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High concentration ratio approximation of linear effective properties of materials with cubic inclusions

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Abstract. This paper establish a high concentration ratio approximation of linear elastic properties of materials with periodic microstructure with cubic inclusions. The approximation is derived using first few terms of power series expansion of the solution of the equivalent eigenstrain problem with a homogeneous eigenstrain approximation. Viability of the approximation at high concentration ratios is proved by comparison with a numerical solution of the homogenization problem. To this end some theoretical result of symmetry properties of the homogenization problem are given. Using these results efficient numerical computation on a reduced computational domain is presented.

Keywords: periodic homogenization; material symmetries; equivalent eigenstrain method; effective elastic properties; asymptotic solution

1. Introduction

A classical approach to find linear effective properties of composite materials is to apply the equivalent inclusion method together with the assumption of uniform eigenstrains. The approach is based on the fact, first observed by Eshelby (1957), that homogeneous macro strain applied to an infinite elastic domain with an ellipsoidal inclusion results in homogeneous eigenstress within the inclusion. Unfortunately, a closed form of the resulting eigenstress is known only for an elliptical inclusion and thus numerous application of the equivalent inclusion method are mainly restricted to problems with ellipsoidal inclusions, see Nemat-Nasser *et al.* (1998). Moreover, the method in its original form usually gives good results only for materials with low concentration ratio as the assumption of homogeneous eigenstrain precludes interaction between inclusions.

For problems with periodic microstructure lack of existence of closed form solutions of the inclusion problem for non-elliptical inclusions is alleviated by the Fourier type methods. Applying it to the problem of cuboidal inclusion within the cuboidal unit cell we found that the uniform eigenstrain approximation gives, not as one might wrongly expect good results for low concentrations, but instead good results for high concentration ratios. For a similar observation concerning closed cell materials that are composed of sheets see Berger *et al.* (2017). Since the assumption of the uniform eigenstrain allows determination of the effective material properties in almost closed form, its

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power series expansion at maximal concentration ratio gives, as is shown in the paper, a closed form approximation of the effective properties at high values of concentration ratio. This has several practical applications, as some important composites are thin walled or are made of plate reinforcements. Nowadays modern manufacturing techniques such as 3D printing allow fabrication of such structures at relatively low cost and availability of a closed form formula that predict their effective properties is of great interest.

On the other hand, it is well known that to determine linear elastic effective material properties of composite materials with a periodic microstructure it suffices to solve a certain system of boundary value problems with periodic boundary conditions, for details see Bensoussan *et al.* (1978). The system can be solved numerically in principle with arbitrary precision. However, for high concentration ratios numerical computation becomes increasingly more involved as it requires more and more fine discretization of the boundary layer that forms around the inclusion boundary. Parametric study of effective properties at high concentrations is thus rather difficult to perform. However, the numerical solution is of fundamental importance in the validation of the closed form approximation as it gives benchmark results to compare with.

The paper is organized as follows. In the first part of the paper homogenization approach with particular attention to its symmetry properties is studied. This is important aspect not only because discretization must preserve symmetry of the problem but also because symmetry of the problem allows its domain reduction, see Hassani (1996) and Lukkassen *et al.* (2008) for a direct method and Barbarosie *et al.* (2017) for a group representation method. It is showed in the paper that instead of solving the problem in the whole cubic domain it suffices to solve a reduced problem only on one eight of the cube. The reduced problem is of the same form but with mixed boundary conditions instead of the periodic one. The reduction of the computational domain greatly reduce the computational cost. In the second part of the paper determination of the effective properties on the basis of the equivalent eigenstrain method with homogenous eigenstrain approximation is presented. A solution in almost a closed form is obtained where only a certain function of the concentration ratio in a form of an infinite sum requires numerical evaluation. However, at high concentration ratios, where the equivalent eigenstrain solution is most accurate, the function is approximated by first few terms of its power series expansion. By comparison with the homogenization solution it is shown that the approximation is reasonably well for concentration ratios above 80%.

2. Notation preliminaries

Throughout the paper tensorial notation is used. Vectors, second and fourth order tensors are denoted by $\underline{a}$, $\underline{\underline{a}}$, and $\underline{\underline{A}}$. In the component notation with respect to the Cartesian basis vectors $\underline{e}_i$ we have $\underline{a} = a_i\,\underline{e}_i$, $\underline{\underline{a}} = a_{ij}\,\underline{e}_i \otimes \underline{e}_j$ and $\underline{\underline{A}} = A_{ijkl}\,\underline{e}_i \otimes \underline{e}_j \otimes \underline{e}_k \otimes \underline{e}_l$. Here and throughout the paper the summation convention over the repeated indices is used. The identity second order tensor is denoted by $\underline{\underline{i}}$ and the fourth order identity tensor by $\underline{\underline{I}}$. Dot product of two tensors or single contraction is denoted by a single dot and the double contraction by a colon.

A group of orthogonal second order tensors is denoted by $O(3)$. Its subgroup of rotations that rotates a cube into itself is called the octahedral or cubic group Bradley *et al.* (2010). The Rayleight product, see for example Bertram (2005), of $\underline{\underline{A}}$ with $Q \in O(3)$ is denoted by $Q * \underline{\underline{A}}$ and is defined by

$$Q * \underline{\underline{A}} = Q * A_{ijkl}\,\underline{e}_i \otimes \underline{e}_j \otimes \underline{e}_k \otimes \underline{e}_l = A_{ijkl}\,Q\underline{e}_i \otimes Q\underline{e}_j \otimes Q\underline{e}_k \otimes Q\underline{e}_l.$$

Similarly is defined $Q * \underline{\underline{a}}$. It follows by direct computation that

$$Q * \left(\underline{\underline{A}} : \underline{\underline{a}}\right) = \left(Q * \underline{\underline{A}}\right) : \left(Q * \underline{\underline{a}}\right) =: Q * \underline{\underline{A}} : Q * \underline{\underline{a}} \tag{1}$$

for arbitrary tensors $\underline{\underline{A}}$, $\underline{\underline{a}}$ and $Q \in \mathcal{O}$.

