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CORRELATION BETWEEN THE ELASTIC MODULI AND CONDUCTIVITY OF TWO-DIMENSIONAL ISOTROPIC TWO-PHASE COMPOSITES

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Abstract. Crosslinks between the elastic moduli and electrical conductivity of two-dimensional composite materials with a variety of random microstructures are obtained with the method of finite elements. The numerical results for two-phase composites are found to be in good agreement with the approximate cross-property relations derived from the Hashin-Shtrikman (HS) bounds. For porous materials (i.e., one of the phases is void), the analytical crosslinks correlate with the numerical predictions only at relatively low porosity levels.

Keywords: cross-property link, two-phase composite, porous material, finite element method, lower and upper bounds.

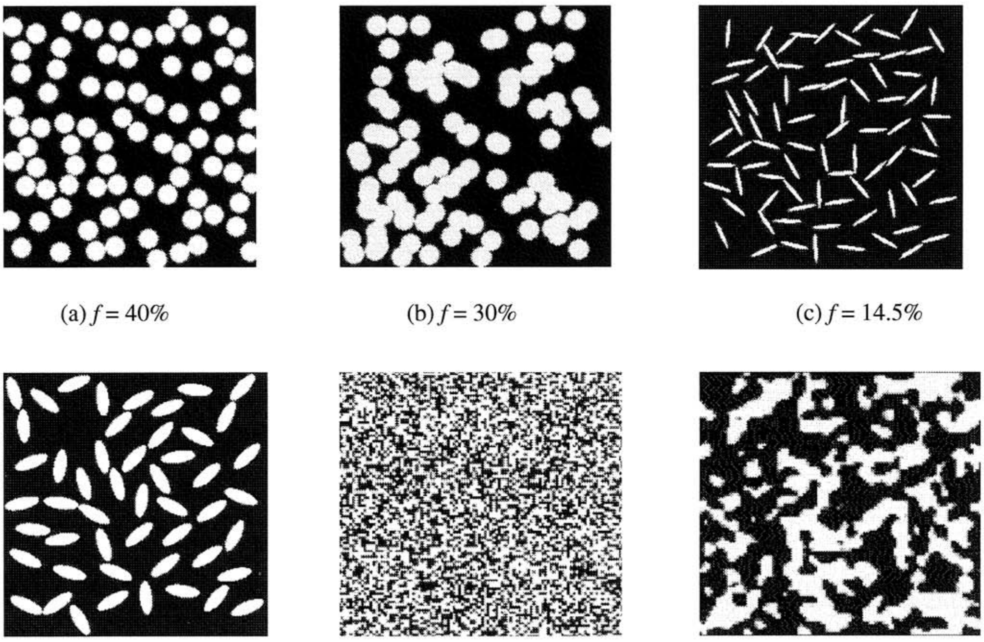
1. Introduction. The effective properties of a composite material having two or more phases depend intimately on its microstructure and constituent properties, thus offering a variety of possibilities to design its functionality by microstructure-tailoring. The elastic moduli of a composite having a given microstructure, and its many other effective properties, such as the electrical/thermal/magnetic conductivity, dielectric coefficient and thermal expansion coefficient, are typically functions of the same microstructural parameters. One can eliminate, at least partially, these parameters to obtain the crosslink between two different classes of properties, e.g. Young's modulus and conductivity. Practically, one can measure one property of the material and deduce the others from the crosslinks.

Cross-property links of a multiphase material were apparently first examined by Bristow (1960) for a solid containing low density, randomly oriented microcracks: crosslinks between elastic modulus and conductivity were obtained. Levin (1967) subsequently gave exact correlations between the effective bulk modulus and thermal expansion coefficient of a composite material. Gibiansky and Torquato (1996) proposed to bound one effective property from the bounds of others: the results are called the cross-property bounds. The correlations between the effective modulus and thermal conductivity of thermal barrier coatings (TBCs) made by physical vapor deposition have been established by Lu et al. (2001) using the non-interaction approximation for a variety of anisotropic pore morphologies; similar work can be found in Sevostianov and Kachanov (2001) for plasma sprayed TBCs. A systematic study on cross-property links was conducted by Kachanov et al. (2001) and Sevostianov and Kachanov (2002). They derived, in the framework of non-interaction approximation, explicit correlations between the effective modulus and electrical conductivity of porous materials as well two-phase composites with anisotropic microstructures. The experimental assessment of the crosslinks was conducted by Sevostianov et al. (2002) for a close-celled metal foam and by Sevostianov and Kachanov (2003) for short fiber-reinforced thermoplastics. It is found that the link between the effective Young's modulus and electrical conductivity can be well predicted.

