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Volodymyr I. Kushch, Sofia G. Mogilevskaya, Henryk K. Stolarski and Steven L. Crouch

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EVALUATION OF THE EFFECTIVE ELASTIC MODULI OF PARTICULATE COMPOSITES BASED ON MAXWELL'S CONCEPT OF EQUIVALENT INHOMOGENEITY: MICROSTRUCTURE-INDUCED ANISOTROPY

VOLODYMYR I. KUSHCH, SOFIA G. MOGILEVSKAYA,
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Maxwell's concept of equivalent inhomogeneity is employed for evaluating the effective elastic properties of macroscopically anisotropic particulate composites with isotropic phases. The effective anisotropic elastic properties of the material are obtained by comparing the far-field solutions for the problem of a finite cluster of isotropic particles embedded in an infinite isotropic matrix with those for the problem of a single anisotropic equivalent inhomogeneity embedded in the same matrix. The former solutions precisely account for the interactions between all particles in the cluster and for their geometrical arrangement. Illustrative examples involving periodic (simple cubic) and random composites suggest that the approach provides accurate estimates of their effective elastic moduli.

1. Introduction

This paper examines Maxwell's concept of equivalent inhomogeneity in the context of the effective elastic properties of macroscopically anisotropic particulate composites with spherical particles. The matrix and the particles are assumed to be isotropic, so the overall anisotropy is entirely due to the geometrical arrangement of particles. Maxwell [1873] originally proposed the concept for evaluating the effective electrical conductivity of isotropic particulate composites. He obtained an approximation formula by equating "the potential at a great distance from the sphere" for two problems: a finite cluster of conducting spherical particles embedded in an infinite conducting matrix, and a single equivalent sphere embedded in the same matrix. The formula did not account for the interaction between the particles and, therefore, for their geometrical arrangement. According to Maxwell, the formula was only valid for materials with low volume fractions of particles. Nonetheless, the formula and analogous estimates (for example, for dielectric, magnetic, optical, and elastic properties) remain extremely popular [Milton 2002; Torquato 2002; McCartney and Kelly 2008; McCartney 2010; Levin et al. 2012] due to their simple, ready-to-use analytical nature. The accuracy of these analytical formulas has been discussed in several publications (for example, [McCartney and Kelly 2008; McCartney 2010; Mogilevskaya et al. 2012]).

It was recently brought to our attention that a concept somewhat similar to that of Maxwell is widely used in the geophysics community. Kuster and Toksöz [1974] (who apparently were not aware of Maxwell's approach) suggested equating the displacement fields for waves scattered by the equivalent

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spherical inhomogeneity and those by a cluster of spherical or spheroidal reinforcements in order to evaluate the effective elastic moduli of two-phase composites. These authors made the assumption that "multiple scattering effects are negligible", which allowed them to neglect interactions between the reinforcements in the cluster and its geometry. The method is discussed in detail in [Berriman and Berge 1996], where it was compared with the Mori–Tanaka approach. Recently, Weng [2010] and Levin et al. [2012] have shown that the approach of [Kuster and Toksöz 1974] is a dynamical analog of the Maxwell scheme.

In a series of recent papers Maxwell's concept was modified to evaluate the effective elastic properties of transversely isotropic composites [Mogilevskaya et al. 2010a; 2010b; 2012; Mogilevskaya and Crouch 2013], the thermal properties of isotropic particulate composites [Koroteeva et al. 2010; Mogilevskaya et al. 2011], and the viscoelastic properties of transversely isotropic composites [Pyatigorets and Mogilevskaya 2011]. The modified concept allowed for a precise account of both the interactions among the constituencies in the cluster and their geometrical arrangement. The comparisons of the estimates obtained using Maxwell's modified approach with benchmark results for periodic and random composites and with the exact solutions demonstrated the estimates' accuracy even for materials with high volume fractions. It has been suggested [Mogilevskaya et al. 2010b; Mogilevskaya and Crouch 2013] that the general methodology presented in those papers would be formally applicable to composite materials exhibiting anisotropic behavior if the solution of a single inhomogeneity with a corresponding degree of anisotropy was used as the reference solution.

The objective of the present paper is to demonstrate that Maxwell's concept is applicable to macroscopically anisotropic particulate composites with isotropic phases (matrix and spherical particles). The formulation involves the solutions for two problems: an infinite isotropic matrix containing a spherical inhomogeneity with an arbitrary degree of anisotropy, and an infinite matrix containing a cluster of nonoverlapping isotropic elastic spherical particles. The effective stiffness tensor of the composite is evaluated by comparing the far-field asymptotic behavior of the displacements for both solutions.

The method of solving the problem of a single anisotropic ellipsoidal inhomogeneity was outlined in Eshelby [1961]; see also [Mura 1987] and the references therein. Closed-form solutions have been reported for the particular cases of material symmetries, for example, by Huang [1968], who considered a problem of a single anisotropic spherical inhomogeneity which possessed cubic symmetry.

The problem of a finite cluster of elastic spherical particles embedded in an infinite elastic matrix has been studied in several publications, but mostly under various simplified assumptions, for example, the assumption that the strains inside the inhomogeneities are uniform [Molinari and El Mouden 1996] and the equivalent transformational strains are polynomial [Moschovidis and Mura 1975]; or the assumption that the interactions are governed by the average equivalent transformational strains [Rodin and Hwang 1991; Shen and Yi 2001]. In several papers the interactions between the inhomogeneities were accounted for in different approximate manners (for example, pairwise interactions in [Ju and Yanase 2010] and eight-particle interactions in [Yin and Sun 2005]). The problem was also solved numerically, for example, in [Fu et al. 1998] with the boundary element method. Complete multipole-type analytical solutions for the problem of a finite cluster of isotropic inhomogeneities were obtained in [Golovchan et al. 1993] for spherical particles, [Kushch 1996] for aligned spheroidal inhomogeneities, [Kushch 1998] for arbitrary oriented spheroidal inhomogeneities, and [Kushch et al. 2011] for spherical inhomogeneities with imperfect, Gurtin–Murdoch type, interfaces.

The solutions for spatially periodic media have been reported for cubic arrays of rigid spheres [Nunan and Keller 1984], for cubic arrays of elastic spheres [Sangani and Lu 1987], for a medium with arbitrary periodic arrays of elastic spheres [Kushch 1985; 1987; Sangani and Mo 1997], for a medium with periodic arrays of elastic spheroids [Kushch 1997], and for a transversely isotropic medium with finite or infinite periodic arrays of transversely isotropic spheres [Kushch 2003; Kushch and Sevostianov 2004]. These solutions were used to calculate the effective elasticity tensors of periodic and quasirandom composites.

The three-dimensional effective elastic properties (isotropic and anisotropic) of particulate composite and porous materials were also calculated in [Nemat-Nasser and Taya 1981; Nemat-Nasser et al. 1982; Iwakuma and Nemat-Nasser 1983; Luciano and Barbero 1994; Cohen and Bergman 2003; Cohen 2004]. Those estimates were obtained using the simplifying assumptions of constant equivalent strains within each inhomogeneity. Torquato [1997] obtained exact series expansions for the effective stiffness tensor of macroscopically anisotropic, two-phase composite media in terms of the powers of the "elastic polarizabilities". Numerical estimates are also available, for example, with the finite element method in [Segurado and Llorca 2002; 2006; Zohdi and Wriggers 2005] and with boundary element method in [Grzhibovskis et al. 2010]. In addition, various effective medium theories and variational bounds have been generalized to estimate the overall three-dimensional anisotropic elastic properties (for example, [Willis 1977; Benveniste 1987; Ponte Castañeda and Willis 1995; Milton 2002; Torquato 2002]).

In the present paper the cluster problem is solved semianalytically using the multipole expansion method of [Kushch et al. 2011]. The reference solution for a single anisotropic spherical inhomogeneity is rederived in a form more suitable for comparison with the cluster problem. A numerical procedure for calculating the effective stiffness tensor is described for materials with an arbitrary degree of overall anisotropy. Closed-form expressions are given for the particular case of cubic symmetry. The effective moduli obtained with the generalized Maxwell method are compared with those obtained by periodic homogenization [Kushch 1987; Sangani and Lu 1987] and with the various approximate estimates and bounding methods.

The paper is structured as follows. Sections 2–4 summarize the statement of the problem, governing equations, and numerical solution (with details provided in the Appendix). These are followed by illustrative examples involving periodic (simple cubic) and random composites in Section 5 and conclusions in Section 6.

2. The equivalent anisotropic inhomogeneity problem

Consider an infinite isotropic elastic matrix with shear modulus μ_0 and Poisson's ratio ν_0 containing an anisotropic spherical elastic inhomogeneity of radius R_{eff} perfectly bonded to the matrix material. The entire system is subjected to the uniform far-field strain $\boldsymbol{E} = E_{ij}\boldsymbol{i}_i\boldsymbol{i}_j$. This is the standard Eshelby problem whose analytical solution is outlined elsewhere (for example, in [Eshelby 1961; Mura 1987]). Below it is derived in a somewhat different form, more suitable for our purposes. The derivation procedure is essentially that of [Kushch et al. 2011], with minor modifications.

