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MICROSTRESSES AND EFFECTIVE ELASTIC MODULI OF A SOLID REINFORCED BY PERIODICALLY DISTRIBUTED SPHEROIDAL PARTICLES

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Abstract—The particle composite consisting of a continuous matrix with the spheroidal particles arranged in several triply periodic arrays is considered. The problem on macroscopically uniform stressed state of this composite is solved accurately. The essence of the method used is the representation of a displacement vector by a series of triply periodic partial vectorial solutions of Lame's equation written in a spheroidal basis. Exact satisfaction of the interfacial boundary conditions reduces the primary boundary-value problem to an infinite set of linear algebraic equations. By solving it numerically the displacements, strains and stresses at an arbitrary point of composite can be determined with any desirable accuracy. Analytical averaging of the strain and stress tensors gives the exact expressions for all components of effective elasticity tensor of composite considered. The influence on stress concentration and effective moduli of the structural parameters of composite is investigated and the comparison is made with known approximate solutions.

1. INTRODUCTION

In this paper the elastic isotropic medium containing several triply periodic lattices of aligned spheroidal inclusions is chosen as a model of composite. The choice was made due to the following reasons. First, a spheroid is often used in the theoretical studies as the model shape of disperse phase particles because it allows us to describe within one unified model the variety of inhomogenities, i.e. short fibres, spherical and platelet particles, needle-like and disk cracks, martensite and precipitate blades, etc. Second, the lattice model of composite is very attractive because it provides the estimation of interaction effects for a large number of particles. This interaction greatly influences the composite's properties, especially for the strongly heterogeneous materials with a high volume content of disperse phase. Moreover, the uniform external loading of such a composite produces the periodic strain–stress field. This circumstance gives the possibility of finding an accurate theoretical solution of corresponding periodic boundary-value problem. Third, because the structure model contains the inclusions with different size, shape and properties, it seems to be suitable for the modelling of multiphase and polydisperse composites.

There are several papers where the lattice model was used for a composite with spherical particles and the accurate solutions have been obtained. The effective elastic moduli of a periodic composite with rigid spherical inclusions were found by Nunan and Keller (1984), with non-rigid ones by Kushch (1987) and Sangani and Lu (1987). The microstresses in a periodic composite with spherical particles were studied by Kushch (1985; 1986). As it is shown in these and other papers where the conductivity of periodic composites was studied (e.g. McPhedran and McKenzie, 1978; Suen *et al.*, 1979; Sangani and Yao, 1988), in most cases the lattice model of composite together with the rigorous method of analysis gives a good correlation with experimental data even for the highly heterogeneous materials with near-to-dense packing of disperse phase.

For the periodic composites with a more general ellipsoidal shape of particles only an approximate solution for effective moduli is available (Iwakuma and Nemat-Nasser, 1983). The elastic stresses in such composites were not studied before. The approximate solution of this problem has been obtained by Kushch (1995b), who solved rigorously the problem for a medium with a finite number of spheroidal inclusions. This approach, however, has the following disadvantage: with the number of inclusions increased the numerical solving procedure becomes more and more time-consuming. The only exception here is the case when particles are arranged in a periodic array. For this structure we can generalise the solution mentioned above on an infinite number of inclusions. By this way the single-, doubly- and triply-periodic structures can be considered.

Below we consider the periodic composite consisting of a continuous matrix phase and N lattices of aligned spheroidal particles. This structure is more general in comparison with the single lattice model used commonly. The only exception here is the paper of Sangani and Yao (1988) who studied the conductivity of a medium containing the identical spherical particles arranged in a finite number of simple cubic lattices. These lattices were placed to agree with the particle distribution rule (Percus–Yevick's law) in a real disordered composite material and this model has given good correlation with the experimental data. Within the model proposed in this paper the particles belonging to different lattices may differ by shape, size and properties. Hence, a real opportunity exists to adapt this model closely to a specific real composite material considered by the proper choice of structural parameters.

2. STATEMENT OF THE PROBLEM

Let us consider the homogeneous isotropic elastic medium containing the spheroidal inclusions of N kinds. The inclusions of each kind are ordered in a triply periodic array so that their centres lie in the nodes of lattice with periods a, b and c along three main lattice vectors $\mathbf{e}_a$, $\mathbf{e}_b$ and $\mathbf{e}_c$, respectively. The following two geometrical restrictions are imposed on the structure of the composite. They are the identical orientation of all spheroids and the non-intersecting of any two inclusions. Because the lattice vectors $\mathbf{e}_a$, $\mathbf{e}_b$ and $\mathbf{e}_c$ are the same for each of the N lattices, the resulting structure of the composite is also periodic. Hence, it is possible to define the elementary periodicity unit (structure cell) of this composite containing the centres of exactly one inclusion of each kind (Fig. 1). It should be noted that this periodicity unit is not uniquely defined. We do not suppose the whole inclusion to be lying completely inside the cell. Intersection of the inclusions with the sides of a parallelepiped is possible; the only requirement is that the centres of inclusions do not lie on the boundary of the cell.

Now we introduce N local Cartesian coordinate system (x_p, y_p, z_p) with the origin in the centre of the pth particle and with the O_pz_p axis coinciding with the rotation axis of the spheroid (Fig. 1). We also define the spheroidal coordinates $(f_p, \xi_p, \eta_p, \varphi_p)$ connected with Cartesian ones by (Hobson, 1931)

$$x_p + \mathrm{i}y_p = f_p\bar{\xi}_p\bar{\eta}_p \exp(\mathrm{i}\varphi_p), \quad z_p = f_p\xi_p\eta_p; \tag{1}$$

where

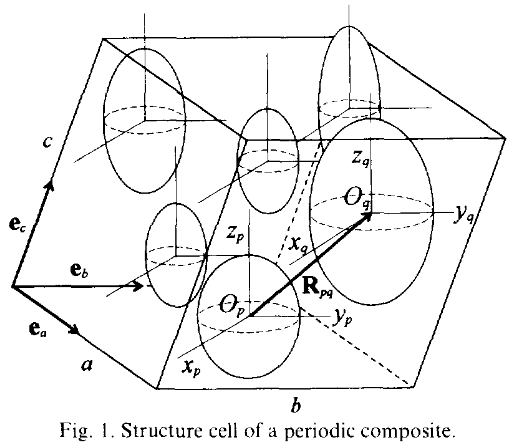


Fig. 1. Structure cell of a periodic composite.

$$\bar{\xi}^2 = \xi^2 - 1, \bar{\eta}^2 = 1-\eta^2; \quad 1 < \xi < \infty, |\eta| \leqslant 1, 0 \leqslant \varphi \leqslant 2\pi.$$

The equalities (1) at fixed $\xi_p = \xi_p^{(0)}$ and $\mathrm{Re}(f_p) > 0$ describe the prolate spheroid with inter-foci distance $2f_p$. To consider the oblate case one must replace ξ_p on $\mathrm{i}\bar{\xi}_p$ and f_p on $(-\mathrm{i}f_p)$ in eqn (1) and all following formulae. The local radius-vectors of the pth and qth coordinate basis are tied by the relation $\mathbf{r}_p = \mathbf{r}_q + \mathbf{R}_{pq}$, where $\mathbf{R}_{pq}$ is the constant vector connecting points O_p and O_q, and determining the reference position of particles with indexes p and q within the elementary structure cell. The placement of the rest of the particles is determined by adding to $\mathbf{R}_{pq}$ of the translation vector $\mathbf{V}_\mathbf{n} = n_1 a\mathbf{e}_a + n_2 b\mathbf{e}_b + n_3 c\mathbf{e}_c$, where n_i are the integers, $-\infty < n_1, n_2, n_3 < \infty$.