There are many micromechanics methods that can be used to predict the effective moduli and conductivity of composite materials. In this letter, we will first derive analytical crosslinks from the Hashin-Shtrikman bounds (Hashin and Shtrikman, 1963), although these are only exactly realized by certain hierarchy laminate structures (Milton, 2002). These crosslinks will then be compared with those calculated with the finite element (FE) method for two-dimensional isotropic two-phase composites having different phase morphologies (including pores in the limiting case).

2. Microstructure and numerical method. The microstructures of the composites to be analyzed are two-dimensional (planar), random and macroscopically isotropic, including impenetrated mono-spheres, penetrated spheres, randomly oriented ellipses with different aspect ratios, Checkerboard model (Ziman, 1979), and Cellular automata model (Rothman and Zaleski, 1997), as shown in Fig. 1. Each of the images in Fig. 1 is taken as a representative volume element (RVE) of the corresponding material. Inclusions (the white phase in Fig. 1) with different physical properties and volume fractions will be examined.

To compute the effective properties of the composites, the FE-based numerical method of Garboczi (1998) is employed. For numerical accuracy, each image of Fig. 1 is divided into 64×64 pixels of the square form, with each pixel considered an element in the FE formulation. With a unit macroscopic shear strain imposed, the local shear stress and its spatial average over the RVE are evaluated to calculate the effective shear modulus μ_c of the material. Throughout this study, the subscripts c, 0 and 1 are used to denote quantities associated with the composite, matrix and inclusions, respectively. The same procedure is applied to compute the effective in-plane bulk modulus k_c and the effective electrical conductivity σ_c. For each microstructure considered, the effective Young's modulus and Poisson's ratio of the composite are computed by the isotropic relations $E_c = 4\mu_c k_c/(\mu_c + k_c)$ and $\nu_c = (k_c - \mu_c)/(\mu_c + k_c)$. The accuracy of the numerical results is checked with the universal relations obtained recently for isotropic planar composites and porous materials having arbitrary phase morphologies (Cherkaev et al., 1993; Hu and Weng, 2001).



(d) $f = 23.5\%$　　(e) $f = 50\%$　　(f) $f = 51\%$

Figure 1. Microstructures of two-dimensional isotropic two-phase planar composites: (a) impenetrated mono-spheres; (b) penetrated mono-spheres; (c) randomly oriented ellipses (aspect ratio 1:10); (d) randomly oriented ellipses (aspect ratio 1:3); (e) Checkerboard; (f) cellular Automata porous material.

3. Correlation relation. The Hashin-Shtrikman (HS) bounds are used first to estimate the effective modulus and effective electrical conductivity of an isotropic planar composite (or a porous material). The results will be approximate, since Milton (2002) has demonstrated that the HS bounds are only exactly realized by some hierarchy laminate structures. Generally speaking, the HS bounds become wider as the contrast of the phases increases. However, it has been accepted that for a inclusion/matrix type composite, one of the HS bounds depends on the properties of the continuos phase, and can provide an reasonable estimate for its overall effective properties. Furthermore, Kachanov et al. (2001) found that the crosslink is rather insensitive to the exact form of the shape distribution of the inclusions. The accuracy of the cross-property links established by the HS bounds will be checked with the numerical experiments performed on the composites shown in Fig. 1.