The displacement vector $\boldsymbol{u}^{(0)}$ in the matrix domain is sought as a sum of the far field and the disturbance field caused by the inhomogeneity

$$\boldsymbol{u}^{(0)}(\boldsymbol{r}) = \boldsymbol{E}\cdot\boldsymbol{r} + \boldsymbol{u}_{\mathrm{dis}}(\boldsymbol{r}), \tag{1}$$

where $\boldsymbol{r}$ is a position vector relative to the Cartesian coordinate system with origin at the center of the inhomogeneity, and $\boldsymbol{u}_{\mathrm{dis}}$ is the displacement disturbance field that should obey the condition $\boldsymbol{u}_{\mathrm{dis}}(\boldsymbol{r}) \to 0$ as $\|\boldsymbol{r}\| \to \infty$. To assure that this condition is satisfied, $\boldsymbol{u}_{\mathrm{dis}}$ is taken in the form

$$\boldsymbol{u}_{\mathrm{dis}}(\boldsymbol{r}) = \sum_{i,t,s} B_{ts}^{(i)} \boldsymbol{U}_{ts}^{(i)}(\boldsymbol{r}) \quad \Bigl(\sum_{i,t,s} = \sum_{i=1}^{3} \sum_{t=0}^{\infty} \sum_{s=-t}^{t}\Bigr), \tag{2}$$

where $B_{ts}^{(i)}$ are the unknown complex coefficients, and the complex-value irregular vector functions $\boldsymbol{U}_{ts}^{(i)}$ ($i = 1, 2, 3$) are defined by (A.7). Specifically, $\boldsymbol{U}_{ts}^{(1)}$ are the potential vectors (gradients of scalar potential), $\boldsymbol{U}_{ts}^{(2)}$ are harmonic vectors with nonzero curl, and $\boldsymbol{U}_{ts}^{(3)}$ are the biharmonic vectors with harmonic divergence. In particular, $\boldsymbol{U}_{1s}^{(2)}$ and $\boldsymbol{U}_{1s}^{(3)}$ represent the displacements due to the concentrated moment and force, respectively (see the Appendix). For a single inhomogeneity problem the series of (2) involves only the functions with $t \le 2$, see [Kushch et al. 2011]. In addition, equilibrium conditions for the inhomogeneity, with the resultant force $T = 0$ and the resultant torque $M = 0$, require that some coefficients with $t \le 2$ also be excluded (see the Appendix). Thus $\boldsymbol{u}_{\mathrm{dis}}$ involves only the functions possessing nonzero vector dipole moment:

$$\boldsymbol{u}_{\mathrm{dis}}(\boldsymbol{r}) = B_{00}^{(1)} \boldsymbol{U}_{00}^{(1)}(\boldsymbol{r}) + \sum_{|s| \le 2} B_{2s}^{(3)} \boldsymbol{U}_{3s}^{(3)}(\boldsymbol{r}). \tag{3}$$

The Cartesian projections of $\boldsymbol{u}_{\mathrm{dis}}$ are real numbers, which implies that $B_{2,-s}^{(3)} = (-1)^s \overline{B_{2s}^{(3)}}$. Thus, the total number of unknown coefficients includes two real ($B_{00}^{(1)}$ and $B_{20}^{(3)}$) and two complex ($B_{21}^{(3)}$ and $B_{22}^{(3)}$) coefficients in (3).

The linear far-field displacement field $\boldsymbol{u}_{\mathrm{far}} = \boldsymbol{E} \cdot \boldsymbol{r}$ is expressed as follows [Kushch et al. 2011]:

$$\boldsymbol{E} \cdot \boldsymbol{r} = c_{00}^{(3)} \boldsymbol{u}_{00}^{(3)}(\boldsymbol{r}) + \sum_{|s| \le 2} c_{2s}^{(1)} \boldsymbol{u}_{2s}^{(1)}(\boldsymbol{r}), \tag{4}$$

where $\boldsymbol{u}_{ts}^{(i)}$ are the regular vector functions defined by (A.5), and the coefficients $c_{ts}^{(i)}$ are defined as follows

$$\begin{aligned} c_{00}^{(3)} &= \frac{(E_{11} + E_{22} + E_{33})}{3\gamma_0(\nu_0)}, & c_{20}^{(1)} &= \frac{(2E_{33} - E_{11} - E_{22})}{3}, \\ c_{21}^{(1)} &= -\overline{c_{2,-1}^{(1)}} = E_{13} - \mathrm{i}E_{23}, & c_{22}^{(1)} &= \overline{c_{2,-2}^{(1)}} = E_{11} - E_{22} - 2\mathrm{i}E_{12}, \end{aligned} \tag{5}$$

where the coefficients $\gamma_t = \gamma_t(\nu_0)$ are given by (A.6) and $i^2 = -1$.

It is well-known [Eshelby 1961] that the strains D_{ij} in the inhomogeneity are uniform, thus the displacement $\boldsymbol{u}^{(1)}(\boldsymbol{r})$ inside the inhomogeneity can be presented as the following linear function of Cartesian coordinates ($\boldsymbol{r} = x_j \boldsymbol{i}_j$):

$$\boldsymbol{u}^{(1)}(\boldsymbol{r}) = \boldsymbol{D} \cdot \boldsymbol{r} = D_{ij} x_j \boldsymbol{i}_i. \tag{6}$$

By analogy with (4), $\boldsymbol{u}^{(1)}(\boldsymbol{r})$ can be written as

$$\boldsymbol{u}^{(1)}(\boldsymbol{r}) = d_{00}^{(3)} \boldsymbol{u}_{00}^{(3)}(\boldsymbol{r}) + \sum_{|s| \le 2} d_{2s}^{(1)} \boldsymbol{u}_{2s}^{(1)}(\boldsymbol{r}), \tag{7}$$

where

$$\begin{aligned} \gamma_0 d_{00}^{(3)} &= \frac{(D_{11}+D_{22}+D_{33})}{3}, & d_{20}^{(1)} &= \frac{(2D_{33}-D_{11}-D_{22})}{3}, \\ d_{21}^{(1)} &= D_{13}-\mathrm{i}D_{23}, & d_{22}^{(1)} &= D_{11}-D_{22}-2\mathrm{i}D_{12}, \end{aligned} \tag{8}$$

and $d_{2,-s}^{(1)} = (-1)^s \overline{d_{2s}^{(1)}}$. The corresponding uniform stress tensor inside the inhomogeneity is

$$\sigma^{(1)}(\boldsymbol{r}) = \boldsymbol{S} = S_{ij}\boldsymbol{i}_i\boldsymbol{i}_j = \boldsymbol{C}^* : \boldsymbol{D}, \tag{9}$$

where $\boldsymbol{C}^*$ is the stiffness tensor (anisotropic, in the general case).

The twelve unknowns that govern the problem of a single inhomogeneity include six real coefficients D_{ij} of (8), and two real ($B_{00}^{(1)}$ and $B_{20}^{(3)}$) and two complex ($B_{21}^{(3)}$ and $B_{22}^{(3)}$) coefficients of (3). They can be obtained from the following conditions of perfect bonding at the matrix/inhomogeneity interface $S_{\text{eff}}(r = R_{\text{eff}})$:

$$[\![\boldsymbol{u}]\!]_{S_{\text{eff}}} = 0, \quad [\![\boldsymbol{T}_r(\boldsymbol{u})]\!]_{S_{\text{eff}}} = 0, \tag{10}$$

where $[\![f]\!]_{S_{\text{eff}}} = \left(f^{(0)} - f^{(1)}\right)_{S_{\text{eff}}}$ is a jump of the quantity f across the interface S_{eff} and $\boldsymbol{T}_r(\boldsymbol{u})$ is the traction vector at S_{eff}. The latter has the following form ($\boldsymbol{n} = \boldsymbol{e}_r = n_j\boldsymbol{i}_j$):

$$\boldsymbol{T}_r\left(\boldsymbol{u}^{(1)}\right) = \boldsymbol{S}\cdot\boldsymbol{e}_r = S_{ij}\boldsymbol{i}_i\boldsymbol{i}_j\cdot\boldsymbol{e}_r = S_{ij}n_j\boldsymbol{i}_i. \tag{11}$$

In view of $\boldsymbol{r} = r\boldsymbol{e}_r$, the tractions $\boldsymbol{T}_r\left(\boldsymbol{u}^{(1)}\right)$ can be expanded in series analogous to that of (7):

$$r\boldsymbol{T}_r\left(\boldsymbol{u}^{(1)}\right) = s_{00}^{(3)}\boldsymbol{u}_{00}^{(3)}(\boldsymbol{r}) + \sum_{|s|\le 2} s_{2s}^{(1)}\boldsymbol{u}_{2s}^{(1)}(\boldsymbol{r}), \tag{12}$$

where

$$\begin{aligned} \gamma_0 s_{00}^{(3)} &= \frac{(S_{11}+S_{22}+S_{33})}{3}, & s_{20}^{(1)} &= \frac{(2S_{33}-S_{11}-S_{22})}{3}, \\ s_{21}^{(1)} &= S_{13}-\mathrm{i}S_{23}, & s_{22}^{(1)} &= S_{11}-S_{22}-2\mathrm{i}S_{12}. \end{aligned} \tag{13}$$

