 from (22), (23) in the two-dimensional space) and

$$\mu_*^u = \frac{K_0^u \mu_0^u}{K_0^u + 2\mu_0^u}, \quad \mu_*^l = \frac{K_0^l \mu_0^l}{K_0^l + 2\mu_0^l};$$

the counterparts of (35), (37) are:

$$\bar{f}_1 \sum_\alpha v_\alpha \left[\tfrac{1}{2}(K_\alpha - K_0^u) - \frac{(K_0^u)^2}{(\mu_0^u)^2}(\mu_\alpha - \mu_0^u)\right]\left(\sum_\beta \frac{v_\beta}{\mu_\beta + \mu_*^u} - \frac{1}{\mu_\alpha + \mu_*^u}\right)^2$$

$$+ \bar{f}_2 \sum_\alpha v_\alpha \left[\tfrac{1}{2}(K_\alpha - K_0^u) - \frac{(K_0^u)^2}{(\mu_0^u)^2}(\mu_\alpha - \mu_0^u)\right]\sum_\beta v_\beta \left(\sum_\gamma \frac{v_\gamma}{\mu_\gamma + \mu_*^u} - \frac{1}{\mu_\beta + \mu_*^u}\right)^2 = 0$$

$$\bar{f}_1 \sum_\alpha v_\alpha \left[\frac{1}{2}\left(\frac{1}{K_\alpha} - \frac{1}{K_0^l}\right) - \left(\frac{1}{\mu_\alpha} - \frac{1}{\mu_0^l}\right)\right]\left(\sum_\beta \frac{v_\beta}{\mu_\beta + \mu_*^l} - \frac{1}{\mu_\alpha + \mu_*^l}\right)^2$$

$$+\bar{f}_2 \sum_\alpha v_\alpha \left[\frac{1}{2}\left(\frac{1}{K_\alpha} - \frac{1}{K_0^l}\right) - \left(\frac{1}{\mu_\alpha} - \frac{1}{\mu_0^l}\right)\right]\sum_\beta v_\beta \left(\sum_\gamma \frac{v_\gamma}{\mu_\gamma + \mu_*^l} - \frac{1}{\mu_\beta + \mu_*^l}\right)^2 = 0$$

$\bar{g}_{12} = \bar{g}_1/\bar{g}_2 = 0$ for circular cell materials and $\bar{g}_{12} = \infty$ for striped cell materials. The bounds on the effective conductivity of two-dimensional random polycrystals are very simple (for all $\bar{f}_1, \bar{f}_2$, not only those of circular cell polycrystals!):

$$P_\sigma^p(\sigma_0^{pu}) \geqslant \sigma_c \geqslant P_\sigma^p(\sigma_0^{pl}),$$

$$P_\sigma^p(\sigma_0) = 2\left(\frac{1}{\sigma_1^p + \sigma_0} + \frac{1}{\sigma_2^p + \sigma_0}\right)^{-1} - \sigma_0,$$

$$\sigma_0^{pu} = \frac{\sigma_1^p + \sigma_2^p}{2}, \quad \sigma_0^{pl} = 2\left(\frac{1}{\sigma_1^p} + \frac{1}{\sigma_2^p}\right)^{-1}.$$

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