We suppose that the stressed state of a composite medium is induced by the remote constant strain tensor $\hat{\mathrm{E}} = \{E_{ij}\}$ prescribed. The displacement vector $\mathbf{u}$ in each phase of the composite satisfies the Lame's equation

$$\frac{2(1-\nu)}{1-2\nu}\nabla(\nabla\cdot\mathbf{u}) - \nabla\times\nabla\times\mathbf{u} = 0, \tag{2}$$

where ν is Poisson's ratio; $\mathbf{u} = \mathbf{u}^{(0)}$, $\nu = \nu_0$ in a matrix, $\mathbf{u} = \mathbf{u}^{(q)}$, $\nu = \nu_q$ in the particle of the qth kind. On interfacial surfaces the continuity conditions of the displacement vector $\mathbf{u}$ and normal stress vector

$$\mathbf{T}_\xi = \sigma_\xi \mathbf{e}_\xi + \tau_{\xi\eta}\mathbf{e}_\eta + \tau_{\xi\varphi}\mathbf{e}_\varphi = 2\mu\left[\frac{\nu}{(1-2\nu)}\mathbf{e}_\xi\nabla\cdot\mathbf{u} + \frac{\bar{\xi}\bar{\eta}}{f}\frac{\partial}{\partial\xi}\mathbf{u} + \frac{1}{2}\mathbf{e}_\xi\times\nabla\times\mathbf{u}\right] \tag{3}$$

are prescribed:

$$[\mathbf{u}^{(0)} - \mathbf{u}^{(q)}]_{\xi_q = \xi_q^{(0)}} = 0; \quad [\mathbf{T}_{\xi_q}(\mathbf{u}^{(0)}) - \mathbf{T}_{\xi_q}(\mathbf{u}^{(q)})]_{\xi_q = \xi_q^{(0)}} = 0; \quad q = 1, 2, \ldots, N. \tag{4}$$

As it is easy to prove, due to the periodicity of the structure, the solution also has periodicity features. So, the displacement vector in a continuous phase (matrix) can be presented as a sum of the linear far field and the periodic disturbance field caused by the presence of inhomogeneities:

$$\mathbf{u}^{(0)} = \hat{\mathrm{E}}\cdot\mathbf{r} + \mathbf{u}_1, \tag{5}$$

where

$$\mathbf{u}_1(\mathbf{r} - a\mathbf{e}_a) = \mathbf{u}_1(\mathbf{r} - b\mathbf{e}_b) = \mathbf{u}_1(\mathbf{r} - c\mathbf{e}_c) = \mathbf{u}_1(\mathbf{r}). \tag{6}$$

It was shown elsewhere (e.g. Kushch, 1985; Sangani and Lu, 1987) that in this case the tensor $\hat{\mathrm{E}}$ has a sense of the average strain tensor of the composite, i.e.

$$E_{ij} = \langle\varepsilon_{ij}\rangle = \frac{1}{V}\int_V \varepsilon_{ij}\,\mathrm{d}V. \tag{7}$$

where $\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ and V is the representative volume of the composite. Taking into account eqns (5) and (6), the periodicity unit (Fig. 1) may be chosen as a representative volume. Also it follows from eqn (6) that the satisfaction of contact conditions (4) for the particles with centres lying inside the structure cell means their equal satisfaction for the rest of inclusions in a medium. Thus, the problem here is to construct the solution of eqn (2) satisfying the periodicity conditions (5) and (6), and the interfacial conditions (4).

3. METHOD OF SOLUTION

The analytical method applied here to solve the boundary-value problem (2)–(6) is, in fact, the modified variant of the approach used by Kushch (1995b) to solve the elasticity problem for a medium containing a finite number of aligned spheroidal inclusions. The essence of the method, in few words, is the representation of the displacement vector in a multiply-connected region by a series of partial vectorial solutions of Lame's equation, and use of addition theorems for these solutions to reduce the boundary-value problem to an infinite set of linear algebraic equations. It is evident that the same approach can be used when the medium with an infinite number of inclusions is considered and no additional mathematical results are needed to solve this problem. Taking into account that the majority of the notations and the detailed description of the method are given by Kushch (1995b), we do not reproduce them here. Below, only the main idea of the method and some details specific for the problem considered will be described.

According to the generalised superposition principle (Golovchan *et al.*, 1993), we present the triply periodic disturbance field by the series

$$\mathbf{u}_1 = \sum_{p=1}^{N} \mathbf{U}^{(p)}, \tag{8}$$

where

$$\mathbf{U}^{(p)} = \sum_{i=1}^{3} \sum_{t=0}^{\infty} \sum_{s=-t}^{t} A_{ts}^{(i)(p)} \mathbf{S}_{ts}^{*(i)}(\mathbf{r}_p, f_p), \tag{9}$$

$A_{ts}^{(i)(p)}$ are the arbitrary constants and $\mathbf{S}_{ts}^{*(i)}$ are the external triply-periodic solutions of Lame's equation given in the Appendix, eqn (A5). The series expansion of the displacement vector, limited in the volume of inclusion of the qth type, contains the internal partial solutions $\mathbf{s}_{ts}^{(i)}$ only:

$$\mathbf{u}^{(q)} = \sum_{i=1}^{3} \sum_{t=0}^{\infty} \sum_{s=-t}^{t} D_{ts}^{(i)(q)} \mathbf{s}_{ts}^{(i)}(\mathbf{r}_q, f_q), \tag{10}$$

where $D_{ts}^{(i)(q)}$ are the unknown coefficients.

Because the $\mathbf{S}_{ts}^{*(i)}$ (A5) and $\mathbf{S}_{ts}^{(i)}$ (A2) are the partial solutions of Lame's equation, the displacement vector in a matrix (5) and in the inclusions (10) are satisfied by eqn (2) exactly. Furthermore, taking into account eqn (7) and the properties of $\mathbf{S}_{ts}^{*(i)}$ we find that $\mathbf{u}_1$ (8) also satisfies the periodicity conditions (6). To execute the interfacial conditions (4) the unknowns $A_{ts}^{(i)(q)}$ and $D_{ts}^{(i)(q)}$ must be determined properly. The obtaining of the resolving set of linear algebraic equations includes the representation of expressions for $\mathbf{u}^{(0)}$ and $\mathbf{u}^{(q)}$ in a qth local coordinate basis, their substitution into eqns (4) and then the reducing of the functional equalities obtained to the algebraic ones by using the orthogonality property of spherical harmonics.