In order to fulfill the interface conditions of (10), we express $\boldsymbol{u}^{(0)}$ and $\boldsymbol{u}^{(1)}$ in terms of vector spherical harmonics $\boldsymbol{S}_{ts}^{(i)}$ (see (A.1)) and use their orthogonality at the spherical surface S_{eff}. With the aid of (A.5) and (A.7) we find that

$$\boldsymbol{u}_{\text{far}}(\boldsymbol{r}) = \gamma_0 c_{00}^{(3)} r\boldsymbol{S}_{00}^{(3)} + \sum_{|s|\le 2} c_{2s}^{(1)} \frac{r}{(2+s)!}\left(\boldsymbol{S}_{2s}^{(1)} + 2\boldsymbol{S}_{2s}^{(3)}\right), \tag{14}$$

$$\boldsymbol{u}_{\text{dis}}(\boldsymbol{r}) = -B_{00}^{(1)}\frac{1}{r^2}\boldsymbol{S}_{00}^{(3)} + \sum_{|s|\le 2}\frac{(2-s)!}{r^2}\left[B_{2s}^{(1)}\frac{1}{r^2}\left(\boldsymbol{S}_{2s}^{(1)} - 3\boldsymbol{S}_{2s}^{(3)}\right) + B_{2s}^{(3)}\left(\beta_{-3}\boldsymbol{S}_{2s}^{(1)} + \gamma_{-3}\boldsymbol{S}_{ts}^{(3)}\right)\right], \tag{15}$$

and

$$\boldsymbol{u}^{(1)}(\boldsymbol{r}) = \boldsymbol{D}\cdot\boldsymbol{r} = \gamma_0 d_{00}^{(3)} r\boldsymbol{S}_{00}^{(3)} + \sum_{|s|\le 2} d_{2s}^{(1)}\frac{r}{(2+s)!}\left(\boldsymbol{S}_{2s}^{(1)} + 2\boldsymbol{S}_{2s}^{(3)}\right), \tag{16}$$

where the coefficients $\gamma_t = \gamma_t(\nu_0)$ and $\beta_t = \beta_t(\nu_0)$ involved in (15) are defined by (A.6).

By equating the coefficients of $\boldsymbol{S}_{00}^{(3)}$ on both sides of the equality $\boldsymbol{u}^{(0)} = \boldsymbol{u}_{\text{far}} + \boldsymbol{u}_{\text{dis}} = \boldsymbol{u}^{(1)}$, we obtain the algebraic equation

$$\gamma_0 c_{00}^{(3)} - \frac{1}{R_{\text{eff}}^3} B_{00}^{(1)} = \gamma_0 d_{00}^{(3)}. \tag{17}$$

Similarly, by equating the coefficients of $\boldsymbol{S}_{2s}^{(1)}$ and $\boldsymbol{S}_{2s}^{(3)}$ ($s = 0, 1, 2$), one obtains

$$\begin{aligned} 2c_{2s}^{(1)} + \frac{(2+s)!(2-s)!}{R_{\text{eff}}^3}\left(\frac{2}{R_{\text{eff}}^2} B_{2s}^{(1)} + 2\beta_{-3} B_{2s}^{(3)}\right) &= 2d_{2s}^{(1)}, \\ 2c_{2s}^{(1)} + \frac{(2+s)!(2-s)!}{R_{\text{eff}}^3}\left(-\frac{3}{R_{\text{eff}}^2} B_{2s}^{(1)} + \gamma_{-3} B_{2s}^{(3)}\right) &= 2d_{2s}^{(1)}, \end{aligned} \tag{18}$$

In view of $\gamma_{-3} - 2\beta_{-3} = 1$, we find that

$$\frac{B_{2s}^{(1)}}{R_{\text{eff}}^2} = \frac{1}{5} B_{2s}^{(3)}. \tag{19}$$

By eliminating $B_{2s}^{(1)}$ using (19) and taking into account that $\beta_{-3}(\nu) = (1-2\nu)/3$, (18) reduces to

$$c_{2s}^{(1)} + \frac{(2+s)!(2-s)!}{R_{\text{eff}}^3} \frac{(8-10\nu_0)}{15} B_{2s}^{(3)} = d_{2s}^{(1)}. \tag{20}$$

The same procedure is employed to fulfill the second condition in (10), namely $\boldsymbol{T}_r\big(\boldsymbol{u}^{(0)}\big) = \boldsymbol{T}_r\big(\boldsymbol{u}^{(1)}\big)$. With the aid of (A.9) and (A.11) we write

$$\boldsymbol{T}_r(\boldsymbol{u}_{\text{far}}) = c_{00}^{(3)} 2\mu_0 g_0(\nu_0) \boldsymbol{S}_{00}^{(3)} + 2\mu_0 \sum_{|s|\le 2} c_{2s}^{(1)} \frac{1}{(2+s)!}\big(\boldsymbol{S}_{2s}^{(1)} + 2\boldsymbol{S}_{2s}^{(3)}\big), \tag{21}$$

$$\boldsymbol{T}_r(\boldsymbol{u}_{\text{dis}}) = B_{00}^{(1)} \frac{4\mu_0}{R_{\text{eff}}^3} \boldsymbol{S}_{00}^{(3)} + 2\mu_0 \sum_{|s|\le 2} \frac{(2-s)!}{r^3}\left[-B_{2s}^{(1)} 4 \frac{1}{R_{\text{eff}}^2}\big(\boldsymbol{S}_{2s}^{(1)} - 3\boldsymbol{S}_{2s}^{(3)}\big) + B_{2s}^{(3)}\big(b_{-3}\boldsymbol{S}_{2s}^{(1)} + g_{-3}\boldsymbol{S}_{2s}^{(3)}\big)\right], \tag{22}$$

and

$$\boldsymbol{T}_r\big(\boldsymbol{u}^{(1)}\big) = \gamma_0 s_{00}^{(3)} \boldsymbol{S}_{00}^{(3)} + \sum_{|s|\le 2} s_{2s}^{(1)} \frac{1}{(2+s)!}\big(\boldsymbol{S}_{2s}^{(1)} + 2\boldsymbol{S}_{2s}^{(3)}\big). \tag{23}$$

The coefficients $b_t = b_t(\nu_0)$ and $g_t = g_t(\nu_0)$ involved in (22) are defined by (A.10). By using (18), as well as the equalities $2b_{-3} - g_{-3} = 4$ and $b_{-3}(\nu) = (1+\nu)/3$, we obtain the following linear equations:

$$2\mu_0 g_0 c_{00}^{(3)} + \frac{4\mu_0}{R_{\text{eff}}^3} B_{00}^{(1)} = \gamma_0 s_{00}^{(3)}, \tag{24}$$

$$c_{2s}^{(1)} - \frac{(2+s)!(2-s)!}{R_{\text{eff}}^3} \frac{(7-5\nu_0)}{15} B_{2s}^{(3)} = \frac{s_{2s}^{(1)}}{2\mu_0} \quad (s = 0, 1, 2). \tag{25}$$

The system of (17), (18), (24), and (25) represents a complete set of four real and four complex algebraic equations (twelve real equations in total) needed to find all the unknown coefficients (six real coefficients D_{ij} of (8) and two real ($B_{00}^{(1)}$ and $B_{20}^{(3)}$) and two complex ($B_{21}^{(3)}$ and $B_{22}^{(3)}$) coefficients of (3)). This system is uniquely resolved to get all the series expansion coefficients in (2) and (7).

3. The cluster problem

Consider an infinite elastic isotropic matrix with shear modulus μ_0 and Poisson's ratio ν_0 containing a cluster of N nonoverlapping isotropic elastic spherical particles, of the same radii R and elastic properties μ_1 and ν_1, perfectly bonded to the matrix. In the global Cartesian coordinate frame $Ox_1x_2x_3$, the center of p-th particle is specified by vector $\boldsymbol{R}_p$. The entire system is subjected to the uniform far-field strain $\boldsymbol{E} = E_{ij}\boldsymbol{i}_i\boldsymbol{i}_j$. In the following this problem is referred to as a finite cluster model (FCM) of the composite.