Evidently, $Q * \underline{\underline{i}} = \underline{\underline{i}}$ and $Q * \underline{\underline{I}} = \underline{\underline{I}}$. Tensors with this property are called isotropic tensors. If $\mathcal{O}$ is a subgroup of $O(3)$ such that $Q * \underline{\underline{C}} = \underline{\underline{C}}$ for all $Q \in \mathcal{O}$, then $\mathcal{O}$ is call a material symmetry group of $\underline{\underline{C}}$. It is also said that $\underline{\underline{C}}$ posses $\mathcal{O}$ symmetry. In particular, if $\mathcal{O}$ is a cubic group, then $\underline{\underline{C}}$ has cubic symmetry.

Symmetric fourth order tensors have two minor symmetries, between the first and the second pair of indices. In component notation $C_{ijkl} = C_{jikl} = C_{ijlk}$. They constitute an algebra where the multiplication is understood as the double contraction. It is well known, see for example Walpole (1981) or Jaric *et al.* (2008), that the subalgebra of tensors with both the cubic and major symmetry is three dimensional. However, assumption of the major symmetry is redundant as the cubic and minor symmetry imply the major symmetry. Symmetric fourth order tensors with the cubic symmetry are called cubic tensors. The space of cubic tensors is thus three dimensional. Its basis tensors are denoted by $\underline{\underline{E}}_i, i = 1, 2, 3$. In the paper is chosen a base $\{\underline{\underline{E}}_i, i = 1, 2, 3\}$ such that components of a cubic tensor $\underline{\underline{A}}$ in this base are components A_{1111}, A_{1122} and A_{1212}. Thus

$$\underline{\underline{A}} = A_{1111}\,\underline{\underline{E}}_1 + A_{1122}\,\underline{\underline{E}}_2 + A_{1212}\,\underline{\underline{E}}_3. \tag{2}$$

Multiplication of two cubic tensors $\underline{\underline{A}}$ and $\underline{\underline{B}}$ is given by

$$\underline{\underline{A}} : \underline{\underline{B}} = a_i\,\underline{\underline{E}}_i : b_j\,\underline{\underline{E}}_j = (a_1 b_1 + 2a_2 b_2)\underline{\underline{E}}_1 + (a_1 b_2 + a_2 b_1 + a_2 b_2)\underline{\underline{E}}_2 + 2a_3 b_3\,\underline{\underline{E}}_3. \tag{3}$$

Therefore the algebra of fourth order symmetric tensors with the cubic symmetry is isomorphic to algebra $(\mathbb{R}^3, +, :)$ with the multiplication given as

$$(a_1, a_2, a_3) : (b_1, b_2, b_3) = (a_1 b_1 + 2a_2 b_2, a_1 b_2 + a_2 b_1 + a_2 b_2, 2a_3 b_3)\,. \tag{4}$$

Clearly, the algebra is commutative. In the cubic basis an isotropic tensor $\lambda\,\underline{\underline{i}} \otimes \underline{\underline{i}} + 2\mu\,\underline{\underline{I}}$ has a representation

$$(\lambda + 2\mu)\underline{\underline{E}}_1 + \lambda\,\underline{\underline{E}}_2 + \mu\,\underline{\underline{E}}_3. \tag{5}$$

3. Homogenization theory

We begin this section with a remark that the homogenization theory is only scarcely presented in the standard micromechanical literature, see for example Nemat-Nasser *et al.* (1998). The reason is that it requires some higher mathematics and also, apart from some simple cases, that it doesn't give a closed form solution but only a set of boundary value problems that have to be solved to obtain desired effective material properties. Nevertheless, the system of boundary value problems can be reliably solved numerically and this gives benchmark results for any other method to compare with. The aim of the present section is to show how this can be done.

3.1 Symmetries of the effective elasticity tensor

Let $Y = Y_{\mathrm{m}} \cup Y_{\mathrm{i}} \subset \mathbb{R}^3$ be a basic periodic cell which defines the periodic microstructure. On Y is defined the elasticity tensor $\underline{\underline{C}}$ such that it is piecewise constant with values $\underline{\underline{C}}_{\mathrm{m}}$ and $\underline{\underline{C}}_{\mathrm{i}}$ on Y_{m} and Y_{i}, respectively. A domain Y_{m} is called the matrix phase and Y_{i} the inclusion phase. It is well known Cioranescu *et al.* (1999), Bensoussan *et al.* (1978) that the effective elastic tensor of the corresponding material with the periodic microstructure is given by

$$C^{\mathrm{eff}}_{ijkh} = \langle C_{ijkh} \rangle - \left\langle C_{ijlm} e_{lm}(\underline{\chi}_{kh}) \right\rangle . \tag{6}$$

Here $\langle \bullet \rangle$ is a volume average over the basic cell Y, $e_{lm}(\underline{\chi}_{kh})$ are components of the deformation tensor of the displacement $\underline{\chi}_{kh}$ and $\underline{\chi}_{kh}$ are solutions of a set of boundary value problems:

Problem 1. *For each pair of Cartesian basis vectors $\underline{e}_k$ and $\underline{e}_h$ find $\underline{\chi}_{kh} \in H^1_\#(Y)$ such that $\left\langle \underline{\chi}_{kh} \right\rangle = \underline{0}$ and*

$$\operatorname{div}\left(\underline{\underline{C}} : \underline{\underline{e}}\left(\underline{\chi}_{kh}\right)\right) = \operatorname{div}\left(\underline{\underline{C}} : \underline{\underline{e}}\left(\underline{e}_k \otimes \underline{e}_h \cdot \underline{y}\right)\right). \tag{7}$$

Here $H^1_\#(Y)$ is a Sobolev space of weakly differentiable functions with periodic boundary conditions on the boundary of Y.

It is well known that the above problem has a unique solution in $H^1_\#(Y)$, Oleinik *et al.* (1992). Due to the symmetry it suffices to solve the above problem only for $k \leq h$. Therefore we have to solve 6 boundary value problems for 6 different right hand sides of (7). Since $\underline{\underline{C}}$ is piecewise constant, the boundary value problem has to be understood in the distributional sense.

Let $\mathcal{O}$ be s symmetry group. It is said that $\mathcal{O}$ is a geometrical symmetry if the microstructure is invariant with respect to $\mathcal{O}$. In particular, $\mathcal{O}$ is a geometrical symmetry of the periodic microstructure with the base cell if $QY = Y$ for all $Q \in \mathcal{O}$. Obviously, geometrical symmetry of the microstructure and material symmetry of material phases of the composite determine symmetry of the effective elasticity tensor. System (6) is to be solved numerically. To solve it effectively, we first inquire after symmetry properties of its solutions $\underline{\chi}_{kh}$.

