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Microstructure and Macroscopic Behavior of Random Heterogeneous Materials

6. AUTHOR(S)
Salvatore Torquato

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Princeton University
5 New South Building
Princeton, NJ 08544

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/MAK
110 Duncan Avenue, Room B115
Bolling AFB, DC 20332-8080

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This project attempted to systematically and quantitatively characterize the microstructure of heterogeneous materials and to use such information to predict rigorously the macroscopic behavior (e.g., effective moduli). By employing homogenization theory and the methods of statistical mechanics, we were able to mathematically describe the microstructure and, as a result, accurately determine the macroscopic response under a wide range of conditions. A goal was to treat seemingly disparate problems using a unified methodology. The generality of our approach enabled us to treat a wide class of two- and three-phase isotropic and anisotropic heterogeneous materials. This work will aid in leading to a highly cost-effective means of optimally designing heterogeneous materials for a particular application.

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Final Report

Microstructure and Macroscopic Behavior of Random Heterogeneous Materials
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Salvatore Torquato

Department of Civil Engineering and Operations Research
and Princeton Materials Institute
Princeton University
Princeton, NJ 08540

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ABSTRACT

This project attempted to systematically and quantitatively characterize the microstructure of heterogeneous materials and to use such information to predict rigorously the macroscopic behavior (e.g., effective moduli). By employing homogenization theory and the methods of statistical mechanics, we were able to mathematically describe the microstructure and, as a result, accurately determine the macroscopic response under a wide range of conditions. A goal was to treat seemingly disparate problems using a unified methodology. The generality of our approach enabled us to treat a wide class of two- and three-phase isotropic and anisotropic heterogeneous materials. This work will aid in leading to a highly cost-effective means of optimally designing heterogeneous materials for a particular application.
I. GRANT ACCOMPLISHMENTS

In what follows we describe the accomplishments that we made on the AFOSR Grant No. F49620-92-J-0501. We published 11 refereed journal articles and gave 25 invited presentations on our AFOSR-related work.

1. Cross-Property Relations

An intriguing fundamental as well as practical question in the study of composite materials is the following: What can be said about various unknown effective properties when different properties of the composite are known? Such cross-property relations become especially useful if one property is more easily measured than another property. Since the effective properties of random media reflect important microstructural information about the medium, one might expect that one could extract useful information about one effective property given an exact determination of another property. Employing the so-called translation method (see Ref. 2 and references therein), we have derived the sharpest rigorous upper and lower bounds on the effective elastic moduli for two-dimensional, two-phase isotropic composites (i.e., transversely isotropic fiber-reinforced materials) in terms of the effective conductivity $\sigma_e$ [2,6]. The former bounds are defined in the elastic moduli-conductivity planes by hyperbolas. Certain boundaries of these regions are realized by specific microgeometries and thus represent optimal bounds. We have also found the best available cross-property bounds for three-dimensional isotropic composites that link the effective bulk modulus $\kappa_e$ to the effective conductivity $\sigma_e$ [8].

How sharp are our cross-property estimates given an exact determination of one of the effective properties? To examine this question we use exact conductivity data and our cross-property relations to predict the effective bulk modulus $\kappa_e$ for hexagonal arrays of superconducting, superrigid cylindrical fibers (phase 2) in a matrix. Our predictions are compared to exact bulk modulus data [1] (see Fig. 1). The agreement between our conductivity predictions and elastic moduli data is excellent (see Fig. 1). It is noteworthy
that \textit{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 \textit{infinite-contrast phase is disconnected via conductivity information}. In summary, cross-property relations provide a new and powerful way to extract important microstructural information on composites.

![Graph showing comparison of bounds with exact data](image)

**Figure 1:** Comparison of the bulk modulus-conductivity bounds with the exact bulk modulus data (circles) [1] for a superrigid, superconducting hexagonal array of circular inclusions. Curves are the bounds using exact conductivity data.

More recently, we have applied the cross-property realtions to solid bodies that are damaged by cracks [7]. These are the first rigorous bounds on the effective moduli of cracked solids that do not require information about the crack density and geometry, quantities which are usually difficult to measure.
2. Imperfect Interfaces

The preponderance of theoretical predictions of the effective moduli of composites have been carried out assuming that the interface plays no role in determining the effective behavior of the materials, i.e., perfect interfaces. In real materials, interfacial effects can dramatically alter the effective behavior. For example, the Kapitza thermal resistance at the interface can be significant at sufficiently low temperatures, interfacial roughness can be appreciable enough to result in electrical resistance at the interface, and debonding at the interface can erode the effective elastic behavior of the composite.

