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Elastic moduli of composites containing a low concentration of complex-shaped particles having a general property contrast with the matrix

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ABSTRACT

There are diverse materials science problems concerned with how the presence of a low concentration of particulate inclusions having mechanical properties distinct from the matrix in which they are placed influences the elasticity of the resulting composite material. There is a classical treatment of the calculation of the leading order virial coefficient for the bulk modulus K and shear modulus G, or intrinsic moduli $[K]$ and $[G]$, for ellipsoidal inclusions having a general contrast between the elastic properties of the particle inclusions and the matrix. However, the treatment of more physically interesting shapes, such as gravel in concrete, is analytically intractable. With literal concrete applications in mind, we treat construction gravel as being composed of block-like particles having an equivalent length, width, and thickness, and we develop numerical approximants for $[K]$ and $[G]$ for these block structures based on finite element calculations and limiting analytic information. The approach generalizes our previous treatment of the electrical conductivity and elastic moduli of composites containing complex-shaped objects, in the dilute limit, having a general property contrast with the suspending matrix, and corrects an error in the previous elastic moduli calculation. We verify that our approximants provide an accurate description of $[K]$ and $[G]$ for general property contrast conditions and extensive tabulations of data based on finite element calculation for a wide range of object shapes.

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1. Introduction

Many applications in science and engineering involve the addition of particles to a matrix to change the overall properties of the resulting composite material. These properties include bulk and shear moduli, compressive and tensile strength, electrical and thermal conductivity, dielectric constant, and shear viscosity (inclusions in fluids). In any composite made from a low concentration of essentially isolated inclusions (volume fraction, c_i) embedded in a matrix (volume fraction, c_m), the effect of each inclusion on the overall properties is mainly controlled by inclusion shape and the contrast in its properties compared to the matrix. For a general property P, the contrast is defined by the ratio, $\Delta_P \equiv P_i/P_m$, which is a basic quantity governing the change in composite material properties. The importance of particle shape in composite property changes also depends on Δ_P (Torquato, 2002; Milton, 2002; Christensen, 1991; Douglas and Garboczi, 1995). The 'dilute limit' can be rigorously and formally defined by having a particle volume fraction small enough so that the elastic fields around a given inclusion do not affect the elastic fields around other inclusions. For linear isotropic elasticity, we define the property contrast ratios as, $\Delta_K = K_i/K_m$, $\Delta_G = G_i/G_m$, and $\Delta_E = E_i/E_m$, where K is the isotropic bulk modulus, G is the

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isotropic shear modulus, and E is the isotropic Young's modulus. In the dilute limit, the composite elastic properties K and G are described by virial expansions (Torquato, 2002) in the inclusion concentration:

$$\begin{aligned} K/K_m &= 1 + [K]c_i + O(c_i^2) \\ G/G_m &= 1 + [G]c_i + O(c_i^2) \end{aligned} \quad (1)$$

where $[K]$ and $[G]$ are dimensionless functions of matrix and inclusion elastic properties and particle shape. Higher order c_i terms become important when the elastic field of the particles start to interact. For particles having an anisotropic shape, we assume that the particles are distributed with isotropic orientational distributions so that $[K]$ and $[G]$ become scalar quantities (Douglas and Garboczi, 1995; Garboczi and Douglas, 1996; Mansfield et al., 2001). The 'intrinsic moduli' $[K]$ and $[G]$ have the following functional forms,

$$\begin{aligned} [K] &= [K](K_m, K_i, G_m, G_i, shape) \\ [G] &= [G](K_m, K_i, G_m, G_i, shape) \end{aligned} \quad (2)$$

In general, intrinsic moduli depends on the elastic properties of both matrix and inclusion, as well as particle shape. However, if we use the common equations relating K, G, the Young's modulus E, and the Poisson's ratio, v,

$$K = \frac{E}{3(1-2v)}, \quad G = \frac{E}{2(1+v)}, \quad \frac{9}{E} = \frac{1}{K} + \frac{3}{G}, \quad v = \frac{(3K-2G)}{2(3K+G)} \quad (3)$$

and make the additional assumption that the intrinsic moduli depend only on the property contrast between the inclusion and matrix ($\Delta_E = E_i/E_m$ is defined to be the "stiffness contrast" between the two phases), we can write $[K]$ and $[G]$ formally as,