Theorem 1. *Let $\mathcal{O} \subset O(3)$ be geometrical and material symmetry of (7). Then for all $Q \in \mathcal{O}$*

$$\underline{\chi}(\underline{e}_k \otimes \underline{e}_h, \underline{y}) = Q^T \underline{\chi}(Q\underline{e}_k \otimes Q\underline{e}_h, Q\underline{y}), \tag{8}$$

where $\underline{\chi}(\underline{e}_k \otimes \underline{e}_h, \underline{y}) = \underline{\chi}_{kh}(\underline{y})$.

Proof. Variational formulation of (7) is

$$\int_Y \nabla \underline{\chi}_{kh} : \underline{\underline{C}} : \nabla \underline{w}\, d\underline{y} = \int_Y \underline{e}_k \otimes \underline{e}_h : \underline{\underline{C}} : \nabla \underline{w}\, d\underline{y}, \qquad \forall \underline{w} \in H^1_\#(Y). \tag{9}$$

Due to the geometrical symmetry we have $QY = Y$ and thus we can introduction a new variable $\hat{\underline{y}} = Q\underline{y}$ with the same domain of integration in (9) as the original $\underline{y}$. Let us define

$$\hat{\underline{w}}(\hat{\underline{y}}) = Q\underline{w}(Q^T \hat{\underline{y}}) \qquad \text{and} \qquad \hat{\underline{\chi}}_{kh}(\hat{\underline{y}}) = Q\underline{\chi}_{kh}(Q^T \hat{\underline{y}}). \tag{10}$$

It follows from the chain rule that

$$\nabla_{\underline{y}}\underline{w}(\underline{y}) = \frac{\partial \underline{w}}{\partial \underline{y}}(\underline{y}) = Q^T \frac{\partial \hat{\underline{w}}}{\partial \hat{\underline{y}}}(\hat{\underline{y}})Q = Q^T \nabla_{\hat{\underline{y}}}\hat{\underline{w}}(\hat{\underline{y}})Q = Q_*^T \nabla_{\hat{\underline{y}}}\hat{\underline{w}}. \tag{11}$$

A similar result holds for $\underline{\chi}_{kh}$. Introducing (11) into (9) we obtain

$$\int_Y Q_*^T \nabla_{\hat{\underline{y}}}\hat{\underline{\chi}}_{kh} : \underline{\underline{C}} : Q_*^T \nabla_{\hat{\underline{y}}}\hat{\underline{w}}\, d\hat{\underline{y}} = \int_Y \underline{e}_k \otimes \underline{e}_h : \underline{\underline{C}} : Q_*^T \nabla_{\hat{\underline{y}}}\hat{\underline{w}}\, d\hat{\underline{y}}. \tag{12}$$

Due to the material symmetry $Q_*^T \underline{\underline{C}} = \underline{\underline{C}}$. Therefore, it follows from (12) that

$$\int_Y \nabla_{\hat{\underline{y}}}\hat{\underline{\chi}}_{kh} : \underline{\underline{C}} : \nabla_{\hat{\underline{y}}}\hat{\underline{w}}\, d\hat{\underline{y}} = \int_Y Q_* \underline{e}_k \otimes \underline{e}_h : \underline{\underline{C}} : \nabla_{\hat{\underline{y}}}\hat{\underline{w}}\, d\hat{\underline{y}}. \tag{13}$$

Since solution of (7) is unique, it follows that

$$\hat{\underline{\chi}}_{kh}(\hat{\underline{y}}) = \underline{\chi}(Q\underline{e}_k \otimes Q\underline{e}_h, \hat{\underline{y}}). \tag{14}$$

Using (14) in (10) we obtain (8) and the theorem is proved. □

We can now prove that geometrical and material symmetries indeed determine symmetry of the effective elasticity tensor.

Theorem 2. *Let be $\mathcal{O}_1$ a material symmetry group and $\mathcal{O}_2$ geometrical symmetry of the microstructure. Then $\mathcal{O} = \mathcal{O}_1 \cap \mathcal{O}_2$ is the symmetry group of the effective elasticity tensor.*

Proof. We first rewrite (6) into

$$\underline{\underline{C}}^{\text{eff}} : \underline{e}_k \otimes \underline{e}_h = \left\langle \underline{\underline{C}} \right\rangle : \underline{e}_k \otimes \underline{e}_h - \left\langle \underline{\underline{C}} : \underline{\underline{e}}\left(\underline{\chi}(\underline{e}_k \otimes \underline{e}_h, \bullet)\right)\right\rangle \tag{15}$$

Applying the Rayleight product $Q*$ on both sides of (15), $Q \in \mathcal{O}$ and using (1) we obtain

$$Q_* \underline{\underline{C}}^{\text{eff}} : Q_* \underline{e}_k \otimes \underline{e}_h = \left\langle \underline{\underline{C}} \right\rangle : Q_* \underline{e}_k \otimes \underline{e}_h - \left\langle \underline{\underline{C}} : Q_* \nabla_{\underline{y}} \underline{\chi}(\underline{e}_k \otimes \underline{e}_h, \underline{y})\right\rangle, \tag{16}$$

since $Q_* \underline{\underline{C}} = \underline{\underline{C}}$. Using (10) in (14) it follows

$$\begin{aligned} Q_* \underline{\underline{C}}^{\text{eff}} : Q_* \underline{e}_k \otimes \underline{e}_h &= \left\langle \underline{\underline{C}} \right\rangle : Q_* \underline{e}_k \otimes \underline{e}_h - \left\langle \underline{\underline{C}} : \nabla_{\hat{\underline{y}}} \underline{\chi}(Q\underline{e}_k \otimes Q\underline{e}_h, \hat{\underline{y}})\right\rangle \\ &= \left\langle \underline{\underline{C}} \right\rangle : Q_* \underline{e}_k \otimes \underline{e}_h - \left\langle \underline{\underline{C}} : \nabla_{\underline{y}} \underline{\chi}(Q\underline{e}_k \otimes Q\underline{e}_h, \underline{y})\right\rangle \\ &= \underline{\underline{C}}^{\text{eff}} : Q_* \underline{e}_k \otimes \underline{e}_h. \end{aligned} \tag{17}$$