Note that $\mathbf{u}^{(q)}$ is already written in a qth local spheroidal basis and therefore does not need any additional transformation. The representation of the linear part of $\mathbf{u}^{(0)}$ (to concretise, we put $\mathbf{r} = \mathbf{r}_1$) has a form

$$\hat{E} \cdot \mathbf{r}_1 = \sum_{i=1}^{3} \sum_{t=0}^{\infty} \sum_{s=-t}^{t} b_{ts}^{(i)(q)} \mathbf{s}_{ts}^{(i)}(\mathbf{r}_q, f_q), \tag{11}$$

where

$$e_{10}^{(1)(q)} = E_{13} X_{1q} + E_{23} Y_{1q} + E_{33} Z_{1q},$$

$$e_{11}^{(1)(q)} = -\overline{e_{1,-1}^{(1)(q)}} = (E_{11} - \mathrm{i}E_{12}) X_{1q} + (E_{12} - \mathrm{i}E_{22}) Y_{1q} + (E_{13} - \mathrm{i}E_{23}) Z_{1q},$$

$$e_{00}^{(3)(q)} = \frac{f_q}{2(2\nu_0-1)}(E_{11}+E_{22}+E_{33}), e_{20}^{(1)(q)} = \frac{f_q}{3}(2E_{33}-E_{11}-E_{22}),$$

$$e_{21}^{(1)(q)} = -\overline{e_{2,-1}^{(1)(q)}} = f_q(E_{13}-\mathrm{i}E_{23}), e_{22}^{(1)(q)} = \overline{e_{2,-2}^{(1)(q)}} = f_q(E_{11}-E_{22}-2\mathrm{i}E_{12}), \tag{12}$$

X_{1q}, Y_{1q} and Z_{1q} are the Cartesian coordinates of vector $\mathbf{R}_{1q}$, all other $e_{ts}^{(i)(q)}$ are equal to zero.

The series expansion of the disturbance field $\mathbf{u}_1$ on a surface $\xi_q = \xi_q^{(0)}$ follows from the eqns (A10) and (A11) in the Appendix. Their substitution into eqn (6) and change of the summation order gives us, together with eqn (11), the representation of $\mathbf{u}^{(0)}$:

$$\mathbf{u}^{(0)}(\mathbf{r}_q, f_q) = \sum_{i=1}^{3}\sum_{t=0}^{\infty}\sum_{s=-t}^{t}[A_{ts}^{(i)(q)}\mathbf{S}_{ts}^{(i)}(\mathbf{r}_q, f_q) + (a_{ts}^{(i)(q)} + e_{ts}^{(i)(q)})\mathbf{s}_{ts}^{(i)}(\mathbf{r}_q, f_q)], \tag{13}$$

where

$$a_{ts}^{(i)(q)} = \sum_{j=1}^{3}\sum_{k=0}^{\infty}\sum_{l=-k}^{k}\sum_{p=1}^{N}\eta_{ktls}^{*(j)(i)}(\mathbf{R}_{pq}, f_p, f_q)A_{kl}^{(j)(p)}. \tag{14}$$

To obtain the algebraic set of equations for the determination of $A_{ts}^{(i)(q)}$ and $D_{ts}^{(i)(q)}$ one needs to substitute eqns (13) and (10) into (6), and decompose the functional equalities obtained into scalar ones, and then, over the set of spherical harmonics. Because this procedure coincides fully with that exposed by Kushch (1995b), we omit the details of transformations and write only the final matrix form of the resolving system:

$$\mathrm{UG}_t^{(q)}(\nu_0)\cdot\mathbf{A}_t^{(q)} + \mathrm{UM}_t^{(q)}(\nu_0)\cdot(\mathbf{a}_t^{(q)}+\mathbf{e}_t^{(q)}) = \mathrm{UM}_t^{(q)}(\nu_q)\cdot\mathbf{D}_t^{(q)};$$

$$\mathrm{TG}_t^{(q)}(\nu_0)\cdot\mathbf{A}_t^{(q)} + \mathrm{TM}_t^{(q)}(\nu_0)\cdot(\mathbf{a}_t^{(q)}+\mathbf{e}_t^{(q)}) = \omega_q\mathrm{TM}_t^{(q)}(\nu_q)\cdot\mathbf{D}_t^{(q)};$$

$$q = 1, 2, \ldots, N; \tag{15}$$

where $\omega_q = \mu_q/\mu_0$, μ_q is the shear modulus of the qth phase. Vector $\mathbf{A}_t^{(q)}$ contains unknowns $A_{t+i-2,s}^{(i)(q)}$, vector $\mathbf{D}_t^{(q)}$ contains unknowns $D_{t-i+2,s}^{(i)(q)}$, vectors $\mathbf{a}_t^{(q)}$ and $\mathbf{e}_t^{(q)}$ include values $a_{(t-i+2,s}^{(i)(q)}$ and $e_{t-i+2,s}^{(i)(q)}$, respectively. These vectors, as well as the matrices $\mathrm{UM}_t^{(q)}$, $\mathrm{UG}_t^{(q)}$, $\mathrm{TM}_t^{(q)}$ and $\mathrm{TG}_t^{(q)}$ are defined in Kushch (1995b).

The numerical realisation of the method exposed is rather simple. The most difficult thing here is the estimation of lattice sums $\eta_{tksl}^{*(i)(j)}$ (A12). For the rational organisation of computations we write these sums as

$$\eta_{tksl}^{*(i)(j)} = \sum_{|\mathbf{R}_{pq}+\mathbf{V}_\mathbf{n}|\leqslant \mathrm{Re}(f_p+f_q)} {}^{(1)}\eta_{tksl}^{*(i)(j)} + \sum_{|\mathbf{R}_{pq}-\mathbf{V}_\mathbf{n}|>\mathrm{Re}(f_p-f_q)} {}^{(2)}\eta_{tksl}^{*(i)(j)} \tag{16}$$

where ${}^{(1)}\eta_{tksl}^{(i)(j)}$ and ${}^{(2)}\eta_{tksl}^{(i)(j)}$ are expressed by the formulae (A7) with $\eta_{tk}^{s-l} = {}^{(1)}\eta_{tk}^{s-l}$ (A8) and $\eta_{tk}^{s-l} = {}^{(2)}\eta_{tk}^{s-l}$ (A9), respectively. The presence of two different representations of η_{tk}^{s-l} (and, hence, of $\eta_{tksl}^{(i)(j)}$) greatly simplifies this problem. So, the expression (A8) is used only for a small finite number of points in the case of the prolate spheroid. For the oblate case $\mathrm{Re}f_p = \mathrm{Re}f_q \equiv 0$ the first sum in eqn (16) is absent. For the rest of the lattice poles the more simple expression (A9) can be used. As a result, the second sums in eqn (16) are expressed through

$$\eta_{tj}^{*s-l} = \sum_{|\mathbf{R}_{pq}+\mathbf{V}_\mathbf{n}|>\mathrm{Re}(f_p+f_q)} {}^{(2)}\eta_{tk}^{s-l} = \sqrt{\pi}a_{tk}\sum_{r=0}^{\infty}(f_p/2)^{2r}M_{tkr}(f_p, f_q)Y_{t+k+2r}^{*s-l}, \tag{17}$$

where the sums

$$Y_t^{*s} = \sum_{|\mathbf{R}_{pq}+\mathbf{V}_\mathbf{n}| > \mathrm{Re}(f_p - f_q)} Y_t^s(\mathbf{R}_{pq} + \mathbf{V}_\mathbf{n}) \tag{18}$$

are practically the same ones that arise when the conductivity problem for a composite with the spherical particles is considered. Their calculation was discussed many times (e.g. McPhedran and McKenzie, 1978; Suen *et al.*, 1979). In part, it is well known that the series Y_2^{*s} converges only conditionally. As it is easy to see, the series (17) for $t+k = 2$ also converges only conditionally, and Y_2^{*s} is the only conditionally convergent term. The rest of this sum, as well as η_{tk}^{*s-l} for $t+k > 2$ converges absolutely and no additional problems arise here in comparison with the case of spherical inclusions. Note only that some additional transformations are needed for the estimation of $\eta_{tksl}^{*(3)(1)}$. To this end we must compute the lattice sums similar to eqn (18) for the biharmonic functions zY_t^s and $(x+iy)$ Y_t^s also arising when a composite with the spherical inclusions is considered.