The solution of the problem is described in detail in [Kushch et al. 2011], where it was obtained for the case of more general interface conditions. The solution procedure employs the superposition principle. Specifically, $\boldsymbol{u}_{\text{dis}}(\boldsymbol{r})$ of (1) is sought as a superposition of the disturbance fields of (2) (vanishing at infinity) caused by each particle separately:

$$\boldsymbol{u}_{\text{dis}}(\boldsymbol{r}) = \sum_{p=1}^{N} \sum_{i,t,s} A_{ts}^{(i)(p)} \boldsymbol{U}_{ts}^{(i)}(\boldsymbol{r} - \boldsymbol{R}_p), \tag{26}$$

where $\boldsymbol{U}_{ts}^{(i)}$ are the irregular vector functions (vanishing at infinity) defined by (A.7) and $A_{ts}^{(i)(p)}$ are the multipole expansion coefficients related to the p-th particle. The displacement vector within the particle is bounded but not linear (due to the interactions between the particles in the cluster) and, therefore, is represented by the *infinite* series of the regular functions $\boldsymbol{u}_{ts}^{(i)}$ defined by (A.5):

$$\boldsymbol{u}^{(p)}(\boldsymbol{r}) = \sum_{i,t,s} d_{ts}^{(i)(p)} \boldsymbol{u}_{ts}^{(i)}(\boldsymbol{r}). \tag{27}$$

An infinite system of linear equations for the unknown coefficients $A_{ts}^{(i)(p)}$ and $d_{ts}^{(i)(p)}$ is obtained from the interface conditions of (10), written for each particle, using the orthogonality properties of vector spherical harmonics. For this purpose, the matrix displacement $\boldsymbol{u}^{(0)}$ given by (1) and (26) should be expanded in the local spherical coordinates of each specific particle with the aid of the reexpansion formulas for $\boldsymbol{U}_{ts}^{(i)}$ due to shift of the coordinate frame [Kushch 1985; 2013] The system is solved numerically after the series of (26) and (27) are truncated (see [Kushch et al. 2011] for more details).

4. Effective stiffness of the composite using the generalized Maxwell approach

The generalized Maxwell concept of equivalent inhomogeneity implies that the effective stiffness tensor of the composite can be obtained by comparing the far-field asymptotic behavior of the displacements for the solutions obtained in Sections 2 and 3. Specifically, we equate the dipole moments of an entire cluster of particles to those of an equivalent spherical inhomogeneity with the effective elastic moduli to be found. The radius R_{eff} of the equivalent inhomogeneity is defined by Maxwell [1873] so as to preserve the volume fraction c of the inhomogeneities in the cluster, which results in

$$R_{\text{eff}}^3 = NR^3/c. \tag{28}$$

A comparison of the displacements given by (2) and (26) yields the following relation:

$$B_{i-1,s}^{(i)} = \sum_{p=1}^{N} A_{i-1,s}^{(i)(p)}, \quad i = 1, 2, 3. \tag{29}$$

In fact, (29) for $i = 2$ is a trivial identity because $B_{1s}^{(2)} = A_{1s}^{(2)} = 0$, due to the equilibrium conditions (see the Appendix and the text preceding (3)). Equation (29) is a formal expression of the generalized Maxwell concept which consists in equating the dipole moments of an entire cluster to those of an equivalent inhomogeneity whose the effective elastic moduli are to be found.

The complete numerical procedure that utilizes the generalized Maxwell concept includes the following steps:

(a) identification of the cluster of N inhomogeneities that adequately represent the composite material in question,

(b) solution of the cluster problem for any given $\boldsymbol{E}$ to get a whole set of the series expansion coefficients $A_{ts}^{(i)(p)}$,

(c) evaluation of the dipole coefficients $B_{i-1,s}^{(i)}$ of the equivalent inhomogeneity from the relation (29),

(d) substitution of the coefficients $B_{i-1,s}^{(i)}$ into (17) and (18) to obtain the coefficients $d_{00}^{(3)}$ and $d_{2s}^{(1)}$ (these are later used to recover the coefficients D_{ij} from (8)),

(e) substitution of the coefficients $B_{i-1,s}^{(i)}$ into (24) and (25) to obtain the coefficients $s_{00}^{(3)}$ and $s_{2s}^{(1)}$ (these are later used to recover the coefficients S_{ij} from (13)), and

(f) determination of the effective stiffness tensor $\boldsymbol{C}^*$ from the constitutive relation $\boldsymbol{S} = \boldsymbol{C}^* : \boldsymbol{D}$. In order to determine all the components of this tensor, steps (b)–(e) need to be performed for six linearly independent realizations of the tensor $\boldsymbol{E}$, for example, for $E_{11}\boldsymbol{i}_1\boldsymbol{i}_1$, $E_{22}\boldsymbol{i}_2\boldsymbol{i}_2$, $E_{33}\boldsymbol{i}_3\boldsymbol{i}_3$, $E_{13}(\boldsymbol{i}_1\boldsymbol{i}_3 + \boldsymbol{i}_3\boldsymbol{i}_1)$, $E_{23}(\boldsymbol{i}_2\boldsymbol{i}_3 + \boldsymbol{i}_3\boldsymbol{i}_2)$, and $E_{12}(\boldsymbol{i}_1\boldsymbol{i}_2 + \boldsymbol{i}_2\boldsymbol{i}_1)$.

This procedure is illustrated below for the case of periodic composite material with simple cubic (SC) packing of isotropic spherical particles embedded into isotropic matrix.

4.1. ***Cubic symmetry.*** Consider the periodic composite with SC packing of spherical elastic particles. The cluster of $N = n^3$ particles representing the material is shown on the left in Figure 1 (n is the number of particles in each of the coordinate directions). This composite is known to be macroscopically anisotropic and is characterized by three independent elastic moduli C_{1111}^*, C_{1122}^*, and C_{1212}^* ($C_{2222}^* = C_{3333}^* = C_{1111}^*$, $C_{2233}^* = C_{3311}^* = C_{1122}^*$, and $C_{2323}^* = C_{3131}^* = C_{1212}^*$). Alternatively, the overall behavior can be characterized by the effective bulk modulus k^* and two shear moduli μ_1^* and μ_2^* as follows:

$$k^* = \frac{(C_{1111}^* + 2C_{1122}^*)}{3}, \quad \mu_1^* = \frac{(C_{1111}^* - C_{1122}^*)}{2}, \quad \mu_2^* = C_{1212}^*. \tag{30}$$

In these notations, the generalized Hooke's law $\boldsymbol{S} = \boldsymbol{C}^* : \boldsymbol{D}$ is written as

$$\begin{aligned} S_{11} + S_{22} + S_{33} &= 3k^*(D_{11} + D_{22} + D_{33}), \\ 2S_{33} - S_{11} - S_{22} &= 2\mu_1^*(2D_{33} - D_{11} - D_{22}), \\ S_{11} - S_{22} - 2\mathrm{i}S_{12} &= 2\mu_1^*(D_{11} - D_{22}) - 4\mathrm{i}\mu_2^* D_{12}. \end{aligned} \tag{31}$$

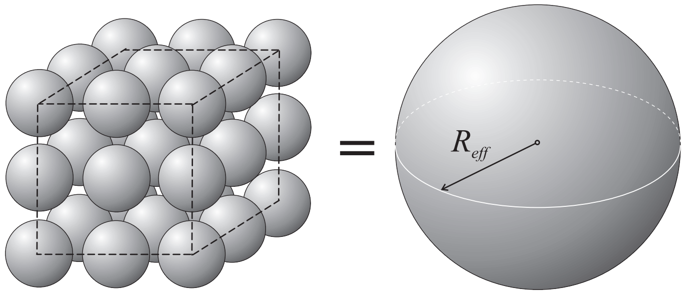

Figure 1. Maxwell's equivalence principle: (left) the finite cluster model (FCM) and (right) the equivalent inhomogeneity.

4.1.1. *Effective bulk modulus.* Consider the far-field strain field characterized by nonzero components $E_{11} = E_{22} = E_{33} = 1$. The algebraic manipulations with (5), (8), (17), (24), and (31) and the use of the identity

$$\frac{g_0(\nu_0)}{\gamma_0(\nu_0)} = \frac{1+\nu_0}{1-2\nu_0} = \frac{3k_0}{2\mu_0} \tag{32}$$

yield the following relations:

$$1 - B_{00}^{(1)} \frac{1}{R_{\text{eff}}^3} = \frac{(D_{11}+D_{22}+D_{33})}{3}, \quad 3k_0 + \frac{4\mu_0}{R_{\text{eff}}^3} B_{00}^{(1)} = 3k^* \frac{(D_{11}+D_{22}+D_{33})}{3}, \tag{33}$$

which reduce to

$$3k_0 + 4\mu_0 \frac{B_{00}^{(1)}}{R_{\text{eff}}^3} = 3k^* \left(1 - \frac{B_{00}^{(1)}}{R_{\text{eff}}^3}\right). \tag{34}$$

Using (29) and the Maxwell definition of volume fraction given by (28), one gets

$$\frac{B_{00}^{(1)}}{R_{\text{eff}}^3} = \frac{c}{NR^3} \sum_{p=1}^{N} A_{00}^{(1)(p)} = c\langle A_{00}^{(1)} \rangle, \tag{35}$$

where $\langle A_{00}^{(1)} \rangle$ is the mean dipole moment. Combination of the last two equations leads to the following expression for the effective bulk modulus k^*:

$$\frac{k^*}{k_0} = \frac{1 + (4\mu_0)/(3k_0) c\langle A_{00}^{(1)} \rangle}{1 - c\langle A_{00}^{(1)} \rangle}. \tag{36}$$