Since k and h are arbitrary, we deduce $Q_* \underline{\underline{C}}^{\text{eff}} = \underline{\underline{C}}^{\text{eff}}$ for all $Q \in \mathcal{O}$ and the proof is concluded. □

It is well known, see for example Ting (1996), that each one of eight elastic symmetry classes has a minimal subset of its symmetry group such that invariance of $\underline{\underline{C}}$ with respect to this subset guarantees the invariance to the whole group. In particular, $\underline{\underline{C}}$ has cubic symmetry provided that it is invariant with respect to $Q_1 = R(\underline{e}_1, \pi/2)$ and $Q_3 = R(\underline{e}_3, \pi/2)$, where $R(\underline{e}, \theta)$ is a rotation of θ around $\underline{e}$. That is, conditions $Q_1 * \underline{\underline{C}} = \underline{\underline{C}}$ and $Q_3 * \underline{\underline{C}} = \underline{\underline{C}}$ imply that $Q * \underline{\underline{C}} = \underline{\underline{C}}$ for all elements of the cubic group. With this remark, it follows that material and geometrical invariance with respect to the minimal set guarantees a material symmetry of the effective elasticity tensor. Moreover, elastic symmetries can be also characterized by a set of planes of mirror symmetry Chadwic *et al.* (2001). Assuming that the basic cell is invariant with respect to the central inversion, i.e., $-Y = Y$, geometrical symmetries of the basic cell can be also characterized by a set of planes of mirror symmetry.

3.2 Cubic symmetry

Let us assume that $Y = [-1, 1]^3$ is a cube and that $\underline{\underline{C}}$ has at least cubic symmetry. Then it follows from Theorem 2 that $\underline{\underline{C}}^{\text{eff}}$ is a cubic tensor. Moreover, it follows from Theorem 1 that it suffices to know values of the auxiliary functions $\underline{\chi}_{kh}$ only in the first octant Y_1 of Y since for any $\underline{y}$ there exists $\underline{y}_1 \in Y_1$ and an orthogonal transformation Q which preserves symmetry of the problem, such that $\underline{y} = Q\underline{y}_1$. There exist several different covers of Y. For example

$$\begin{aligned} Y &= Y_1 \cup Z_1 Y_1 \cup Z_2 (Y_1 \cup Z_1 Y_1) \cup (Y_1 \cup Z_1 Y_1 \cup Z_2 (Y_1 \cup Z_1 Y_1)) \\ &= Y_1 \cup (-Y_1) \cup Z_1 Y_1 \cup Z_2 Y_1 \cup Z_3 Y_1 \cup R(\underline{e}_1, \pi) Y_1 \cup R(\underline{e}_2, \pi) Y_1 \cup R(\underline{e}_3, \pi) Y_1, \end{aligned} \tag{18}$$

where Z_k denotes a reflection across the plane through the origin with the normal in the direction of $\underline{e}_k$.

Covering of Y by rigid transformation of Y_1 implies that it is enough to solve systems (7) only for functions defined on Y_1. However, functions $\underline{\chi}_{kh}$ have boundary conditions prescribed on the boundary of Y and thus in order to transform (7) to the boundary value problem on Y_1 we have to transform also the boundary conditions from Y to Y_1. To this end, let us choose $\underline{y}^+ \in Y_1$. Using (8) for $\underline{y}^- = Z_k \underline{y}^+$, $k \in \{1, 2, 3\}$ it follows that

$$\underline{\chi}_{ij}(\underline{y}^-) = \underline{\chi}(\underline{e}_i \otimes \underline{e}_j, Z_k \underline{y}^+) = Z_k \underline{\chi}(Z_k \underline{e}_i \otimes Z_k \underline{e}_j, \underline{y}^+). \tag{19}$$

Now, for $i = j$ or $i \neq k$ and $j \neq k$ it follows that $Z_k \underline{e}_i \otimes Z_k \underline{e}_j = \underline{e}_i \otimes \underline{e}_j$ and $Z_k \underline{e}_i \otimes Z_k \underline{e}_j = -\underline{e}_i \otimes \underline{e}_j$ for all other pairs of i and j. Therefore

$$\begin{aligned} i = j \vee (i \neq k \wedge j \neq k) \quad &\Longrightarrow \quad \underline{\chi}_{ij}(\underline{y}^-) = Z_k \underline{\chi}_{ij}(\underline{y}^+), \\ (i = k \wedge j \neq k) \vee (j = k \wedge i \neq k) \quad &\Longrightarrow \quad \underline{\chi}_{ij}(\underline{y}^-) = -Z_k \underline{\chi}_{ij}(\underline{y}^+). \end{aligned} \tag{20}$$

On the symmetry plane $\underline{y}^+ = \underline{y}^-$. Denoting by Σ_k the symmetry plane of Z_k we obtain from (20) the boundary conditions on $\Sigma_k^0 = \Sigma_k \cap Y_1$:

$$\begin{aligned} \chi_k(\underline{e}_i \otimes \underline{e}_i, \underline{y}) = 0 \quad &\text{for} \quad i \in \{1, 2, 3\}, \\ \chi_k(\underline{e}_l \otimes \underline{e}_k, \underline{y}) = 0 \quad &\text{for} \quad l \neq k, l \in \{1, 2, 3\}, \end{aligned}$$

$$\chi_k(\underline{e}_i \otimes \underline{e}_j, \underline{y}) = 0 \quad \text{for} \quad i \neq k \wedge j \neq k, i, j \in \{1,2,3\}, \tag{21}$$

no summation over repeated i and l. From (20) we obtain also boundary conditions on the faces $\Sigma_k^+ = \{(y_1, y_2, y_3) : y_k = 1\} \cap Y_1$ of the same form as (21) since due to the periodicity of $\underline{\chi}_{ij}$, we have $\underline{\chi}_{ij}(\underline{y}^+) = \underline{\chi}_{ij}(\underline{y}^-)$ for $\underline{y}^+ \in \Sigma_k^+$. Summarizing, boundary conditions for the restriction $\hat{\chi}$ of χ to Y_1 are