4. AVERAGE ELASTIC MODULI TENSOR

The solution obtained is sufficient for the calculation of the four-rank tensor $\hat{C} = \{C_{ijkl}\}$ of the effective elastic moduli defined by the relation

$$\langle\sigma_{ij}\rangle = C_{ijkl}\langle\varepsilon_{kl}\rangle, \tag{19}$$

where $\langle\varepsilon_{kl}\rangle = E_{kl}$ (7),

$$\langle\sigma_{ij}\rangle = \frac{1}{V}\int_V \sigma_{ij}\,\mathrm{d}V, \tag{20}$$

V is the volume of the elementary structure cell (Fig. 1). Hence, for determination of $\hat{C}$ it is sufficient to find the expressions for $\langle\sigma_{ij}\rangle$ and calculate them for the corresponding values of E_{kl}:

$$C_{ijkl} = \langle\sigma_{ij}\rangle \quad \text{for } E_{kl} = 1, E_{k'l'} = 0 \quad (k \neq k', l \neq l'). \tag{21}$$

By the use of Hooke's law for the material of each composite phase we have

$$V\langle\sigma_{ij}\rangle = \sum_{p=0}^{N}\int_{V_p}\sigma_{ij}^{(p)}\,\mathrm{d}V = \sum_{p=0}^{N} 2\mu_p\int_{V_0}\left(\varepsilon_{ij}^{(p)} + \delta_i^j\frac{\nu_p}{1-2\nu_p}\theta^{(p)}\right)\mathrm{d}V \tag{22}$$

where $\varepsilon_{ij}^{(p)} = \varepsilon_{ij}(\mathbf{u}^{(p)})$, $\sigma_{ij}^{(p)} = \sigma_{ij}(\mathbf{u}^{(p)})$, $\theta = \varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33}$ and V_p is the volume of the pth phase within the elementary cell, equal in total to the volume of the pth inclusion. Thus

$$V = \sum_{p=0}^{N} V_p, d_p = V_p/V$$

is the volume fraction of the pth phase. The equality (22) may be rewritten in the following form

$$\langle\sigma_{ij}\rangle = 2\mu_0\left(E_{ij}+\delta_i^j\frac{\nu_0}{1-2\nu_0}E_{kk}\right) + \sum_{p=1}^{N}\left[2(\mu_p-\mu_0)\frac{1}{V}\int_{V_p}\varepsilon_{ij}^{(p)}\,\mathrm{d}V + \delta_i^j\left(\frac{2\mu_p\nu_p}{1-2\nu_p} - \frac{2\mu_0\nu_0}{1-2\nu_0}\right)\frac{1}{V}\int_{V_p}\theta^{(p)}\,\mathrm{d}V\right]. \tag{23}$$

Hence, we need to integrate strains over the volume of inclusions only. With the aid of Gauss' theorem the volume integrals are reduced easily to surface ones:

$$\int_{V_p} \varepsilon_{ij}^{(p)} \, dV = \int_{V_p} \frac{1}{2}(u_{i,j}^{(p)} + u_{j,i}^{(p)}) \, dV = \int_{S_p} \frac{1}{2}(u_i^{(p)} n_j + u_j^{(p)} n_i) \, dS, \tag{24}$$

where S_p is the surface $\xi_p = \xi_p^{(0)}$, $u_i^{(p)}$ and n_i are the Cartesian components of displacement vector $\mathbf{u}^{(p)}$ and of unit vector $\mathbf{n}$ normal to this surface, respectively. Calculation of the surface integrals in eqn (24) is not a problem taking into account the representation of internal partial solutions (A2) on the surface S_p (Kushch, 1995b) and the use of orthogonality of harmonics $\chi_t^s(\eta, \varphi)$ on this surface. The integration gives us the exact analytical formulae

$$\int_{V_p} \varepsilon_{11}^{(p)} \, dV = \frac{V_p}{f_p}\left[\gamma D_{00}^{(3)(p)} - \frac{1}{2}(D_{20}^{(1)(p)} - \mathrm{Re} D_{22}^{(1)(p)})\right];$$

$$\int_{V_p} \varepsilon_{22}^{(p)} \, dV = \frac{V_p}{f_p}\left[\gamma D_{00}^{(3)(p)} - \frac{1}{2}(D_{20}^{(1)(p)} + \mathrm{Re} D_{22}^{(1)(p)})\right];$$

$$\int_{V_p} \varepsilon_{33}^{(p)} \, dV = \frac{V_p}{f_p}(\gamma D_{00}^{(3)(p)} + D_{20}^{(1)(p)});$$

$$\int_{V_p} \varepsilon_{12}^{(p)} \, dV = -\frac{V_p}{f_p} \mathrm{Im} D_{22}^{(1)(p)}; \quad \int_{V_p} (\varepsilon_{13}^{(p)} - i\varepsilon_{23}^{(p)}) \, dV = \frac{V_p}{f_p} D_{21}^{(1)(p)}; \quad \gamma = 2(2\nu_0 - 1)/3. \tag{25}$$

Substitution of eqn (25) into (23) gives the necessary expressions for effective moduli. Finally, we replace in these formulae $D_{ts}^{(i)(p)}$ with $A_{ts}^{(i)(p)}$ using eqns (15) for $t = 1$ and obtain

$$\frac{\langle\sigma_{11}\rangle + \langle\sigma_{22}\rangle + \langle\sigma_{33}\rangle}{3k_0} = E_{11} + E_{22} + E_{33} - \left(1 + \frac{4\mu_0}{3k_0}\right) \sum_{p=1}^{N} \tilde{d}_p A_{00}^{(1)(p)};$$

$$\frac{2\langle\sigma_{33}\rangle - \langle\sigma_{11}\rangle - \langle\sigma_{22}\rangle}{2\mu_0} = 2E_{33} - E_{11} - E_{22} + 4(1-\nu_0) \sum_{p=1}^{N} \tilde{d}_p A_{20}^{(3)(p)};$$

$$\frac{\langle\sigma_{11}\rangle - \langle\sigma_{22}\rangle - 2i\langle\sigma_{12}\rangle}{2\mu_0} = E_{11} - E_{22} - 2iE_{33} + 8(1-\nu_0) \sum_{p=1}^{N} \tilde{d}_p A_{22}^{(3)(p)};$$

$$\frac{\langle\sigma_{13}\rangle - i\langle\sigma_{23}\rangle}{2\mu_0} = E_{13} - iE_{23} + 4(1-\nu_0) \sum_{p=1}^{N} \tilde{d}_p A_{21}^{(3)(p)}; \tag{26}$$

where

$$\tilde{d}_p = \frac{4\pi(f_p)^2}{3V}, \quad k_0 = \frac{2\mu_0(1+\nu_0)}{3(1-2\nu_0)}$$

is the bulk modulus of a matrix material.