4.1.2. *Effective shear modulus μ_1^*.* Consider the far-field strain field characterized by nonzero components $E_{33} = 1$ and $E_{11} = E_{22} = -E_{33}/2$. The only nonzero coefficient of (5) is $c_{20}^{(1)} = 1$. Using (20) and (25) with $s = 0$ as well as (31), one gets the following system of equations:

$$\begin{aligned} 1 + \frac{4}{R_{\text{eff}}^3} \frac{(8-10\nu_0)}{15} B_{20}^{(3)} &= \frac{(2D_{33} - D_{11} - D_{22})}{3}, \\ 1 - \frac{4}{R_{\text{eff}}^3} \frac{(7-5\nu_0)}{15} B_{20}^{(3)} &= \frac{\mu_1^*}{\mu_0} \frac{(2D_{33} - D_{11} - D_{22})}{3}. \end{aligned} \tag{37}$$

The system of (37), with the use of expression (29), yields the following solution for the effective shear modulus μ_1^*:

$$\frac{\mu_1^*}{\mu_0} = \frac{1-(7-5\nu_0)\frac{4}{15}c\langle A_{20}^{(1)}\rangle}{1+(8-10\nu_0)\frac{4}{15}c\langle A_{20}^{(1)}\rangle}, \tag{38}$$

where the mean dipole $\langle A_{2s}^{(1)}\rangle$ is defined as

$$\langle A_{2s}^{(1)}\rangle = \frac{1}{NR^3}\sum_{p=1}^{N} A_{2s}^{(1)(p)}. \tag{39}$$

4.1.3. *Effective shear modulus μ_2^*.* Now consider the far-field strain field characterized by nonzero component $E_{12}=1$. The only nonzero coefficient of (5) is $c_{22}^{(1)}=-2\mathrm{i}$. Using (20) and (25) with $s=2$ as well as (31), one gets the following system of equations:

$$\begin{aligned} -2\mathrm{i}+24\frac{(8-10\nu_0)}{15}\frac{B_{22}^{(3)}}{R_{\text{eff}}^3} &= D_{11}-D_{22}-2\mathrm{i}D_{12},\\ -2\mathrm{i}+24\frac{(-7+5\nu_0)}{15}\frac{B_{22}^{(3)}}{R_{\text{eff}}^3} &= \frac{\mu_1^*}{\mu_0}(D_{11}-D_{22})-2\mathrm{i}\frac{\mu_2^*}{\mu_0}D_{12}. \end{aligned} \tag{40}$$

Using (29) and separating the imaginary parts in the equations of system (40), the following solution for the effective shear modulus μ_2^* is obtained:

$$\frac{\mu_2^*}{\mu_0} = \frac{1+(7-5\nu_0)\frac{4}{5}c\langle \operatorname{Im} A_{22}^{(1)}\rangle}{1-(8-10\nu_0)\frac{4}{5}c\langle \operatorname{Im} A_{22}^{(1)}\rangle}. \tag{41}$$

4.1.4. *Noninteracting estimates.* In the case when the interactions between the particles are neglected, the cluster problem reduces to a set of N uncoupled single-particle problems, as in the original Maxwell approach. Hence,

$$\langle A_{00}^{(1)}\rangle = \frac{k_1-k_0}{k_1+\frac{4}{3}\mu_0}, \tag{42}$$

$$\langle A_{20}^{(1)}\rangle = \frac{15}{4}\,\frac{\mu_0-\mu_1}{(8-10\nu_0)\mu_1+(7-5\nu_0)\mu_0}, \tag{43}$$

$$\langle \operatorname{Im} A_{22}^{(1)}\rangle = \frac{5}{4}\,\frac{\mu_0-\mu_1}{(8-10\nu_0)\mu_1+(7-5\nu_0)\mu_0}. \tag{44}$$

It could be shown that, in this case, the estimates of (36) for the effective bulk modulus reduce to those of [Kerner 1956; McCartney and Kelly 2008; McCartney 2010], and to one of the Hashin and Shtrikman [1963] bounds. They also coincide with the estimates of the composite sphere assemblage, the Mori–Tanaka method, and those of the generalized self-consistent method (for example, [Milton 2002; McCartney and Kelly 2008]). The estimates of (38) for the effective shear modulus μ_1^* and the estimates of (41) for the effective shear modulus μ_2^* coincide and reduce to those of [Kerner 1956; McCartney and Kelly 2008; McCartney 2010] and to the one of the Hashin and Shtrikman [1963] bounds. They also coincide with the estimates of the composite sphere assemblage and the Mori–Tanaka method (for example, [Milton 2002; McCartney and Kelly 2008]).

It can be concluded that noninteracting estimates *cannot* capture the overall, microstructure induced, anisotropy of the composite material.

5. Numerical study

5.1. ***Periodic (SC) composite.*** In order to test the developed approach, we evaluate three effective elastic moduli of the periodic composite with simple cubic (SC) arrangement of particles considered in Section 4.1 (the representative cluster is depicted in Figure 1, left). Accurate values of the effective moduli of such composites are reported by Kushch [1987] and Sangani and Lu [1987], who provided complete solutions of the triple periodic homogenization problem. Their results are practically identical except for in the value of $\mu_2^*(c)/\mu_0$ for porous material. It was suggested by Cohen [2004] that the estimates of [Sangani and Lu 1987] might be inaccurate. Therefore, in the subsequent analysis, all the periodic (SC) solutions have been recalculated with $t_{\max} = 20$ and used as reference solutions. In addition, various bounds and approximate estimates are available (for example, [Milton 2002; Cohen and Bergman 2003; Cohen 2004]) and are used for comparison.

In order to provide comparison with the numerical data reported in the above cited works, in the following studies, as in [Kushch 1987; Sangani and Lu 1987], we assume $\nu_0 = \nu_1 = 0.3$. The equivalent inhomogeneity (Figure 1, right) is assumed to be anisotropic and to possess cubic symmetry of elastic properties with three independent elastic moduli defined by (30).

First simulations are conducted to analyze the convergence rate of the generalized Maxwell solution in terms of the cluster's size. The three effective elastic moduli for high-contrast composite ($\mu_1/\mu_0 = 100$) are presented in Table 1 for the values $n = 1, 2, 3, 4$ and two volume fractions c ($c = 0.1$ and $c = 0.5$). The packing limit for the SC composite is $c_{\max} = \pi/6 \approx 0.5236$. The extreme cases we study in this part are deliberately designed to test the developed method.

Here and below, the series of (26) and (27) are truncated at $t_{\max} = 13$. This number was sufficient to provide numerical solutions for dipole coefficients $A_{0s}^{(1)(p)}$ and $A_{2s}^{(3)(p)}$ that are accurate up to four significant digits for $c \le 0.45$ and up to at least three significant digits for $c = 0.5$. The last row of Table 1 contains values of SC results from [Kushch 1987; Sangani and Lu 1987] that are accurate up to four significant digits. It is seen from Table 1 that for $c = 0.5$ the value of $n = 4$ is sufficient to estimate all three moduli with accuracy of about 5%. This seems to be a good result, in view of the fact that $c = 0.5$ is near the packing limit ($c_{\max} = 0.5236$) and the contrast between the particles and the matrix is very high (almost rigid particles). For $c = 0.1$ the convergence rate is higher, especially for the relative bulk modulus k^*/k_0. Therefore, in the subsequent numerical studies the value $n = 4$ has been adopted.

The generalized Maxwell approach is capable of capturing the microstructure-induced overall anisotropy of the material (quite pronounced for $c = 0.5$, $\mu_1^*/\mu_2^* \approx 2$), whereas the noninteracting approach predicts macroscopic isotropy ($\mu_2^* = \mu_1^*$).

The simulations to follow are conducted for porous ($\mu_1 = 0$), moderate contrast ($\mu_1/\mu_0 = 10$), and high-contrast ($\mu_1/\mu_0 = 100$) composite materials and for a wide range of volume fractions. The normalized effective moduli k^*/k_0, $\mu_1^*(c)/\mu_0$, and $\mu_2^*(c)/\mu_0$ obtained using the generalized Maxwell approach, labeled FCM, are presented in Tables 2, 3, and 4, respectively, where they are compared with the SC

	$c = 0.1$			$c = 0.5$		
n	k^*/k_0	μ_1^*/μ_0	μ_2^*/μ_0	k^*/k_0	μ_1^*/μ_0	μ_2^*/μ_0
1	1.176	1.228	1.228	2.564	3.015	3.015
2	1.176	1.247	1.217	2.928	4.881	3.242
3	1.176	1.254	1.214	3.098	6.160	3.301
4	1.176	1.258	1.212	3.184	7.024	3.330
SC	1.176	1.263	1.209	3.287	6.697	3.399

Table 1. Convergence of the FCM solution to the exact solution in terms of the cluster size, n.

	k^*/k_0			μ_1^*/μ_0			μ_2^*/μ_0		
c	SC	FCM	C&B	SC	FCM	C&B	SC	FCM	C&B
0.10	0.774	0.774	0.774	0.841	0.839	0.841	0.812	0.814	0.812
0.20	0.602	0.601	0.604	0.718	0.712	0.719	0.640	0.644	0.641
0.30	0.465	0.462	0.471	0.609	0.600	0.612	0.490	0.494	0.496
0.40	0.348	0.343	0.364	0.504	0.495	0.512	0.360	0.360	0.379
0.45	0.295	0.289	0.318	0.450	0.443	0.463	0.301	0.298	0.330
0.50	0.242	0.238	0.276	0.393	0.389	0.413	0.243	0.237	0.288

Table 2. Comparison of normalized effective moduli of porous solid.

solutions. In addition, these tables contain the results predicted by the approximate formulas proposed for the cubic arrays by Cohen and Bergman [2003] and Cohen [2004], labeled C&B.