$$\begin{aligned}
\chi_k(\underline{e}_i \otimes \underline{e}_i, \underline{y}) = 0 \quad &\text{for} \quad \underline{y} \in \Sigma_k^0 \cup \Sigma_k^+ \quad \text{and} \quad i \in \{1,2,3\}, \\
\chi_k(\underline{e}_l \otimes \underline{e}_k, \underline{y}) = 0 \quad &\text{for} \quad \underline{y} \in \Sigma_k^0 \cup \Sigma_k^+ \quad \text{and} \quad l \neq k, l \in \{1,2,3\}, \\
\chi_k(\underline{e}_i \otimes \underline{e}_j, \underline{y}) = 0 \quad &\text{for} \quad \underline{y} \in \Sigma_k^0 \cup \Sigma_k^+ \quad \text{and} \quad i \neq k \wedge j \neq k, i, j \in \{1,2,3\}.
\end{aligned} \tag{22}$$

no summation over i and l. Dirichlet boundary conditions (22) are complimented with Neumann boundary conditions on components of $\underline{\chi}_{kh}$ which are free of Dirichlet boundary conditions. Since they don't appear explicitly in the variational formulation of Problem 1, we shall not write them down here.

Let us now denote by $\underline{\hat{\chi}}_{kh}$, $1 \leq k \leq h \leq 3$ a set of functions defined on Y_1 such that transformation rules (8) apply. Using the covering (18) and (8) functions $\underline{\hat{\chi}}_{kh}$ can be extended from Y_1 to functions $\underline{\chi}_{kh}$ defined on the whole cube Y. In Problem 1 it is required that $\underline{\chi}_{kh}$ have the zero average. We shall now show that due to the construction of $\underline{\chi}_{kh}$ the zero average condition is automatically satisfied without further requirements on $\underline{\hat{\chi}}_{kh}$. Indeed,

$$\begin{aligned}
\int_Y \underline{\chi}_{kh}\, d\underline{y} \;=\; & \int_{Y_1} \underline{\chi}_{kh}\, d\underline{y} + \int_{-Y_1} \underline{\chi}_{kh}\, d\underline{y} + \int_{Z_1 Y_1} \underline{\chi}_{kh}\, d\underline{y} + \int_{Z_2 Y_1} \underline{\chi}_{kh}\, d\underline{y} + \int_{Z_3 Y_1} \underline{\chi}_{kh}\, d\underline{y} + \\
& \int_{R(\underline{e}_1,\pi) Y_1} \underline{\chi}_{kh}\, d\underline{y} + \int_{R(\underline{e}_2,\pi) Y_1} \underline{\chi}_{kh}\, d\underline{y} + \int_{R(\underline{e}_3,\pi) Y_1} \underline{\chi}_{kh}\, d\underline{y}.
\end{aligned} \tag{23}$$

Using (8) and taking into account that $Q \in O(3)$ we have

$$\int_{QY_1} \underline{\chi}_{kh}(\underline{y})\, d\underline{y} = \int_{Y_1} \underline{\chi}(\underline{e}_k \otimes \underline{e}_h, Q\underline{y})\, d\underline{y} = Q \int_{Y_1} \underline{\hat{\chi}}(Q^T \underline{e}_k \otimes Q^T \underline{e}_h, \underline{y})\, d\underline{y}. \tag{24}$$

Considering a case $k = h = 1$ it follows for $i \in \{1,2,3\}$ that

$$\begin{aligned}
\int_{-Y_1} \underline{\chi}_{11}(\underline{y})\, d\underline{y} &= -\int_{Y_1} \underline{\hat{\chi}}_{11}(\underline{y})\, d\underline{y}, \\
\int_{Z_i Y_1} \underline{\chi}_{11}(\underline{y})\, d\underline{y} &= Z_i \int_{Y_1} \underline{\hat{\chi}}_{11}(\underline{y})\, d\underline{y}, \\
\int_{R(\underline{e}_i,\pi) Y_1} \underline{\chi}_{11}(\underline{y})\, d\underline{y} &= R(\underline{e}_i, \pi) \int_{Y_1} \underline{\hat{\chi}}_{11}(\underline{y})\, d\underline{y}
\end{aligned} \tag{25}$$

Inserting (25) into (23) we obtain

$$\int_Y \underline{\chi}_{11}\, d\underline{y} = ((Z_1 + Z_2 + Z_3) + (R(\underline{e}_1, \pi) + R(\underline{e}_2, \pi) + R(\underline{e}_3, \pi))) \int_{Y_1} \underline{\hat{\chi}}_{11}\, d\underline{y} = \underline{0}. \tag{26}$$

For all other cases $k \leq h$ a similar computation holds and thus we have proved that the extensions $\underline{\chi}_{kh}$ have the zero average.

We are now in position to formulate:

Problem 2. *For each pair of Cartesian basis vectors $\underline{e}_k$ and $\underline{e}_h$ find $\hat{\underline{\chi}}_{kh} \in H^1(Y_1)$ such that $\hat{\underline{\chi}}_{kh}$ satisfies boundary conditions (22) and*

$$\operatorname{div}\left(\underline{\underline{C}} : \underline{\underline{e}}\left(\hat{\underline{\chi}}_{kh}\right)\right) = \operatorname{div}\left(\underline{\underline{C}} : \underline{\underline{e}}\left(\underline{e}_k \otimes \underline{e}_h \cdot \underline{y}\right)\right). \tag{27}$$

It is clear from our discussion that restriction of a solution of Problem 1 to Y_1 is also a solution of Problem 2. Moreover, as it was shown, solutions of Problem 2 can be extended to functions defined on Y. It is not difficult to show that in this way the solution of Problem 1 is obtained and this proves that Problem 2 is unequally solvable.