The expressions (26) are rather simple, they contain only the first few unknowns $A_{ts}^{(i)(p)}$ that can be computed with a high accuracy from a truncated system (15) of a relatively small size. Moreover, relations (26) can be inverted to express the E_{ij} through $\langle\sigma_{ij}\rangle$. Their substitution in eqns (15) gives a set of equations with the average stresses as governing parameters. Hence, we can also consider the macroscopically uniform stressed state of a periodic composite when the constant average stress tensor is prescribed.

5. NUMERICAL RESULTS

The problem considered has many parameters. They are the number of lattices and their mutual position, lattice angles and periods, size and shape of particles, phase properties

Table 1. Convergence of $A_{00}^{(1)}(d, t_{max})$ for the uniaxial deformation $\langle \varepsilon_{33} \rangle = 1$ of a porous medium with $\nu_0 = 0.3$, $R = 2$

	d				
t_{max}	0.1	0.2	0.3	0.4	0.5
1	0.50234	0.44941	0.40629	0.37008	0.33884
3	0.50264	0.45124	0.41099	0.37913	0.35418
5	0.50264	0.45126	0.41106	0.37941	0.35538
7	0.50264	0.45126	0.41107	0.37944	0.35589
9	0.50264	0.45126	0.41107	0.37945	0.35603
11	0.50264	0.45126	0.41107	0.37945	0.35610
13	0.50264	0.45126	0.41107	0.37945	0.35612
15	0.50264	0.45126	0.41107	0.37945	0.35612

and external loading type. To reduce their number we consider a medium containing a single orthogonal lattice of spheroidal particles; the index denoting the number of phase will be omitted below. Furthermore, we put $f\bar{\xi}_0/a = f\bar{\xi}_0/b = f\xi_0/c$ ($f \equiv f_1$, $\xi_0 \equiv \xi_1^{(0)}$); i.e. the lattice periods are proportional to semiaxes of spheroid. For this type of structure the maximum volume content of the disperse phase is $d_{max} = 0.5236$ ($d \equiv d_1$) for the arbitrary aspect ratio of the spheroid $R = \xi_0/\bar{\xi}_0$. In part, for $R = 1$ we have a simple cubic lattice of spheres. Thus, for the simplest structure given we have only two structure parameters, they are d and R.

The convergence rate of series (8) and (10) depends on the problem parameters specified. When the lattice periods tend to infinity, all unknowns except $\mathbf{A}_1$ tend to zero and the problem is reduced to a simple one-particle problem with a finite expression for $\mathbf{u}$. On the contrary, when particles draw together ($d \to d_{max}$), these series converge more slowly and additional terms must be accounted to obtain the solution with a desired accuracy. To be sure that the results are accurate enough we need to investigate the convergence behaviour of $\mathbf{u}(t_{max})$ with t_{max} increased. Here t_{max} is the maximum value of index t in the above solution retained in a numerical analysis, $\mathbf{u}(t_{max}) \to \mathbf{u}_{exact}$ when $t_{max} \to \infty$. So, in Table 1, the values of the coefficient $A_{00}^{(1)}(d, t_{max})$ for uniaxial deformation along axis Oz of porous medium with $\nu_0 = 0.3$ are presented. It is seen from the table that the convergence rate is rapid enough to exclude only the case when $d = 0.5$ (nearly-touching particles). Because the expressions for effective moduli (23) contain only first series coefficients, this table allows us also to choose the value of t_{max} necessary for calculation of the elastic moduli with a prescribed accuracy.

The series for the stresses converge more slowly than corresponding series for the displacements. Hence, more unknowns must be retained in a truncated system (15) when the stressed state of the composite is investigated. Nevertheless, the numerical studies show that $t_{max} = 15$ provides the calculation of stresses with a relative error less than 3% for $d \leqslant 0.95 d_{max}$. Note, that this error realises only in the points of the maximum stress concentration, for the rest of the domain the accuracy of the solution is higher. The only exception is the dense packing of rigid inclusions when the stresses tend to infinity. This case demands a separate consideration similar to that performed by Nunan and Keller (1984) for a composite with spherical particles.

Tables 2–4 contain the stress concentration coefficients $k_{ijkl} = \max \sigma_{ij}^{(0)} / \langle \sigma_{kl} \rangle$ on the interfacial boundary $\xi = \xi_0$. So, the maximum values of $\sigma_{33}^{(0)}$ due to uniaxial tension $\langle \sigma_{33} \rangle = 1$ take place on the equator of the spheroid for the porous material $\omega = 0$ and on the spheroid's poles for the composite, $\omega > 1$. The stress amplitude is greatly influenced by the shape of the inclusions. So, the values of k_{3333} in a porous material are greater for the oblate case, in a composite—for prolate spheroids. At the same time, these dependencies are not simple. The monotonous growth of k_{3333} with increasing d is observed only for the spherical inclusions. For the composite with prolate particles we have at the beginning the decrease of the stress concentration and for $d \geqslant 0.25$— its increase.

The coefficients k_{1111} and k_{2211} in a composite with oblate inhomogeneities due to uniaxial tension $\langle \sigma_{11} \rangle = 1$ vary in an analogous manner (Tables 3 and 4, respectively). The

Table 2. The stress concentration coefficient $k_{3333} = \max\sigma_{33}^{(0)}/\langle\sigma_{33}\rangle$ due to uniaxial tension $\langle\sigma_{33}\rangle = 1$

		d				
R	ω	0	0.15	0.25	0.35	0.5
	0	1.44	1.72	2.14	2.87	4.44
2.0	10	2.62	2.21	2.15	2.37	3.43
	10^6	3.28	2.61	2.51	2.83	4.61
	0	2.07	2.21	2.55	3.31	5.29
1.0	10	1.74	1.93	2.19	2.63	3.50
	10^6	1.94	2.20	2.59	3.35	5.68
	0	3.30	3.25	3.61	4.17	6.01
0.5	10	1.32	2.03	2.36	2.64	2.96
	10^6	1.38	2.04	2.97	3.79	5.91

Table 3. The stress concentration coefficient $k_{1111} = \max\sigma_{11}^{(0)}/\langle\sigma_{11}\rangle$ due to uniaxial tension $\langle\sigma_{11}\rangle = 1$