![Graph](image)

Figure 2: Comparison of the lower bounds of Torquato and Rintoul [5] on the dimensionless conductivity $\sigma_e/\sigma_1$ vs. inclusion volume fraction $\phi_2$ to the experimental data (circles and squares) of De Araujo and Rosenberg for metallic particles in epoxy at 2 resistance values ($R = 0$ is perfect interface) corresponding to two different temperatures.

We assert that in order to get sharp estimates of the effective properties of composites with imperfect interfaces, one must incorporate nontrivial morphological information about the interface. For example, previous elastic-moduli bounds for imperfect interfaces do not incorporate such nontrivial interfacial information and thus are not very sharp bounds. We begin by considering the problem of determining the effective conductivity $\sigma_e$ of dispersions
of spheres with imperfect interfaces since: (i) it is mathematically easier than the elastic problem, and (ii) because (unlike the mechanical problem) experimental data exists for the interface property. For such a system we have developed rigorous bounds on $\sigma_e$ [5] in terms of the conductivity of the inclusions, $\sigma_2$, conductivity of the matrix, $\sigma_1$, the dimensionless interface resistance, $R$, inclusion volume fraction $\phi_2$, and higher-order morphological information, including interfacial statistics. Figure 2 shows that our new bounds give remarkably accurate predictions of the effective thermal conductivity of suspensions of metallic particles in epoxy matrices for two values of the Kapitza resistance $R$ ($R = 0$ corresponds to a perfect interface).

We have recently evaluated the effective conductivity of periodic arrays of spheres with interfacial resistance [10]. Corresponding work was carried out for superconducting interfaces [11].

3. General Property Estimates

It is useful to obtain estimates of the effective mechanical properties that incorporate microstructural information beyond that contained in volume fractions alone. We have recently derived the best possible bounds on the effective elastic moduli of any transversely isotropic fiber-reinforced material (with a perfect interface) that depend upon three-point correlation function information [4]. We also found bounds on the effective bulk and shear moduli of suspensions of overlapping spheres [3].

We have also obtained the first nontrivial phase-interchange relations for the effective elastic moduli of both transversely isotropic and isotropic two-phase composites [9]. These relations are useful in studying such composite materials near their percolation thresholds.
4. Computer Simulations

Compared to theoretical studies, there has been much less research directed toward obtaining effective properties “exactly” from computer simulations, especially for off-lattice or continuum models (e.g., distribution of particles in a matrix). Such “computer experiments” could provide unambiguous tests on theories for well-defined model microstructures. We have applied the boundary element method to determine the effective elastic moduli of an idealized model of hexagonal arrays of infinitely long, aligned cylinders in a matrix (a model of a fiber-reinforced material) or a thin-plate composite consisting of hexagonal arrays of disks in a matrix [1]. This has led to the most comprehensive set of simulation data for the elastic moduli of this useful model system. We intend to apply this technique and related numerical methods (finite elements) to compute the effective moduli of random systems.

II. PUBLICATIONS


6. L. V. Gibiansky and S. Torquato, “Rigorous Link Between the Conductivity and Elastic Moduli of Fiber-Reinforced Composite Materials,” Philosophical Transactions of


III. INVITED TALKS AND CONFERENCE PRESENTATIONS


8. Rigorous Link Between the Effective Elastic Moduli and Effective Conductivity of Composite Materials, MEET'N'93 (Joint ASME, SES, and ASCE Meeting), Charlottesville, Virginia, June, 1993 (with L. V. Gibiansky).

9. Macroscopic Behavior of Random Media from the Microstructure, MEET'N'93 (Joint ASME, SES, and ASCE Meeting), Charlottesville, Virginia, June, 1993


15. Link Between the Conductivity and Elastic Moduli of Heterogeneous Materials, American Institute of Chemical Engineers, St. Louis, Missouri, November, 1993.


IV. PERSONNEL

In addition to the principal investigator, Prof. Salvatore Torquato, the salaried research group at Princeton University consisted of two postdoctoral associates, Dr. Leonid Gibiansky and Dr. Hongwei Cheng, and a graduate student, John Quintanilla, who will complete his Ph.D. degree at the end of the year.