It now only remains to show how to compute the effective elasticity tensor by means of $\hat{\underline{\chi}}_{kh}$. Let us denote in accordance with the covering (23)

$$Q_1 = I, Q_2 = -I, Q_3 = Z_1, Q_4 = Z_2, Q_5 = Z_3, Q_6 = R(\underline{e}_1, \pi), Q_7 = R(\underline{e}_2, \pi), Q_8 = R(\underline{e}_3, \pi).$$

Now,

$$\begin{aligned}
\left\langle \underline{\underline{C}} : \underline{\underline{e}}\left(\underline{\chi}(\underline{e}_k \otimes \underline{e}_h, \bullet)\right)\right\rangle &= \frac{1}{|\,Y\,|} \sum_{i=1}^{8} \int_{Q_i Y_1} \underline{\underline{C}} : \frac{\partial}{\partial \underline{y}}\, \underline{\chi}(\underline{e}_k \otimes \underline{e}_h, \underline{y})\, dy \\
&= \frac{1}{8\,|\,Y_1\,|} \int_{Y_1} \underline{\underline{C}} : \sum_{i=1}^{8} Q_i * \frac{\partial}{\partial \underline{y}_1}\, \hat{\underline{\chi}}(Q_i^T \underline{e}_k \otimes Q_i^T \underline{e}_h, \underline{y}_1)\, dy_1.
\end{aligned} \tag{28}$$

Direct computation shows that

$$\frac{1}{8} \sum_{i=1}^{8} Q_i * \frac{\partial}{\partial \underline{y}_1}\, \hat{\underline{\chi}}(Q_i^T \underline{e}_k \otimes Q_i^T \underline{e}_h, \underline{y}_1) = \underline{\underline{A}}_{kh} \frac{\partial}{\partial \underline{y}_1}\, \hat{\underline{\chi}}(\underline{e}_k \otimes \underline{e}_h, \underline{y}_1), \tag{29}$$

where

$$\begin{aligned}
\underline{\underline{A}}_{ii} &= \sum_{j=1}^{3} \underline{e}_j \otimes \underline{e}_j \otimes \underline{e}_j \otimes \underline{e}_j, \\
\underline{\underline{A}}_{12} &= \underline{e}_1 \otimes \underline{e}_2 \otimes \underline{e}_1 \otimes \underline{e}_2 + \underline{e}_2 \otimes \underline{e}_1 \otimes \underline{e}_2 \otimes \underline{e}_1, \\
\underline{\underline{A}}_{13} &= \underline{e}_1 \otimes \underline{e}_3 \otimes \underline{e}_1 \otimes \underline{e}_3 + \underline{e}_3 \otimes \underline{e}_1 \otimes \underline{e}_3 \otimes \underline{e}_1, \\
\underline{\underline{A}}_{23} &= \underline{e}_2 \otimes \underline{e}_3 \otimes \underline{e}_2 \otimes \underline{e}_3 + \underline{e}_3 \otimes \underline{e}_2 \otimes \underline{e}_3 \otimes \underline{e}_2.
\end{aligned} \tag{30}$$

Since $\underline{\underline{C}}^{\text{eff}}$ has cubic symmetry, it suffices to evaluate only C^{eff}_{1111}, C^{eff}_{1122} and C^{eff}_{1212}. Using (6), (28-30) and cubic symmetry of $\underline{\underline{C}}$ it follows

$$\begin{aligned}
C^{\text{eff}}_{1111} &= \langle C_{1111} \rangle - \frac{1}{|\,Y_1\,|} \int_{Y_1} \underline{e}_1 \otimes \underline{e}_1 : \underline{\underline{C}} : \underline{\underline{A}}_{11} : \frac{\partial}{\partial \underline{y}_1}\, \hat{\underline{\chi}}(\underline{e}_1 \otimes \underline{e}_1, \underline{y}_1)\, d\underline{y}_1 \\
&= \langle C_{1111} \rangle - \frac{1}{|\,Y_1\,|} \int_{Y_1} \sum_{j=1}^{3} C_{11jj} \left(\nabla_{\underline{y}_1} \hat{\underline{\chi}}_{11}\right)_{jj} d\underline{y}_1
\end{aligned}$$

$$= \langle C_{1111} \rangle - \left\langle C_{11kl} \underline{\underline{e}} \left(\underline{\hat{\chi}}_{11} \right)_{kl} \right\rangle_{Y_1} , \tag{31}$$

where $\langle \bullet \rangle_{Y_1}$ denotes average over Y_1. Similarly,

$$\begin{aligned} C^{\text{eff}}_{1122} &= \langle C_{1122} \rangle - \left\langle C_{11kl} \underline{\underline{e}} \left(\underline{\hat{\chi}}_{22} \right)_{kl} \right\rangle_{Y_1} , \\ C^{\text{eff}}_{1212} &= \langle C_{1212} \rangle - \left\langle C_{12kl} \underline{\underline{e}} \left(\underline{\hat{\chi}}_{12} \right)_{kl} \right\rangle_{Y_1} . \end{aligned} \tag{32}$$

Thus, we have established:

Theorem 3. *Nonzero effective coefficients of the periodic homogenization problem with cubic symmetry are*

$$C^{\text{eff}}_{ijkh} = \langle C_{ijkh} \rangle_{Y_1} - \left\langle C_{ijlm} e_{lm} (\underline{\hat{\chi}}_{kh}) \right\rangle_{Y_1} , \tag{33}$$

where $\underline{\hat{\chi}}_{kh}$ *are solutions of the boundary value Problem 2.*

3.3 Finite element discretization

We have succeeded to reduce a domain of the boundary value problems for the auxiliary functions from the whole cube to one eight of it. Since both Problems 1 and 2, apart from some special cases, don't admit a closed form solution, reduction of the domain is of great computational advantage. Moreover, Problem 1 has prescribed periodic boundary conditions while Problem 2 has Dirichlet boundary conditions, which are much easier to apply. Also Problem 1 has an additional constraint of the zero average. Within the context of the finite element computation the periodic boundary conditions, as well as the zero average condition, are usually imposed by using multipliers which spoil positive definiteness of the stiffness matrix. Problem 2 is thus not only considerably smaller but is also free of the above mentioned nuisances.

In order to consistently discretize determination of the effective material properties discretization of the problem has to conserve symmetry of the problem. Therefore, the finite element mesh has to possess the same symmetry as the problem. A finite element mesh with cubic symmetry can be generated by discretization of the polyhedral angle of the first octant and then by rotation of it around the symmetry axes of the cube, see Fig. 1 of a FEM mesh with 12531 tetrahedral elements. In order to obtain a valid finite element mesh, faces of the polyhedral angle have to be consistently discretized. Alternatively, it suffices to generate a finite element mesh which is invariant only with respect to the defining minimal set of the symmetry, see the last paragraph in Section 3.1. We remark that it is even possible to reduce the computational domain from the octant to the polyhedral angle of the cube. However, in this reduction boundary value problems for the auxiliary functions are not separated and thus the reduction is of minor importance.