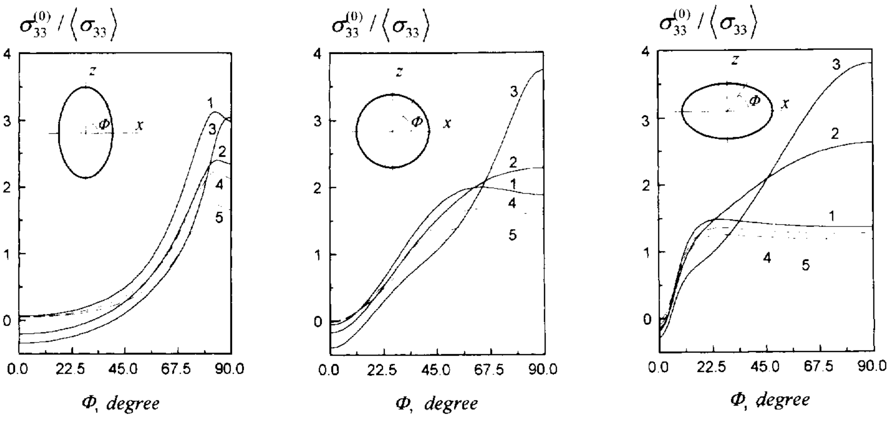
		d				
R	ω	0	0.15	0.25	0.35	0.5
	0	2.41	2.72	3.10	3.61	5.01
2.0	10	1.54	1.96	2.27	2.65	3.24
	10^6	1.65	2.25	2.75	3.56	5.77
	0	2.07	2.21	2.55	3.31	5.29
1.0	10	1.74	1.93	2.19	2.63	3.50
	10^6	1.94	2.20	2.59	3.35	5.68
	0	1.66	1.95	2.54	3.34	5.41
0.5	10	2.18	2.07	2.16	2.49	3.49
	10^6	2.56	2.39	2.53	3.05	5.05

Table 4. The stress concentration coefficient $k_{2211} = \max\sigma_{22}^{(0)}/\langle\sigma_{11}\rangle$ due to uniaxial tension $\langle\sigma_{11}\rangle = 1$

		d				
R	ω	0	0.15	0.25	0.35	0.5
	0	0.12	0.30	0.40	0.51	0.83
2.0	10	0.60	0.77	0.92	1.11	1.43
	10^6	0.71	0.97	1.18	1.53	2.47
	0	0.14	0.20	0.27	0.48	1.04
1.0	10	0.68	0.76	0.88	1.09	1.53
	10^6	0.83	0.94	1.11	1.44	2.44
	0	0.11	0.13	0.26	0.52	1.19
0.5	10	0.84	0.81	0.86	1.02	1.49
	10^6	1.09	1.03	1.08	1.30	2.16

analysis of these data allows us to estimate the possible stress concentrations in a composite depending on its structure and loading type.

Until now there are no studies where the microstress fields in a periodic composite were investigated. For the non-ordered materials their number is rather limited. So, for the composite with uniformly distributed aligned spheroidal particles, the interface stresses were estimated by Tandon and Weng (1986). Their analysis is based on the single spheroidal particle model and uses the theory combining Eshelby's solution and Mori–Tanaka's mean stress theorem. Note that its model differs from that considered here. Nevertheless, because



a) $R = 2$; b) $R = 1$; c) $R = 0,5$;

Fig. 2. Stress $\sigma_{33}^{(0)}$ distribution on the surface $\xi = \xi_0$ due to uniaxial tension $\langle \sigma_{33} \rangle = 1$.

it is practically the only work where stress distribution was evaluated, it is of interest to compare the results obtained by these two ways.

So in Fig. 2 the stress $\sigma_{33}^{(0)}$ distribution on a surface $\xi = \xi_0(\varphi = 0)$ due to uniaxial tension of a composite material with parameters $v_0 = 0.35$; $\mu_0 = 1.02$ GPa; $\mu_1 = 30.2$ GPa; $v_1 = 0.2$ is depicted. The solid lines 1–3 correspond to our solution, the dashed lines 4 and 5 present the results of Tandon and Weng (1986). The lines 2 and 4 are calculated for $d = 0.2$, lines 2 and 5 are calculated for $d = 0.4$, at $d = 0$ (single inclusion) both solutions coincide (line 1). It is seen from pictures that with increased d the difference between solutions grows significantly, especially for the oblate spheroids [Fig. 2(c)]. Moreover, the approximate solution predicts the monotonous decrease of stress $\sigma_{33}^{(0)}$ with growth of d. The more rigorous analysis shows, however, the rapid growth of stresses at $d \to d_{max}$ caused by interaction of neighbouring particles.

The periodic composite is, as a rule, essentially the anisotropic one. Even in the simplest case (cubic lattice of spherical particles) its behaviour is described by three moduli. For the orthogonal lattice of spheroidal inclusions we have the macroscopically orthotropic material with nine independent components of tensor $\hat{C}$. The effective moduli tensor of a periodic composite with ellipsoidal inclusions was evaluated by Iwakuma and Nemat-Nasser (1983). Their approach was based on the assumption that the strains in the inclusions are uniform. Note that this assumption corresponds to $t_{max} = 1$ in eqn (15). Really, the internal solutions $\mathbf{s}_{3-i,s}^{(i)}$ are the linear functions of coordinates [see eqns (11) and (12)] producing the constant strain and stress tensors. As it was to be expected, the numerical results obtained with the use of Iwakuma and Nemat-Nasser's technique, and by our method for $t_{max} = 1$ coincide with a high accuracy. In Table 5 the values of modulus C_{3333} are obtained from eqn (23)

Table 5. The values of C_{3333} calculated by accurate ($t_{max} = 15$) and approximate (Iwakuma and Nemat-Nasser, 1983) method

		$d = 0.1$		$d = 0.3$		$d = 0.5$	
R	ω	$t_{max} = 1$	$t_{max} = 15$	$t_{max} = 1$	$t_{max} = 15$	$t_{max} = 1$	$t_{max} = 15$
	0	2.807	2.799	1.846	1.818	1.158	1.048
1.0	10	4.107	4.102	5.899	5.930	8.690	9.646
	1000	4.256	4.248	6.794	6.887	11.56	17.71
	0	2.767	2.656	1.735	1.667	1.072	0.945
0.5	10	4.023	4.021	5.657	5.675	8.229	9.228
	1000	4.130	4.128	6.349	6.652	10.46	17.73
	0	2.583	2.523	1.648	1.518	1.004	0.829
0.2	10	4.000	4.005	5.564	5.737	8.014	9.102
	1000	4.104	4.115	6.222	6.708	10.09	17.81

Table 6. Modulus C_{1111} for a composite with a simple cubic lattice of inclusions, $d = 0.1$

	ω				
R	0	0.5	2.0	10	1000
0.25	2.856	3.291	3.782	4.645	5.482
0.5	2.877	3.281	3.756	4.267	4.536
0.75	2.839	3.274	3.744	4.155	4.336
1.0	2.799	3.278	3.736	4.102	4.248
1.25	2.762	3.264	3.732	4.070	4.199
1.5	2.732	3.261	3.728	4.049	4.167
1.75	2.705	3.258	3.726	4.035	4.145
2.0	2.681	3.256	3.724	4.023	4.128
2.25	2.653	3.253	3.722	4.012	4.113

Table 7. Modulus C_{3333} for a composite with a simple cubic lattice of inclusions, $d = 0.1$

	ω				
R	0	0.5	2.0	10	1000
0.25	1.843	3.211	3.696	3.889	3.944
0.5	2.474	3.239	3.711	3.956	4.032
0.75	2.693	3.256	3.725	4.026	4.132
1.0	2.799	3.278	3.736	4.102	4.248
1.25	2.859	3.276	3.747	4.185	4.388
1.5	2.897	3.282	3.757	4.281	4.565
1.75	2.923	3.287	3.767	4.397	4.810
2.0	2.941	3.291	3.776	4.555	5.225
2.25	2.954	3.295	3.787	4.868	6.765

for $t_{max} = 1$ and $t_{max} = 15$ (accurate solution), $\nu_0 = \nu_1 = 0.3$. These data allow us to estimate the relative error of the approximate approach.

