Determining elastic behavior of composites by the boundary element method

J. W. Eischen
Department of Mechanical and Aerospace Engineering, North Carolina State University, Raleigh, North Carolina 27695-7910

S. Torquato
Department of Civil Engineering and Operations Research and the Princeton Materials Institute, Princeton University, Princeton, New Jersey 08544

(Received 11 November 1992; accepted for publication 2 March 1993)

The *boundary element method* is applied to determine the effective elastic moduli of continuum models of composite materials. In this paper, we specialize to the 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. Thus, one need only consider two-dimensional elasticity, i.e., either plane-strain or plane-stress elasticity. This paper examines a variety of cases in which the inclusions are either stiffer or weaker than the matrix for a wide range of inclusion volume fractions ϕ_2. Our comprehensive set of simulation data for the elastic moduli are tabulated. Using the boundary element method, a key microstructural parameter η_2 that arises in rigorous three-point bounds on the effective shear modulus is also computed. Our numerical simulations of the elastic moduli for the hexagonal array are compared to rigorous two-point and three-point bounds on the respective effective properties. In the extreme instances of either superrigid particles or voids, we compare analytical relations for the elastic moduli near dilute and close packing limits to our simulation results.

I. INTRODUCTION

The problem of determining the effective transport and mechanical properties of disordered composite materials is a classical subject of research in science and engineering, dating back to the work of Maxwell,[1] Rayleigh,[2] and Einstein.[3] The complexity of the microstructure of random composite media makes an exact theoretical determination of the effective properties generally not possible. This naturally leads one to attempt to estimate the properties from partial statistical information on the sample in the form of correlation functions, and in particular, to establish the range of possible values the effective properties can take given such limited morphological information, i.e., to determine rigorous upper and lower bounds on the properties. In the last decade, considerable theoretical progress has been made on the derivation of rigorous bounds,[4–6] identification of the microstructures that correspond to the extreme values (i.e., optimal bounds),[7–10] and the systematic characterization and determination of the statistical correlation functions that arise in bounds.[11] There has been relatively 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.

In the case of static composite media, most numerical studies have focused on obtaining effective diffusion parameters such as the effective conductivity, effective diffusion coefficient, and effective time scales associated with diffusion and reaction among traps. An efficient means of computing effective diffusion properties is by employing first-passage-time algorithms.[12] Comparatively speaking, there is a dearth of numerical simulations of the effective elastic moduli of continuum models of composites.

Approximately 20 years ago, numerical data for the effective elastic moduli were obtained for square[13,14] and hexagonal arrays[15] arrays of cylinders in a matrix for a limited selection of material properties. Most of these studies made use of finite difference procedures. Very recently, Day *et al.*[16] have devised a discretized-spring scheme that is realized on digital-image-based model of a two-dimensional, two-phase material in which one of the phases has zero elastic moduli (i.e., holes) to compute the effective elastic moduli. This method has recently been extended to treat cases in which both phases have nonzero moduli.[17]

The purpose of this paper is to begin a program to provide accurate and comprehensive numerical data for the effective elastic moduli of continuum models of composite materials by employing the *boundary element method*.[18] In the first paper of this series, we specialize to the 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.[13] (In the sequel to this paper, random arrays will be studied.[19]) In all cases we seek to determine the effective elastic properties in a plane perpendicular to the generators and thus need only consider two-dimensional elasticity (i.e., either plane-strain or plane-stress elasticity). We examine a number of instances in which the inclusions are either stiffer or weaker than the matrix for a wide range of inclusion volume fractions ϕ_2. Because the method is accurate, we tabulate all of the simulation data for the elastic moduli. Using the boundary

 0021-8979/93/74(1)/159/12/$6.00

element method, we also compute a key microstructural parameter η_2 that arises in rigorous three-point bounds on the effective shear modulus. Our numerical simulations of the elastic moduli for the hexagonal array are compared to rigorous two-point and three-point bounds on the respective effective properties. Finally, in the extreme instances of superrigid particles or voids, we compare analytical relations for the elastic moduli near close packing to our simulation results.

The remainder of the paper is organized as follows. In Sec. II we review some pertinent theoretical results and obtain an asymptotic relation near close packing for the effective shear modulus in the case of superrigid inclusions in an incompressible matrix. In Sec. III the boundary element method is described for the problem at hand, i.e., for two-dimensional arrays of inclusions. In Sec. IV we present our simulation results for the in-plane elastic moduli of hexagonal arrays. Here we also present numerical data for the aforementioned three-point microstructural parameter η_2 arising in bounds for the shear modulus. Our data are compared to rigorous bounds and analytical asymptotic relations. Finally, in Sec. V we make concluding remarks.