Finite element discretization of the problem results in a large linear system. To solve it we used a direct linear solver from the HSL Mathematical Software Library, A collection of Fortran codes for large scale scientific computation (2016). The solver was found to be very effective with good parallel performance. Correctness of the results was confirmed by comparison with results from the literature Heitkam *et al.* (2016) for a spherical inclusion and by comparing results for different meshes, basis functions and also material properties. Note that the homogenization problem has for composites with a constant shear modulus of phases a closed form solution for an arbitrary shape of the inclusion, see Hill (1964), what gives an ideal benchmark problem for certifying the code. On the basis of performed tests it is concluded that our finite element computation gives correct results with high accuracy. Results are presented later in the paper together with the comparison with results obtained by the equivalent eigenstrain method. Tetrahedral elements with quadratic basis functions with a fine mesh consisting of around 12000 elements per the polyhedral angle of the cube was used.

4. Fourier representation of Eshelby operator

After obtaining a finite element solution for the effective elasticity tensor we now proceed to a completely different method which gives an approximate solution in almost a closed form. A range of applicability of the approximation will be determined by comparison with the finite element solution.

Since Fourier series expansion is used, it is convenient to use $\Omega = [-\pi, \pi]^3$ for the basic periodic cell instead of $Y = [-1, 1]^3$. The inclusion problem amounts to solve the following boundary value problem: for a given $\underline{\underline{\epsilon}}^* \in \mathrm{Sym}_2$ find $\underline{\underline{e}} \in \mathrm{Sym}_2$ with periodic boundary conditions on $\partial\Omega$ such that

$$\operatorname{div} \underline{\underline{C}} : (\underline{\underline{e}} - \underline{\underline{\epsilon}}^*) = \underline{0} \quad \text{in} \quad \Omega \quad \text{and} \quad \left\langle \underline{\underline{e}} \right\rangle_\Omega = \underline{\underline{0}}. \tag{34}$$

Here Sym_2 is the space of second order symmetric tensors, $\underline{\underline{C}}$ is the elasticity tensor and $\left\langle \underline{\underline{e}} \right\rangle_\Omega$ is

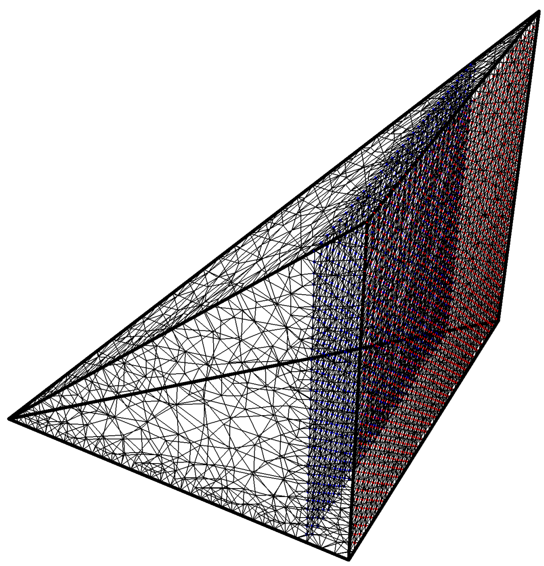


Fig. 1 Finite element mesh of the polyhedral angle. Nodes at inclusion face are coloured blue, at the cell face red

the average over Ω. It is well known that the solution of the problem is given by

$$\underline{\underline{e}}(\underline{x}) = \sum_{|\underline{m}|\neq 0} \underline{\underline{K}}(\underline{m}) : \underline{\underline{\epsilon}}^*(\underline{m}) e^{i\,\underline{m}\cdot\underline{x}}, \tag{35}$$

where $\underline{m} \in \mathbb{Z}^3$ is a multi index, $\underline{\underline{\epsilon}}^*(\underline{m})$ is m-nth Fourier coefficient of $\underline{\underline{\epsilon}}^*$ and

$$\underline{\underline{K}}(\underline{m}) = \frac{2}{|\underline{m}|^2} \underline{m} \hat{\otimes} \underline{\underline{i}} \hat{\otimes} \underline{m} + \frac{\nu}{1-\nu} \cdot \frac{1}{|\underline{m}|^2} \underline{m} \otimes \underline{m} \otimes \underline{\underline{i}} - \frac{1}{1-\nu} \cdot \frac{1}{|\underline{m}|^4} \underline{m} \otimes \underline{m} \otimes \underline{m} \otimes \underline{m}. \tag{36}$$

Here $\hat{\otimes}$ is the symmetric dyadic product, $\underline{\underline{i}}$ is the identity second order tensor and ν is the Poisson ratio. Eq. (34) defines Eshelby operator $\mathcal{S}$ which maps $\underline{\underline{\epsilon}}^*$ to $\underline{\underline{e}} = \mathcal{S}\,\underline{\underline{\epsilon}}^*$ while (36) gives its Fourier form.

Usually $\underline{\underline{\epsilon}}^*$ is nonzero only on a part of the domain Ω. The support of $\underline{\underline{\epsilon}}^*$ is called the inclusion and is denoted by Ω_{i}. In the language of composite materials the compliment $\Omega_{\mathrm{m}} = \Omega \setminus \Omega_{\mathrm{i}}$ is called the matrix.