These formulas have the following forms [Cohen and Bergman 2003; Cohen 2004]:

$$\frac{k^*}{k_0} = 1 - \frac{c}{k_0/(k_0 - k_1) - 3k_0(1-c)/(3k_0 + 4\mu_0)}, \tag{45}$$

$$\frac{\mu_1^*}{\mu_0} = 1 - \frac{c(1 - \mu_1/\mu_0)}{1 - (1 - c + G_1)s_2}, \tag{46}$$

$$\frac{\mu_2^*}{\mu_0} = 1 - \frac{c(1 - \mu_1/\mu_0)}{1 - (1 - c + G_2)s_2}, \tag{47}$$

where

$$\begin{aligned} &G_1 = (3k_0 + \mu_0)(-0.929c + 1.1422c^{5/3})/(k_0 + 2\mu_0), \quad G_2 = -2G_1/3, \\ &s_2 = 1.2(k_0 + 2\mu_0)(1 - \mu_1/\mu_0)/(3k_0 + 4\mu_0). \end{aligned} \tag{48}$$

Expression (45) coincides with that of (36) and (42), which means that it does not include the effects of particles' interactions. In the case of porous materials Cohen [2004, Tables 2 and 3] showed that estimates (45)–(47) are in good agreement with those of [Iwakuma and Nemat-Nasser 1983], while the results of [Kushch 1987; Sangani and Lu 1987] for the bulk modulus are in good agreement with those of [Torquato 1998].

	k^*/k_0			μ_1^*/μ_0			μ_2^*/μ_0		
c	SC	FCM	C&B	SC	FCM	C&B	SC	FCM	C&B
0.10	1.150	1.150	1.150	1.208	1.204	1.208	1.173	1.175	1.173
0.20	1.331	1.331	1.330	1.504	1.490	1.500	1.363	1.369	1.361
0.30	1.558	1.561	1.551	1.915	1.890	1.890	1.593	1.604	1.581
0.40	1.869	1.872	1.829	2.492	2.467	2.375	1.907	1.919	1.856
0.45	2.087	2.083	1.996	2.873	2.865	2.646	2.130	2.137	2.024
0.50	2.391	2.378	2.189	3.348	3.381	2.927	2.463	2.446	2.222

Table 3. Comparison of normalized effective moduli of moderate contrast ($\mu_1/\mu_0 = 10$) composite.

	k^*/k_0			μ_1^*/μ_0			μ_2^*/μ_0		
c	SC	FCM	C&B	SC	FCM	C&B	SC	FCM	C&B
0.10	1.176	1.176	1.176	1.263	1.258	1.263	1.209	1.212	1.209
0.20	1.397	1.399	1.396	1.676	1.653	1.669	1.445	1.455	1.442
0.30	1.690	1.694	1.677	2.336	2.287	2.270	1.746	1.765	1.723
0.40	2.137	2.139	2.048	3.505	3.449	3.106	2.208	2.230	2.092
0.45	2.514	2.508	2.284	4.556	4.570	3.610	2.599	2.609	2.330
0.50	3.287	3.184	2.564	6.697	7.024	4.156	3.399	3.330	2.623

Table 4. Comparison of normalized effective moduli of high-contrast ($\mu_1/\mu_0 = 100$) composite.

It can be seen from Tables 2–4 that the generalized Maxwell approach provides estimates of the effective stiffnesses of composites consistent with SC results for the considered range of c and μ_1/μ_0. On the other hand, the approximate expressions of [Cohen and Bergman 2003; Cohen 2004], in general, provide accurate estimates only for low volume fractions of particles for high-contrast composites, as suggested by the authors themselves.

The normalized effective moduli $k^*(c)/k_0$, $\mu_1^*(c)/\mu_0$, and $\mu_2^*(c)/\mu_0$ of the high-contrast composite ($\mu_1/\mu_0 = 100$) are also plotted in Figure 2, in which the FCM-based results ($n = 4$) are marked by open and solid circles, the dash-dotted lines represent the noninteracting approach, the solid and dashed lines represent the SC solution of [Kushch 1987], and the open and solid triangles represent the results of [Cohen 2004].

In addition, in Table 5, we verified that the effective shear moduli $\mu_1^*(c)$ and $\mu_2^*(c)$ of high-contrast composite ($\mu_1/\mu_0 = 100$, $\nu_0 = \nu_1 = 0.3$) obtained with both SC and FCM models satisfy the following inequalities developed for a composite with cubic symmetry [Milton 2002]:

$$\frac{3c}{2[\mu_1^*(c)-\mu_0]}+\frac{c}{\mu_2^*(c)-\mu_0}\le\frac{5}{2(\mu_1-\mu_0)}+\frac{3(1-c)(k_0+2\mu_0)}{\mu_0(3k_0+4\mu_0)}, \tag{49}$$

$$\frac{3(1-c)}{2[\mu_1-\mu_1^*(c)]}+\frac{(1-c)}{\mu_1-\mu_2^*(c)}\le\frac{5}{2(\mu_1-\mu_0)}-\frac{3c(k_1+2\mu_1)}{\mu_1(3k_1+4\mu_1)}. \tag{50}$$

As can be seen from Table 5, the noninteracting estimates coincide with the right-hand side of inequality (49), while they also fulfill inequality (50). The estimates based on Cohen and Bergman's formulas

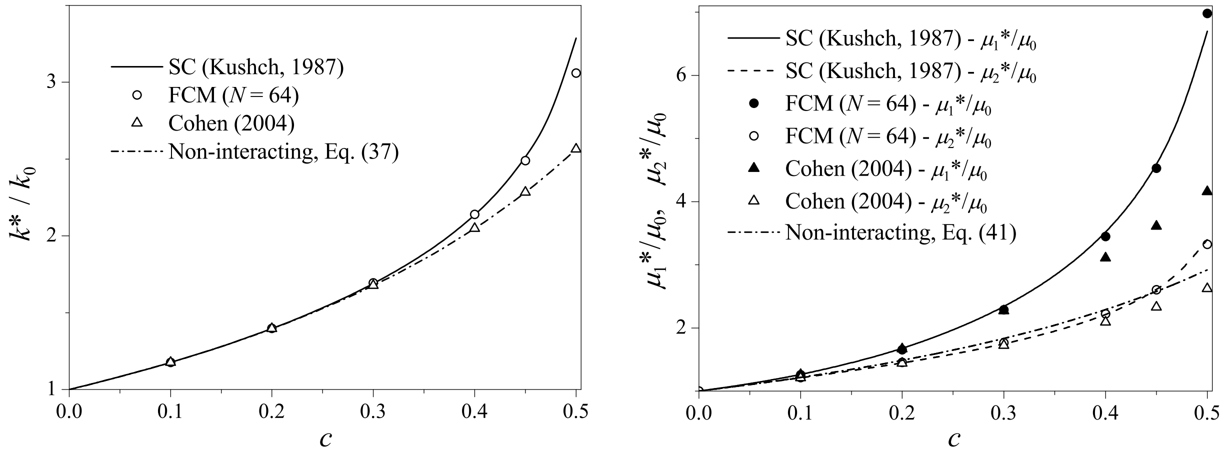

Figure 2. Normalized effective bulk modulus (left) and shear moduli (right) of high-contrast ($\mu_1/\mu_0 = 100$) composite with SC array of spherical particles.

	LHS (49)					LHS (50)				
c	(43)	C&B	FCM	SC	RHS (49)	(43)	C&B	FCM	SC	RHS (50)
0.10	1.0967	1.048	1.053	1.049	1.0967	0.023	0.023	0.023	0.023	0.0241
0.20	0.9776	0.901	0.899	0.893	0.9776	0.020	0.020	0.020	0.020	0.0229
0.30	0.8586	0.769	0.742	0.739	0.8586	0.018	0.018	0.018	0.018	0.0217
0.40	0.7395	0.651	0.570	0.571	0.7395	0.015	0.015	0.015	0.015	0.0205
0.45	0.6800	0.597	0.472	0.471	0.6800	0.014	0.014	0.014	0.014	0.0199
0.50	0.6205	0.546	0.341	0.340	0.6205	0.013	0.013	0.013	0.013	0.0193

Table 5. The values of the left and right-hand sides (LHS and RHS) of (49) and (50) for $\mu_1/\mu_0 = 100$.