For planar isotropic porous materials, the HS upper bounds for the effective in-plane bulk, shear and Young's moduli, and the effective conductivity are

$$\overline{k}_c \equiv \frac{k_c}{k_0} = \frac{(1-f)\mu_0}{fk_0+\mu_0},\ \overline{\mu}_c \equiv \frac{\mu_c}{\mu_0} = \frac{(1-f)k_0}{f(k_0+2\mu_0)+k_0},\ \overline{E}_c \equiv \frac{E_c}{E_0} = \frac{1-f}{1+2f} \quad (1a)$$

$$\overline{\sigma}_c \equiv \frac{\sigma_c}{\sigma_0} = \frac{1-f}{1+f} \quad (1b)$$

From Eq. (1), we eliminate the pore volume fraction to arrive at:

$$\frac{1}{\overline{E}_c} = -\frac{1}{2} + \frac{3}{2}\frac{1}{\overline{\sigma}_c},\ \frac{1}{\overline{k}_c} = -\frac{\nu_0}{1-\nu_0} + \frac{1}{1-\nu_0}\frac{1}{\overline{\sigma}_c} \quad (2)$$

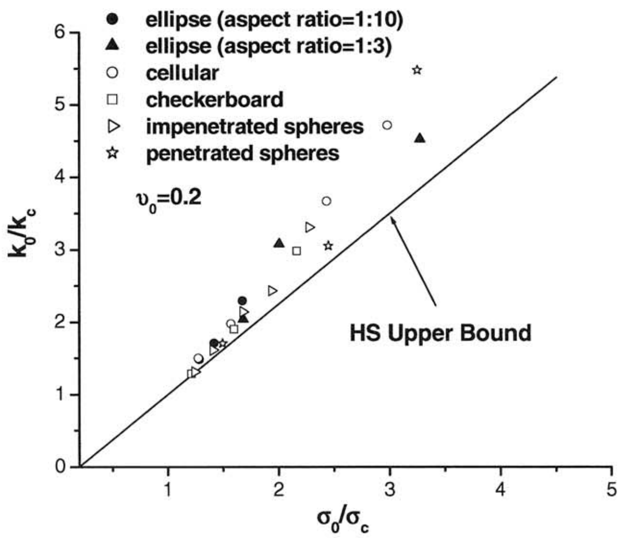


Figure 2. Effective in-plane bulk modulus plotted as a function of effective electrical conductivity for two-dimensional isotropic porous materials. Symbols: FE calculation; solid line: HS upper bound.

Fig. 2 presents the numerically calculated correlation between $1/\bar{k}_c$ and $1/\bar{\sigma}_c$ for $\nu_0 = 0.2$; the correlation derived from the HS upper bound is included. Notice that, at relatively low porosity levels (e.g., $f < 1/3$), $1/\bar{E}_c$ and $1/\bar{k}_c$ are both linear functions of $1/\bar{\sigma}_c$, and are insensitive to the pore morphologies. As the porosity level is increased, the calculated crosslink starts to deviate from that established by using HS upper bound, and becomes clearly microstructure-dependent. Analytical models including more information on the distribution of the phases are needed for improved predictions.

Consider next the case where the microstructures of Fig. 1 each represent a inclusion/matrix type composite, with the matrix being the 'softer' phase in terms of both the mechanical and electrical properties. The dimensionless HS lower bounds for the effective in-plane bulk modulus, shear modulus and electrical conductivity of the composite are:

$$\bar{k}_c \equiv \frac{k_c}{k_0} = 1 + \frac{f}{\dfrac{1}{\bar{k}-1} + \dfrac{(1-f)}{1+v}}, \quad \bar{\mu}_c \equiv \frac{\mu_c}{\mu_0} = 1 + \frac{f}{\dfrac{1}{\bar{\mu}-1} + \dfrac{(1-f)(1+2v)}{2(1+v)}} \tag{3a}$$

$$\bar{\sigma}_c \equiv \frac{\sigma_c}{\sigma_0} = \frac{(1+f)\bar{\sigma} + (1-f)}{(1-f)\bar{\sigma} + (1+f)} \tag{3b}$$

where $\bar{k} = k_1 / k_0$, $\bar{\mu} = \mu_1 / \mu_0$, $\bar{\sigma} = \sigma_1 / \sigma_0$ and $v = \mu_0 / k_0$; k_1, μ_1 and σ_1 are separately the in-plane bulk modulus, shear modulus and electrical conductivity of the inclusion. The cross-property links are obtained from (3) by eliminating the fiber volume concentration f, as:

$$\frac{K(\bar{k}_c)}{K(\bar{k})} = \frac{\Sigma(\bar{\sigma}_c)}{\Sigma(\bar{\sigma})}, \quad \frac{\mathrm{M}(\bar{\mu}_c)}{\mathrm{M}(\bar{\mu})} = \frac{\Sigma(\bar{\sigma}_c)}{\Sigma(\bar{\sigma})} \tag{4}$$

where

$$K(x) = \frac{1}{x-1} + \frac{1}{v+1}, \quad M(x) = \frac{1}{x-1} + \frac{1+2v}{2(v+1)}, \quad \Sigma(x) = \frac{x+1}{x-1} \tag{5}$$

Numerical calculations are carried out for $\bar{k} = 10$, $\bar{\mu} = 10$, $\bar{\sigma} = 10$ and $v = 0.667$, with different inclusion (fiber) volume fractions considered for each composite. Fig. 3 compares the crosslinks etablished by the numerical method with the HS lower bound predictions from Eq. (4). A direct correlation between k_c / k_0 and σ_c / σ_0, evaluated by the FE method, is presented in Fig. 4.

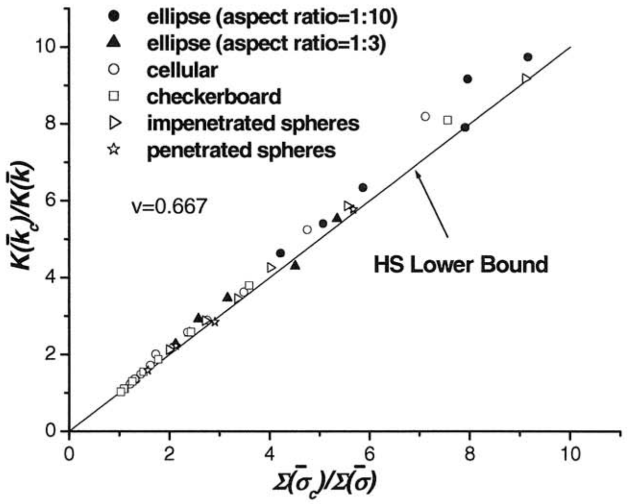


Figure 3. Normalized effective in-plane bulk modulus plotted as a function of normalized effective electrical conductivity for two-dimensional isotropic two-phase composites. Symbols: FE calculation; solid line: HS lower bound.

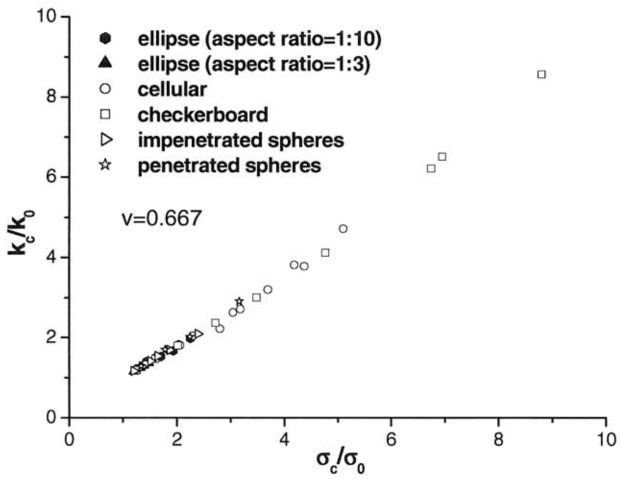


Figure 4. Effective in-plane bulk modulus plotted as a function of effective electrical conductivity for two-dimensional isotropic two-phase composites. Symbols: FE calculation.