II. THEORETICAL RESULTS

Here we discuss some previous theoretical results for the elastic moduli such as the dilute-concentration results, high-concentration results, and rigorous three-point bounds. In the case of nearly touching superrigid inclusions in an incompressible matrix, we derive an analytical expression for the effective shear modulus.

A. Basic definitions for two-dimensional elasticity

Before reviewing some theoretical results pertinent to this paper, it useful to define the elastic moduli for two-dimensional (2D) media. First consider a homogeneous 2D body which is isotropic. For such a material, the relationship between the stress tensor σ_{ij} and strain tensor ϵ_{ij} is given by

$$\sigma_{ij}=(k-G)\epsilon_{kk}\delta_{ij}+2G\epsilon_{ij}, \quad i,j,k=1,2. \tag{1}$$

This relation defines the 2D bulk modulus k and shear modulus G. Note that the symmetric stress and strain tensors have three independent components. Similarly, we write the strain-stress relation as

$$\epsilon_{ij}=\frac{1}{E}[(1+\nu)\sigma_{ij}\delta_{ij}-\nu\sigma_{kk}\delta_{ij}], \quad i,j,k=1,2, \tag{2}$$

where ν and E are the 2D Poisson's ratio and Young's modulus, respectively. Clearly, there are only two independent moduli. Comparing relations (1) and (2) yields, e.g., the following interrelations:

$$G=\frac{E}{2(1+\nu)}, \tag{3}$$

$$\nu=\frac{k-G}{k+G}, \tag{4}$$

$$\frac{4}{E}=\frac{1}{k}+\frac{1}{G}. \tag{5}$$

Equation (4) reveals that the 2D Poisson's ratio lies in the interval $[-1,1]$ as opposed to its three-dimensional (3D) counterpart that lies in the interval $[-1,0.5]$.

Now consider a two-phase 2D body. Denote the corresponding elastic moduli for phase i by k_i, G_i, ν_i, and E_i. Then relations (3)–(5) apply to each phase, i.e., append a subscript i to each of the moduli in Eqs. (3)–(5). Similarly, denote the corresponding 2D effective moduli by k_e, G_e, ν_e, and E_e. Again, relations (3)–(5) apply to the effective properties. The constitutive relations (1) and (2) apply as well except that the stress and strain tensors must be replaced with the *average* stress and *average* strain tensors, respectively.

Thus far we have not had to state whether we are dealing with *plane-strain* or *plane-stress* elasticity. Such specifications only arise when one desires to make contact with 3D elasticity. Plane-strain elasticity is physically relevant when considering a fiber-reinforced material. On the other hand, plane-stress elasticity is physically relevant when considering two-phase composites in the form of thin sheets. It is simple to relate 2D to 3D moduli for a single 3D isotropic material. This is done in the Appendix where it is shown, among other results, that the 2D shear modulus G (either in plane strain or plane stress) is equal to the 3D shear modulus. However, the bulk-moduli relations are not so simple. The plane-strain bulk modulus k is related to the 3D bulk modulus K by the well-known relation

$$k=K+G/3. \tag{6}$$

By contrast the plane-stress bulk modulus k obeys the relation

$$k=\frac{9KG}{3K+4G}. \tag{7}$$

Other interrelations among the 2D and 3D moduli are given in the Appendix. It is important to emphasize that the relations (6) and (7) apply only to individual phases. *Relations (6) and (7) do not apply to the effective properties.* In the Appendix we discuss the interrelations among the effective 2D moduli and the effective 3D moduli.

B. Dilute-concentration results

Consider any macroscopically isotropic 2D composite consisting of a equisized circular disks in matrix. Through first order in the inclusion volume fraction ϕ_2, the following exact asymptotic relations hold for the effective in-plane bulk and shear moduli, respectively,[20]

$$k_e=k_1+(k_2-k_1)\frac{(k_1+G_1)}{(k_2+G_1)}\phi_2, \tag{8}$$

$$G_e=G_1+\frac{2G_1(G_2-G_1)(k_1+G_1)}{G_2(k_1+G_1)+G_1(k_1+G_2)}\phi_2. \tag{9}$$