(46) and (47) also satisfy both inequalities. Interestingly the combination involved in the left-hand side of (50) is the same (up to three significant digits) for all four methods considered.

5.2. ***Random composite.*** In this section the generalized Maxwell approach is used to evaluate the effective elastic stiffness of random particulate composites. In the case of statistically uniform random microstructure, the composite is known to be macroscopically isotropic and characterized by two elastic moduli, k^* and μ^*.

The representative finite clusters of such material are constructed by random generations of particles in a cube by employing the molecular dynamics algorithm for growing particles used in [Sangani and Mo 1997]. To provide statistical validity to the results, the simulation data are averaged over 20 random configurations. The standard error of the mean (the standard deviation divided by the square root of the number of configurations) is indicated in Tables 6 and 7, with the error estimate for the last significant digit enclosed in parentheses. For example, 4.35(3) means 4.35 ± 0.03.

In Table 6, the normalized effective bulk (k^*/k_0) and shear (μ^*/μ_0) moduli of the rigid particle composite ($\mu_1 = \infty$) are presented for a wide range of volume fractions: $c = 0.1, 0.25, 0.45, 0.6$. In order to check isotropy of the model, the normalized shear modulus was estimated using both (38) and

	k^*/k_0			μ^*/μ_0			
c	(36)	S&M	(42)	(38)	(41)	S&M	(43)
0.10	1.184(0)	1.183(1)	1.179	1.245(0)	1.244(0)	1.242(2)	1.233
0.25	1.569(2)	1.60(1)	1.538	1.794(3)	1.775(2)	1.85(2)	1.700
0.45	2.55(1)	2.53(1)	2.322	3.32(2)	3.32(3)	3.42(3)	2.718
0.60	4.22(3)	4.35(3)	3.423	6.5(1)	6.2(2)	6.6(1)	4.15

Table 6. Normalized effective moduli of random composite with rigid particles.

	k^*/k_0			μ^*/μ_0			
c	(36)	S&M	(42)	(38)	(41)	S&M	(43)
0.10	0.771(0)	0.771(1)	0.774	0.821(0)	0.821(0)	0.820(1)	0.825
0.25	0.522(0)	0.520(1)	0.533	0.599(0)	0.596(1)	0.588(3)	0.611
0.45	0.294(1)	0.299(1)	0.318	0.364(1)	0.351(3)	0.355(2)	0.390
0.60	0.168(1)	0.177(1)	0.202	0.219(1)	0.202(4)	0.205(1)	0.259

Table 7. Normalized effective moduli of random porous solid.

(41). Also, Table 6 contains the data obtained by the accurate approach of [Sangani and Mo 1997], labeled S&M, and that obtained by noninteracting method of [McCartney 2010], labeled with (42) and (43).

In order to provide macroscopic isotropy of the composite, the simulations in [Sangani and Mo 1997] have been conducted with $N = 32$ for $c = 0.6$ and with $N = 16$ for other volume fractions. In our computations, as before, $N = 64$ and $t_{\max} = 13$. As seen from Table 6, the modified Maxwell approach provides good estimates for a whole range of c: for $c \leq 0.45$, the difference between the estimates for k^*/k_0 obtained with the generalized Maxwell approach and those reported in [Sangani and Mo 1997] does not exceed the statistical error margins. Note that the configurations with $c > 0.49$ strongly depend on the method used in generating the random microstructure and on the value of N (since, at such high c, the hard-sphere system may be in a metastable fluid state, a semicrystalline state, or a disordered glassy state; for example, [Rintoul and Torquato 1996; Sangani and Mo 1997; Sierou and Brady 2001]). However, even for $c = 0.6$ the relative error in the estimates for k^*/k_0 obtained from (36) is about 4%. At the same time, underestimation of the effective stiffness by the noninteracting Maxwell method is of the order of 22% for the normalized bulk modulus and 38% for the normalized shear modulus. A minor anisotropy (within 5%) predicted by (38) and (41) can be due to the cubic shape of finite cluster we used and/or the specific N ($= 4^3 = 64$) where the semicrystalline arrangement of particles in the generated configuration is likely. This issue deserves separate consideration.

The analogous data for the porous solid are collected in Table 7. Here, we observe the same tendencies and patterns as in the previous case, with the only difference being that this time the standard (noninteracting) Maxwell procedure overestimates k^*/k_0 and μ^*/μ_0 for $c = 0.6$ by 15% and 26%, respectively. The use of the generalized Maxwell procedure reduces the error for k^*/k_0 to 5% and for μ^*/μ_0 to 1–7%. For $c < 0.6$, an accuracy of the suggested method is even higher, see Tables 6 and 7.

6. Conclusions

In this paper the generalized Maxwell approach based on the concept of equivalent anisotropic inhomogeneity is applied for evaluating the anisotropic overall elastic properties of particulate composites with isotropic phases (matrix and spherical particles). A numerical procedure using the approach is outlined for materials with an arbitrary degree of overall anisotropy. This procedure accurately accounts for the geometrical arrangement of particles and their interactions. In a special case of the periodic composite material with simple cubic packing of spherical particles, the closed-form expressions for the three elastic moduli that characterize the overall behavior are provided in terms of dipole coefficients for individual particles. It is demonstrated that noninteracting estimates cannot capture the overall, microstructure-induced anisotropy of the composite materials considered in this work. Illustrative examples involving simple cubic and random composites demonstrate that the approach provides estimates that are consistent with those predicted by the triple-periodic model for the whole range of volume fractions. Based on the results of this work, as well as on the two-dimensional results of [Mogilevskaya and Crouch 2013], it is clear that the approach can be used for the three-dimensional analysis of materials reinforced with particles of arbitrary shapes, if the cluster problem (Section 3) is solved with the boundary element method.

There are several interesting, problem-related issues which are left unresolved/unaddressed in this paper. The first problem is related to the choice of the spherical shape of the equivalent inhomogeneity, which might not adequately represent the shape of the cluster. While this is likely to affect the values of the effective moduli, the reasonable agreement of our results with exact solution for the periodic composite indicates that this effect is rather small. In addition, the recent studies by Sevostianov and Giraud [2012], who investigated the effect of the inhomogeneity's shape on compliance, found that a sphere and a cube of equal volumes possess quite similar compliance tensors. Therefore, it is expected that the dipole moments (apparently expressed in terms of the compliance contribution tensor) would also be similar for the sphere and cube of equal volume. From that point of view, our assumption of spherical shape of the equivalent inhomogeneity should be considered as an approximation which can be refined by taking a more appropriate shape of the cluster or equivalent inhomogeneity. The convergence study in terms of cluster size is a separate problem which also deserves much more attention. In the context of this paper, the most important finding is that macroscopic elastic anisotropy of a composite can be predicted with reasonable accuracy from a relatively small fragment/cluster of the composite structure. In the present work we assumed isotropic constituents of the composite, which means that the macroscopic anisotropy is entirely due to the geometric arrangement of particles. Similar methodology can also be used for composites with anisotropic particles (for example, cubic or transverse isotropic). All of these issues will be addressed in subsequent publications.

Appendix

The vector surface spherical harmonics $\boldsymbol{S}_{ts}^{(i)} = \boldsymbol{S}_{ts}^{(i)}(\boldsymbol{r})$ (for example, [Morse and Feshbach 1953]) are defined in terms of their scalar counterparts, $\chi_t^s = P_t^s(\cos\theta)\exp(\mathrm{i}s\varphi)$, as

$$\boldsymbol{S}_{ts}^{(1)} = r\nabla(\chi_t^s) = \boldsymbol{e}_\theta \frac{\partial}{\partial\theta}\chi_t^s + \frac{\boldsymbol{e}_\varphi}{\sin\theta}\frac{\partial}{\partial\varphi}\chi_t^s,$$
$$\boldsymbol{S}_{ts}^{(2)} = r\nabla\times\left(\boldsymbol{e}_r\chi_t^s\right) = \frac{\boldsymbol{e}_\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\chi_t^s - \boldsymbol{e}_\varphi\frac{\partial}{\partial\theta}\chi_t^s, \tag{A.1}$$

$$\boldsymbol{S}_{ts}^{(3)} = \boldsymbol{e}_r \chi_t^s \quad (t \geq 0, |s| \leq t).$$

These functions constitute a complete and orthogonal set on the sphere S. Specifically,

$$\frac{1}{S}\int_S \boldsymbol{S}_{ts}^{(i)} \cdot \overline{\boldsymbol{S}_{kl}^{(j)}}\, dS = \alpha_{ts}^{(i)} \delta_{tk}\delta_{sl}\delta_{ij}, \tag{A.2}$$

where $\alpha_{ts}^{(1)} = \alpha_{ts}^{(2)} = t(t+1)\alpha_{ts}$ and $\alpha_{ts}^{(3)} = \alpha_{ts} = \dfrac{1}{2t+1}\dfrac{(t+s)!}{(t-s)!}$. The vector surface spherical harmonics satisfy the following useful relations:

$$\boldsymbol{S}_{t,-s}^{(i)} = (-1)^{s+i-1}\overline{\boldsymbol{S}_{ts}^{(i)}}, \quad \boldsymbol{S}_{-(t+1),s}^{(i)} = \boldsymbol{S}_{ts}^{(i)}. \tag{A.3}$$