It is seen from Table 5 that when the lattice periods are proportional to semiaxes of spheroid the effective moduli only slightly depends on the shape of inclusions. Another matter is when the inclusion's shape varies, whereas the lattice is fixed. Tables 6 and 7 contain the values of moduli C_{1111} and C_{3333}, respectively, for the composite with a simple cubic lattice structure $a = b = c$, $\nu_0 = \nu_1 = 0.3$, $d = 0.1$. The data presented in these tables show that in this case even for a relatively small volume fraction of disperse phase the effective elastic properties can vary in a wide range depending on the aspect ratio of the inclusions. So, for a composite with $\omega = 1000$ and $R = 2.25$ the ratio $C_{3333}/C_{1111} = 1.645$, whereas for $R = 0.25$, $C_{3333}/C_{1111} = 0.719$. In a special case when $R = 1$ these moduli coincide with one other and agree with those obtained by other ways (Nunan and Keller, 1984; Kushch, 1987; Sangani and Lu, 1987).

6. CONCLUSIONS

The rigorous analytical method is developed to analyse the microstresses and macroscopic elastic behaviour of a periodic matrix-type composite with the spheroidal disperse phase particles. The structure model proposed is general and flexible enough. It may be used to study a wide class of heterogeneous materials. Besides the shape of inhomogeneities, it allows us to model the spatial distribution of particles in a real disordered composite and to account the size distribution and multi-phaseness of a filler. Among the advantages of the solution obtained we point out the possibility to investigate the singularities of the problem stated. In part, for a dense packing of rigid particles, when both stresses and effective moduli tend to infinity, the asymptotic analysis can be fulfilled analogously to Nunan and Keller's (1984) method. Another extreme case is the materials with needle-like and penny-shaped inclusions or cracks. The proper limit transfer in a general solution gives the accurate results for these materials.

The method is simple and effective from a computational standpoint. It provides computation of field parameters and effective moduli with a high accuracy. The numerical results presented show the effect of inclusion's shape and particle–particle interaction on the stress concentration and the effective elastic response of the composite. The method also can be used to estimate the validity bounds on known approximate approaches and the accuracy of solutions obtained by numerical methods.

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APPENDIX. TRIPLY-PERIODIC VECTORIAL SOLUTIONS OF LAME'S EQUATION

The following partial solutions of eqn (2) are entered by Kushch (1995a): external $\mathbf{S}_{ts}^{(i)} = \mathbf{S}_{ts}^{(i)}(\mathbf{r}, f)$ [constrained at $|\mathbf{r}| \to \infty$]

$$\mathbf{S}_{ts}^{(1)} = \mathbf{e}_1 F_{t+1}^{s-1} - \mathbf{e}_2 F_{t+1}^{s+1} + \mathbf{e}_3 F_{t+1}^{s};$$

$$\mathbf{S}_{ts}^{(2)} = \frac{1}{t}[\mathbf{e}_1 (t+s) F_t^{s-1} + \mathbf{e}_2 (t-s) F_t^{s+1} + \mathbf{e}_3 s F_t^s];$$

$$\mathbf{S}_{ts}^{(3)} = \mathbf{e}_1 \{ -(x-\mathrm{i}y) \mathrm{D}_2 F_{t-1}^{s-1} - [(\xi^{(0)})^2 - 1] \mathrm{D}_1 F_t^s + (t+s-1)(t+s) \beta_{-(t-1)} F_{t-1}^{s-1} \}$$
$$+ \mathbf{e}_2 \{ (x+\mathrm{i}y) \mathrm{D}_1 F_{t-1}^{s+1} - [(\xi^{(0)})^2 - 1] \mathrm{D}_2 F_t^s - (t-s-1)(t-s) \beta_{(t-1)} F_{t-1}^{s+1} \}$$
$$+ \mathbf{e}_3 [z \mathrm{D}_3 F_{t-1}^s - (\xi^{(0)})^2 \mathrm{D}_3 F_t^s - C_{(t-1),s} F_{t-1}^s]; \tag{A1}$$

internal $\mathbf{s}_{ts}^{(i)} = \mathbf{s}_{ts}^{(i)}(\mathbf{r}, f)$ [constrained at $|\mathbf{r}| \to 0$]

$$\mathbf{s}_{ts}^{(1)} = \mathbf{e}_1 f_{t-1}^{s-1} - \mathbf{e}_2 f_{t-1}^{s+1} + \mathbf{e}_3 f_{t-1}^{s};$$

$$\mathbf{s}_{ts}^{(2)} = \frac{1}{(t+1)}[\mathbf{e}_1 (t-s+1) f_t^{s-1} + \mathbf{e}_2 (t+s+1) f_t^{s+1} - \mathbf{e}_3 s f_t^s];$$

$$\mathbf{s}_{ts}^{(3)} = \mathbf{e}_1\{-(x-\mathrm{i}y)\mathrm{D}_2 f_{t-1}^{s-1} - [(\xi^{(0)})^2-1]\mathrm{D}_1 f_t^s + (t-s+1)(t-s+2)\beta_t f_{t+1}^{s-1}\}$$
$$+\mathbf{e}_2\{(x+\mathrm{i}y)\mathrm{D}_1 f_{t+1}^{s+1} - [(\xi^{(0)})^2-1]\mathrm{D}_2 f_t^s - (t+s+1)(t+s+2)\beta_t f_{t+1}^{s+1}\}$$
$$+\mathbf{e}_3[z\mathrm{D}_3 f_{t+1}^s - (\xi^{(0)})^2\mathrm{D}_3 f_t^s - C_{ts} f_{t-1}^s]; \tag{A2}$$

where

$$\beta_t = \frac{t+5-4v}{(t+1)(2t+3)},\ C_{ts} = (t-s+1)(t+s+1)\beta_t;\quad t = 0, 1, \ldots, |s| \leqslant t.$$

In eqns (A1) and (A2) the following notations are used:

$$\mathbf{e}_1 = (\mathbf{e}_x + \mathrm{i}\mathbf{e}_y)/2,\ \mathbf{e}_2 = (\mathbf{e}_x - \mathrm{i}\mathbf{e}_y)/2,\ \mathbf{e}_3 = \mathbf{e}_z;$$
$$\mathrm{D}_1 = (\partial/\partial x - \mathrm{i}\partial/\partial y),\ \mathrm{D}_2 = \bar{\mathrm{D}}_1 = (\partial/\partial x + \mathrm{i}\partial/\partial y),\ \mathrm{D}_3 = \partial/\partial z. \tag{A3}$$

$$f_t^s(\mathbf{r}, f) = \frac{(t-s)!}{(t+s)!}P_t^s(\xi)\chi_t^s(\eta,\varphi),\ F_t^s(\mathbf{r}, f) = \frac{(t-s)!}{(t+s)!}Q_t^s(\xi)\chi_t^s(\eta,\varphi) \tag{A4}$$

are the internal and external solutions of Laplace's equation in spheroidal coordinates. In eqn (A4) $\chi_t^s(\eta,\varphi) = P_t^s(\eta)\exp(\mathrm{i}\varphi)$ are the scalar spherical harmonics, P_t^s and Q_t^s are the associated Legendre's polynomials of first and second kind, respectively.