4. Discussion. The results of Fig. 4 reveals that the crosslink relation of a two-dimensional isotropic composite has a remarkably weak dependence on its microstructure, in agreement with the observation of Kachanov et al. (2001) that the crosslink of a two-phase composite is relatively insensitive to the exact phase shape distribution. Also, the prediction by the HS lower bound agrees well with that calculated by the FE method, irrespective of the microstructure of the composite. For a porous material with high contrast between the phases, however, significant difference exists between the HS upper bound and the FE prediction at relatively large porosity levels (Fig. 2). Analytical models incorporating detailed pore morphologies are needed to address this discrepancy. At sufficiently low porosity levels, there is no need in bounds: exact results can be obtained with the non-interaction approximation (see, e.g., Sevostianov and Kachanov, 2001, 2002; Lu et al., 2001).

More detailed results on two-dimensional multiphase anisotropic composites and porous materials will be reported in a separate study. The implication from the current results of Figs. 2 and 3 that the agreement between the FE prediction and lower bound holds at large fiber volume fractions for two-phase composites whilst the correlation between the FE prediction and upper bound only holds at low porosity levels will be examined in more detail. In addition to the bounds, other analytical crosslinks incorperating more information on the distribution and shape of the phases will also be used to compare with numerical predictions. Furthermore, the threshold porosity (fiber volume fraction) level beyond which the non-interaction approximation is no longer valid will be established.

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References

Bristow, J.R. (1960). Microcracks, and the static and dynamic elastic constants of annealed heavily cold-worked metals, *British J. Appl. Phys.* **11**, 81-85.

Cherkaev, A. V., Lurie, K A. and Milton, G. W. (1992). Invariant properties of the stress in plane elasticity and equivalence classes of composites, *Proc. R. Soc. Lond. A* **438**, 519-529

Garboczi, E. J (1998). *Finite Element and Finite Difference Programs for Computing the Linear Electric and Elastic Properties of Digital Images of Random Materials*, NIST Internal Report 6269.

Gibiansky, L. V. and Torquato, S. (1996). Rigorous link between the conductivity and elastic moduli of fiber reinforced materials, *Proc. R. Soc. Lond.* A**452**, 253-283.

Hashin, Z. and Shtrikman, S. (1963) A variational approach to the theory of the elastic behavior of multiphase materials, *J. Mech. Phys. Solids* **11**, 127-140.

Hu, G. K. and Weng, G. J. (2001). A new derivative on the shift property of effective elastic compliances for planar and 3-D composites, *Proc. R. Soc. Lond.* A**457**, 1675-1684.

Kachanov, M., Sevostianov, I. and Shafiro, B. (2001). Explicit cross-property correlations for porous materials with anisotropic microstructures, *J. Mech. Phys. Solids* **49**, 1-25.

Levin, V. M. (1967). On the coefficients of thermal expansion of heterogeneous material, *Mechanics of Solids* **2**, 58-61

Lu, T. J., Levi, C. G., Wadley, H. N. G. and Evans, A. G. (2001). Distributed porosity as a control parameter for oxide thermal barriers made by physical vapor deposition, *J. Am. Ceram. Soc.* **84**, 2937-2946.

Milton, G. A. (2002). *The Theory of Composite*, Cambridge University Press.

Rothman, D. H. and Zaleski, S. (1997). *Lattice-Gas Cellular Automata Simple Models of Complex Hydrodymamics*, Cambridge University Press.

Sevostianov, I. and Kachanov, M. (2001). Plasma sprayed ceramic coatings: anisotropic elastic and conductive properties in relation to microstructure: cross-property correlations, *Materials Science and Engineering* **A297**, 235-343.

Sevostianov, I., Kovaik, J. and Simanik, F. (2002). Correlation between elastic and electric properties for metal foams: theory and experiment, *Int. J. Fracture* **144**, L23-L28.

Sevostianov, I. and Kachanov, M. (2002). Explicit cross-property correlations for anisotropic two-phase composite materials, *J. Mech. Phys. Solids* **50**, 253-282.

Sevostianov, I. and Kachanov, M. (2003). Connection between elastic moduli and thermal conductivity of anisotropic short fiber reinforced thermoplastics: theory and experimental verification. *Materials Science and Engineering* **A360**, 339-344.

Ziman, J. M. (1979). *Model of Disorder: The Theoretical Physics of Homogeneously Disordered Systems*, Cambridge University Press.