The complete set of the partial solutions of Lamé's equation

$$\frac{2(1-\nu)}{(1-2\nu)}\nabla(\nabla\cdot\boldsymbol{u}) - \nabla\times\nabla\times\boldsymbol{u} = 0, \tag{A.4}$$

where $\boldsymbol{u}$ is the displacement vector and ν is the Poisson ratio, have been introduced in [Kushch 1985]. The regular (bounded everywhere but $r \to \infty$) complex-value vector functions $\boldsymbol{u}_{ts}^{(i)}$ are written in terms of the vector spherical harmonics $\boldsymbol{S}_{ts}^{(i)}$ of (A.1) as

$$\begin{aligned} \boldsymbol{u}_{ts}^{(1)} &= \frac{r^{t-1}}{(t+s)!}\big(\boldsymbol{S}_{ts}^{(1)} + t\boldsymbol{S}_{ts}^{(3)}\big), \quad \boldsymbol{u}_{ts}^{(2)} = -\frac{1}{(t+1)}\frac{r^t}{(t+s)!}\boldsymbol{S}_{ts}^{(2)}, \\ \boldsymbol{u}_{ts}^{(3)} &= \frac{r^{t+1}}{(t+s)!}\big[\beta_t(\nu)\boldsymbol{S}_{ts}^{(1)} + \gamma_t(\nu)\boldsymbol{S}_{ts}^{(3)}\big], \end{aligned} \tag{A.5}$$

where the coefficients

$$\beta_t(\nu) = \frac{t+5-4\nu}{(t+1)(2t+3)} \quad \text{and} \quad \gamma_t(\nu) = \frac{t-2+4\nu}{(2t+3)} \tag{A.6}$$

are related by $\gamma_t + (t+1)\beta_t \equiv 1$. The irregular (infinitely growing at $r \to 0$ and vanishing at infinity) complex-value functions $\boldsymbol{U}_{ts}^{(i)}$ are

$$\begin{aligned} \boldsymbol{U}_{ts}^{(1)} &= \frac{(t-s)!}{r^{t+2}}\big[\boldsymbol{S}_{ts}^{(1)} - (t+1)\boldsymbol{S}_{ts}^{(3)}\big], \quad \boldsymbol{U}_{ts}^{(2)} = \frac{1}{t}\frac{(t-s)!}{r^{t+1}}\boldsymbol{S}_{ts}^{(2)}, \\ \boldsymbol{U}_{ts}^{(3)} &= \frac{(t-s)!}{r^t}\big[\beta_{-(t+1)}(\nu)\boldsymbol{S}_{ts}^{(1)} + \gamma_{-(t+1)}(\nu)\boldsymbol{S}_{ts}^{(3)}\big]. \end{aligned} \tag{A.7}$$

The traction vector $\boldsymbol{T}_n = \sigma\cdot\boldsymbol{n}$ at the surface $S : r = \text{constant}$ is

$$\frac{1}{2\mu}\boldsymbol{T}_r(\boldsymbol{u}) = \frac{\nu}{1-2\nu}\boldsymbol{e}_r(\nabla\cdot\boldsymbol{u}) + \frac{\partial}{\partial r}\boldsymbol{u} + \frac{1}{2}\boldsymbol{e}_r\times(\nabla\times\boldsymbol{u}). \tag{A.8}$$

For the regular vector functions of (A.5), this results in [Kushch 1985]

$$\begin{aligned} \frac{1}{2\mu}\boldsymbol{T}_r(\boldsymbol{u}_{ts}^{(1)}) &= \frac{(t-1)}{r}\boldsymbol{u}_{ts}^{(1)}, \quad \frac{1}{2\mu}\boldsymbol{T}_r(\boldsymbol{u}_{ts}^{(2)}) = \frac{(t-1)}{2r}\boldsymbol{u}_{ts}^{(2)}, \\ \frac{1}{2\mu}\boldsymbol{T}_r(\boldsymbol{u}_{ts}^{(3)}) &= \frac{r^t}{(t+s)!}\big[b_t(\nu)\boldsymbol{S}_{ts}^{(1)} + g_t(\nu)\boldsymbol{S}_{ts}^{(3)}\big], \end{aligned} \tag{A.9}$$

where

$$b_t(\nu) = (t+1)\beta_t - 2(1-\nu)/(t+1), \quad g_t(\nu) = (t+1)\gamma_t - 2\nu. \tag{A.10}$$

For the irregular solutions $\boldsymbol{U}_{ts}^{(i)}$ of (A.7), the vector takes the following form:

$$\begin{aligned} \frac{1}{2\mu}\boldsymbol{T}_r(\boldsymbol{U}_{ts}^{(1)}) &= -\frac{(t+2)}{r}\boldsymbol{U}_{ts}^{(1)}, \quad \frac{1}{2\mu}\boldsymbol{T}_r(\boldsymbol{u}_{ts}^{(2)}) = -\frac{(t+2)}{2r}\boldsymbol{U}_{ts}^{(2)}, \\ \frac{1}{2\mu}\boldsymbol{T}_r(\boldsymbol{U}_{ts}^{(3)}) &= \frac{(t-s)!}{r^{t+1}}\big[b_{-(t+1)}\boldsymbol{S}_{ts}^{(1)} + g_{-(t+1)}\boldsymbol{S}_{ts}^{(3)}\big] \end{aligned} \tag{A.11}$$

In view of (A.5), $\boldsymbol{T}_r(\boldsymbol{u}_{ts}^{(i)})$ can be represented in terms of vector spherical harmonics of (A.1).

The resultant force $\boldsymbol{T}$ and resultant torque (moment) $\boldsymbol{M}$ acting on the spherical surface $S : r = R$ enclosing the point $\boldsymbol{r} = 0$ are

$$\boldsymbol{T} = \int_S \boldsymbol{T}_r \, dS, \quad \boldsymbol{M} = \int_S \boldsymbol{r} \times \boldsymbol{T}_r \, dS. \tag{A.12}$$

It is readily found that $\boldsymbol{T} = \boldsymbol{M} = 0$ for all the regular functions $\boldsymbol{u}_{ts}^{(i)}$. Among the irregular functions $\boldsymbol{U}_{ts}^{(i)}$, only three functions have nonzero resultant force, namely

$$\boldsymbol{T}\big(\boldsymbol{U}_{10}^{(3)}\big) = 16\mu\pi(\nu-1)\boldsymbol{i}_3, \quad \boldsymbol{T}\big(\boldsymbol{U}_{11}^{(3)}\big) = -\overline{\boldsymbol{T}\big(\boldsymbol{U}_{1,-1}^{(3)}\big)} = 32\mu\pi(\nu-1)(\boldsymbol{i}_1 + \mathrm{i}\boldsymbol{i}_2). \tag{A.13}$$

Hence, $\boldsymbol{U}_{1s}^{(3)}$ can be regarded as vector monopoles. The net resultant torque is zero for all the Lamé solutions except for $\boldsymbol{U}_{1s}^{(2)}$, for which

$$\boldsymbol{M}\big(\boldsymbol{U}_{10}^{(2)}\big) = -8\mu\pi\boldsymbol{i}_3, \quad \boldsymbol{M}\big(\boldsymbol{U}_{11}^{(2)}\big) = \overline{\boldsymbol{M}\big(\boldsymbol{U}_{1,-1}^{(2)}\big)} = -16\mu\pi(\boldsymbol{i}_1 + \mathrm{i}\boldsymbol{i}_2). \tag{A.14}$$

Formulas (A.13) and (A.14) provide an insight into the physical meaning of the irregular vector functions $\boldsymbol{U}_{1s}^{(2)}$ and $\boldsymbol{U}_{1s}^{(3)}$, these being the displacements due to concentrated moment and force, respectively, applied at the point $\boldsymbol{r} = 0$.

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VOLODYMYR I. KUSHCH: vkushch@bigmir.net
Institute for Superhard Materials, National Academy of Sciences of Ukraine, 2 Avtozavodskaya St., Kiev 04074, Ukraine

SOFIA G. MOGILEVSKAYA: mogil003@umn.edu
Department of Civil Engineering, University of Minnesota, 500 Pillsbury Drive SE, Minneapolis, MN 55455, United States
http://www.ce.umn.edu/people/faculty/mogilevs/

HENRYK K. STOLARSKI: stola001@umn.edu
Department of Civil Engineering, University of Minnesota, 500 Pillsbury Drive SE, Minneapolis, MN 55455, United States

STEVEN L. CROUCH: crouch@umn.edu
Department of Civil Engineering, University of Minnesota, 500 Pillsbury Drive SE, Minneapolis, MN 55455, United States
http://www.ce.umn.edu/directory/faculty/crouch

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