$$\begin{aligned} [K] &= [K](\Delta_E, v_m, v_i,\ shape) \\ [G] &= [G](\Delta_E, v_m, v_i,\ shape) \end{aligned} \quad (4)$$

where v_m and v_i are the Poisson's ratios of matrix and inclusion, respectively. If the inclusion has the same isotropic elastic properties as the matrix, there is no change in composite properties when the particle inclusions are added and the intrinsic moduli must then be 0. Evidently, the intrinsic moduli depend on only three elastic parameters rather than four. The goal of this paper is to construct general purpose and effective analytical approximations for the functional dependence of $[K]$ and $[G]$ in Eq. (4) on general elastic parameters and on a particular class of particle shape, namely rectangular parallelepipeds (blocks).

A previous paper (Garboczi et al., 2006) used a combination of numerical finite element techniques and approximate analytical techniques to approximate the intrinsic moduli functions given in Eq. (4) for a range of particle geometries and elastic property contrasts. Approximate analytical forms for the property and shape dependence in Eq. (4) were used in this work, where the unknown coefficients were determined by fitting to finite element numerical results for specific shapes. This paper extends the range of property mismatch and shapes considered in this previous work, as well as correcting a mistake and improving the numerical data used. The exact ellipsoid calculation of Eshelby (1957) as implemented by Mura (1982) and Pan and Weng (1995) is used, along with the numerical values of the intrinsic moduli in the infinite and zero contrast limits, to construct an improved analytical approximation for Eq. (4).

The calculation of the intrinsic moduli is a basic input into the development of any approximate treatment of composite materials at higher particle concentrations. For example, differential effective medium theory (McLaughlin, 1977; Garboczi and Berryman, 2001) requires that one be able to determine the intrinsic (dilute) properties for any combination of matrix and composite properties. Providing an approximate analytical form for the intrinsic moduli of various shapes that do not have an exact solution for their intrinsic moduli will allow differential effective medium theory to be applied to composite materials built out of these inclusion shapes.

2. Exact relations for the intrinsic elastic moduli

For intrinsic elastic moduli, the only exact calculations for general contrast are for ellipsoidal particles (Eshelby, 1957; Mura, 1982; Pan and Weng, 1995). Simple formulae are available for axisymmetric ellipsoids including spheres (Berryman, 1980; Christensen, 1991). There are also general exact relations that cover parts of the space of inclusion shape and property contrast.

An expansion exists for the effective properties of the general composite elastic problem, at any volume fraction and for any shape inclusion, in terms of the property contrast (Torquato, 2002, 1997). Up through quadratic order in $(\Delta_K - 1)$ and $(\Delta_G - 1)$, the terms are independent of particle shape (Torquato, 2002, 1997; Garboczi et al., 2006). In this expansion, the intrinsic moduli are formally defined as the limits,

$$[K] = \lim_{c_i \to 0}\left(\frac{K - K_m}{c_i K_m}\right) \quad [G] = \lim_{c_i \to 0}\left(\frac{G - G_m}{c_i G_m}\right) \quad (5)$$

Up to quadratic order, $[K]$ depends only on Δ_K and $[G]$ depends only on Δ_G, independent of inclusion shape. This fact leads to two analytical relations that $[K]$ and $[G]$ must simultaneously obey for any particle. The conditions $\Delta_K = 1$ and $\Delta_G = 1$ imply that $[K] = 0$ and $[G] = 0$, respectively, since under these conditions there is no difference between the inclusion and the matrix material; this assumes the interface is perfect and smooth. We then conclude that there are a total of three relations that must be obeyed by $[K]$ and $[G]$ for any shape. This fact, along with the zero and infinite contrast limits, was used previously in (Garboczi et al., 2006) to construct approximants for $[K]$ and $[G]$. However, we have since realized that there is a *fourth* analytical expression that must be satisfied and which only applies to $[K]$. In particular, there is an exact expression for the bulk modulus K of a two-phase composite medium where $G_i = G_m$, for any contrast Δ_K and any volume fraction of inclusions (Hill, 1963):

$$K = K_m c_m + K_i c_i - \frac{(K_i - K_m)^2 c_m c_i}{K_m c_i + K_i c_m + \frac{4}{3} G_m} \quad (6)$$