Now we introduce functions

$$\mathbf{S}_{ts}^{*(i)}(\mathbf{r}, f) = \sum_{\mathbf{n}} \mathbf{S}_{ts}^{(i)}(\mathbf{r}+\mathbf{V}_{\mathbf{n}}, f), \tag{A5}$$

where $\sum_{\mathbf{n}}$ means summation over all lattice poles $-\infty < n_1, n_2, n_3 < \infty$. As it is easy to see, functions (A6) satisfy eqn (2) in a space with excluded singularity points $\mathbf{V}_{\mathbf{n}} = n_1 a\mathbf{e}_a + n_2 b\mathbf{e}_b + n_3 c\mathbf{e}_c$ and periodicity conditions (6). Hence, they can be considered as external triply-periodic solutions of Lame's equation.

Representation of $\mathbf{S}_{ts}^{*(i)}$ in a local spheroidal basis follows directly from the addition theorems for the external solutions (A1) [Kushch, 1995a]:

$$\mathbf{S}_{ts}^{(i)}(\mathbf{r}_p, f_p) = \sum_{j=1}^{3}\sum_{k=0}^{\infty}\sum_{l=-k}^{k} \eta_{tksl}^{(i)(j)}(\mathbf{R}_{pq}, f_p, f_q)\mathbf{s}_{kl}^{(j)}(\mathbf{r}_q, f_q), \tag{A6}$$

where

$$\eta_{tksl}^{(1)(2)} = \eta_{tksl}^{(1)(3)} = \eta_{tksl}^{(2)(3)} = 0;\quad \eta_{tksl}^{(1)(1)} = \eta_{t+1,k-1}^{s-l};\quad \eta_{tksl}^{(2)(2)} = \eta_{tk}^{s-l};\quad \eta_{tksl}^{(3)(3)} = \eta_{t-1,k+1}^{s-l};$$
$$\eta_{tksl}^{(2)(1)} = \left(\frac{s}{t}+\frac{l}{k}\right)\eta_{t,k-1}^{s-l}\ (k>0),\ \eta_{t0s0}^{(2)(1)} = 0;\quad \eta_{tksl}^{(3)(2)} = 4(1-v)\eta_{tksl}^{(2)(1)};$$
$$\eta_{tksl}^{(3)(1)} = \left\{4(1-v)\frac{l}{k}\left[\frac{s}{t}+\frac{l}{(k-1)}\right]+C_{k-2,l}-C_{(t-1),s}\right\}\eta_{t-1,k-1}^{s-l}$$
$$+(2k-1)\sum_{p=0}^{r}\left[\frac{Z_{pq}}{f_q}\eta_{t-1,k-2p}^{s-l}+f_p(\xi_p^{(0)})^2\eta_{t,k-2p}^{s-l}-f_q(\xi_q^{(0)})^2\eta_{t-1,k-1-2p}^{s-l}\right], k \geqslant 2;$$
$$\eta_{t1s0}^{(3)(1)} = -C_{(t-1),s}\eta_{t-1,0}^{s},$$
$$\eta_{t1s1}^{(3)(1)} = (t+s-1)[1+(t+s)\beta_{(t+1)}]\eta_{t-1,0}^{s-l},$$
$$\eta_{t1s,-1}^{(3)(1)} = (t-s-1)[1+(t-s)\beta_{(t+1)}]\eta_{t-1,0}^{s+l}. \tag{A7}$$

In eqns (A7) η_{tk}^{s-l} are the coefficients in the addition theorem for scalar harmonics F_t^s:

$$\eta_{tk}^{s-l} = {}^{(1)}\eta_{tk}^{s-l}(\mathbf{R}_{pq}, f_p, f_q) = a_{tk}\left(\frac{2}{\tilde{f}}\right)^{t-k+1}\sum_{r=0}^{\infty} F_{t+k+2r}^{s-l}(\mathbf{R}_{pq}, \tilde{f}).$$
$$\sum_{l=0}^{r}\frac{(-1)^{r-l}}{(r-l)!}\left(\frac{\tilde{f}}{f_p}\right)^{2l}(t+k+2r-2l+1/2)\Gamma(t+k+r+l+1/2)M_{tkl}(f_p, f_q), \tag{A8}$$

where

$$a_{tk} = (-1)^{k+s-l}(k+1/2)\sqrt{\pi}(f_p/2)^{t+1}(f_q/2)^{-k},\quad M_{tkr}(f_p, f_q) = \sum_{j=0}^{r}\frac{(f_q/f_p)^{2j}}{j!(r-j)!\Gamma(t+r-j+3/2)\Gamma(k+j+3/2)}.$$

The series (A6) for $\tilde{f} > f_1$ converges when two non-intersecting spheroids of finite size are considered. For more details, see Kushch (1995c). We note that a more simple expression for $\eta_{tk}^{s,l}$ exists at least when $|\mathbf{R}_{pq}| > \mathrm{Re}(f_p+f_q)$. It has the form

$$\eta_{tk}^{s,l} = {}^{(2)}\eta_{tk}^{s,l}(\mathbf{R}_{pq}, f_p, f_q) = \sqrt{\pi}\, a_{tk} \sum_{r=0}^{t} (f_p/2)^{2r} M_{tkr}(f_p, f_q)\, Y_{t+k+2r}^{s-l}(\mathbf{R}_{pq}), \tag{A9}$$

where $Y_t^s(\mathbf{r}) = (t-s)!\,r^{-(t+1)}\chi_t^s(\theta, \varphi)$ are the partial solutions of Laplace's equation in a spherical basis. The presence of these two representations of $\eta_{tk}^{s,l}$ simplifies greatly the calculation of lattice sums. This problem is discussed in the main text of the paper.

Taking into account eqn (A6), we obtain for $p \neq q$

$$\mathbf{S}_{ts}^{*(i)}(\mathbf{r}_p, f_p) = \sum_{j=1}^{3} \sum_{k=0}^{t} \sum_{l=-k}^{k} \eta_{tksl}^{*(i)(j)}(\mathbf{R}_{pq}, f_p, f_q)\, \mathbf{s}_{kl}^{(j)}(\mathbf{r}_q, f_q)\,; \tag{A10}$$

and

$$\mathbf{S}_{ts}^{*(i)}(\mathbf{r}_p, f_p) = \mathbf{S}_{ts}^{(i)}(\mathbf{r}_p, f_p) + \sum_{j=1}^{3} \sum_{k=0}^{t} \sum_{l=-k}^{k} \eta_{tksl}^{*(i)(j)}(\mathbf{0}, f_p, f_p)\, \mathbf{s}_{kl}^{(j)}(\mathbf{r}_p, f_p)\,; \tag{A11}$$

where

$$\eta_{tksl}^{*(i)(j)}(\mathbf{R}_{pq}, f_p, f_q) = \sum_{\mathbf{n}} \eta_{tksl}^{(i)(j)}(\mathbf{R}_{pq} + \mathbf{V}_{\mathbf{n}}, f_p, f_q). \tag{A12}$$

For $p = q$ ($\mathbf{R}_{pp} \equiv 0$) this sum does not contain the term with $n_1 = n_2 = n_3 = 0$. Equations (A10) and (A11) give us the necessary expressions of $\mathbf{S}_{ts}^{*(i)}$ in a local spheroidal basis.