5. Equivalent eigenstrain equation

Let Ω represents a composite material with a piecewise constant elasticity tensor with values $\underline{\underline{C}}$ on the matrix and $\underline{\underline{C}}_{\mathrm{i}}$ on the inclusion. Equivalent eigenstrain equation says that for the prescribed homogeneous macro strain $\underline{\underline{e}}_{\mathrm{b}}$ there exists an equivalent eigenstrain such that

$$\underline{\underline{C}}_{\mathrm{m}} : (\underline{\underline{e}} + \underline{\underline{e}}_{\mathrm{b}}) = \underline{\underline{C}} : (\underline{\underline{e}} + \underline{\underline{e}}_{\mathrm{b}} - \underline{\underline{\epsilon}}^*). \tag{37}$$

Evidently, the mapping $\underline{\underline{e}}_{\mathrm{b}} \mapsto \underline{\underline{\epsilon}}^*$ is linear and is denoted by $\underline{\underline{\epsilon}}^* = \mathcal{Z}\,\underline{\underline{e}}_{\mathrm{b}}$. Equation (37) is solved by the means of variational formulation, Mejak (2014). Assuming homogeneous eigenstrain approximation $\underline{\underline{\epsilon}}^* = \chi(\Omega_{\mathrm{i}})\underline{\underline{\epsilon}}_0^*$, here $\chi(\Omega_{\mathrm{i}})$ is the indicator function of Ω_{i}, the corresponding Lagrange equation is

$$\underline{\underline{\epsilon}}_0^* - \hat{\underline{\underline{C}}} : \langle\, \underline{\underline{e}}\,\rangle_{\Omega_{\mathrm{i}}} = \hat{\underline{\underline{C}}} : \underline{\underline{e}}_{\mathrm{b}}, \tag{38}$$

where $\hat{\underline{\underline{C}}} = \underline{\underline{C}}^{-1} : \left(\underline{\underline{C}} - \underline{\underline{C}}_{\mathrm{i}}\right)$. Putting (35) into (38) it follows

$$\left(\underline{\underline{I}} - \frac{\pi^3}{|\Omega_{\mathrm{i}}|} \hat{\underline{\underline{C}}} : \sum_{|\underline{m}|\neq 0} \underline{\underline{K}}(\underline{m}) \epsilon^*(\underline{m}) \epsilon^*(-\underline{m}) \right) \underline{\underline{\epsilon}}_0^* = \hat{\underline{\underline{C}}} : \underline{\underline{e}}_{\mathrm{b}}. \tag{39}$$

It is known form Mejak (2014) that (39) has a unique solution that can be expressed in a form $\underline{\underline{\epsilon}}_0^* = \underline{\underline{Z}} : \underline{\underline{e}}_{\mathrm{b}}$, where $\underline{\underline{Z}}$ is a fourth order tensor with minor symmetries.

A crucial step to solve (39) is to compute the infinite sum. To this end, although more general cases can be treated, let us assume that Ω_{i} is a centrally placed cube with the side length $2\delta\pi$, $\delta \in [0, 1]$. It follows then that

$$\epsilon^*(\underline{m}) = \frac{\sin(m_1\pi\delta)\sin(m_2\pi\delta)\sin(m_3\pi\delta)}{\pi^3\, m_1 m_2 m_3}. \tag{40}$$

Therefore, $\epsilon^*(\underline{m})$ is an even function of $\underline{m}$ and is invariant to cyclic permutations of $\underline{m}$. The triple sum in (39) is also invariant to the inversions and cyclic permutations and thus $\sum_{|\underline{m}|\neq 0} \underline{\underline{K}}(\underline{m})\epsilon^*(\underline{m})^2$ is a cubic tensor with minor symmetries. It follows then, see (2), that

$$\sum_{|\underline{m}|\neq 0} \underline{\underline{K}}(\underline{m})\epsilon^*(\underline{m})^2 = \frac{1}{3}\sum_{|\underline{m}|\neq 0} \epsilon^*(\underline{m})^2 \left(\underline{\underline{E}}_1 + \frac{\nu}{1-\nu}\underline{\underline{E}}_2 + \underline{\underline{E}}_3\right) + \frac{1}{3(1-\nu)} \sum_{|\underline{m}|\neq 0} \frac{m_1^2 m_2^2 + m_1^2 m_3^2 + m_2^2 m_3^2}{\left(m_1^2+m_2^2+m_3^2\right)^2}\epsilon^*(\underline{m})^2 \left(2\underline{\underline{E}}_1 - \underline{\underline{E}}_2 - \underline{\underline{E}}_3\right). \tag{41}$$

The first sum is evaluated using the Parseval's theorem

$$\sum_{|\underline{m}|\neq 0} \epsilon^*(\underline{m})^2 = \frac{1}{|\Omega_{\mathrm{i}}|}\int_\Omega \chi(\Omega_{\mathrm{i}})^2\, d\Omega - \lim_{\underline{m}\to\underline{0}} \epsilon^*(\underline{m})^2 = \delta^3(1-\delta^3). \tag{42}$$

To evaluate the second sum we first observe that it suffices to compute the sum

$$\beta(\delta) = \frac{1}{\pi^6}\sum_{|\underline{m}|\neq 0} \frac{\sin^2(m_1\pi\delta)\sin^2(m_2\pi\delta)\sin^2(m_3\pi\delta)}{m_3^2\left(m_1^2+m_2^2+m_3^2\right)^2}. \tag{43}$$

Using the residue theorem Henric (1977), summation over m_1 gives

$$\beta(\delta) = \sum_{m_2,m_3=-\infty}^{\infty} b(m_2,m_3) = \frac{1}{8\pi^5}\sum_{m_2,m_3=-\infty}^{\infty} \frac{-2\coth\gamma - 2\sinh(\gamma\delta) + B(\gamma)}{m_3^2\left(m_2^2+m_3^2\right)^{3/2}}\sin^2(m_2\pi\delta)\sin^2(m_3\pi\delta), \tag{44}$$

where $\gamma = \pi\sqrt{m_2^2+m_3^2}$ and

$$B(\gamma) = \frac{\sinh(2\gamma(1-\delta)) + \sinh(2\gamma(\delta+1))}{\cosh(2\gamma)-1} + \frac{4(\gamma\delta\cosh(2\gamma(\delta-1)) - \gamma\delta\cosh(2\gamma\delta) + \gamma\cosh(2\gamma\delta) - \gamma)}{\cosh(2\gamma)-1}. \tag{45}$$

Note that $\lim_{\gamma\to\infty}(B(\gamma) - 2\sinh(\gamma\delta)) = 0$ and thus the sum is absolutely convergent. To the best author knowledge the sum (44) is not analytically summable and is thus approximated by a finite sum

$$\beta(\delta) \doteq 4\sum_{m_2,m_3=1}^{N_1} b(m_2,m_3) + 2\sum_{m_2=1}^{N_2}\lim_{m_3\to 0} b(m_2,m_3) \tag{46}$$

for sufficiently large N_1 and N_2.

Putting (42-43) into (41) we have

$$\sum_{|\underline{m}|\neq 0} \underline{\underline{K}}(\underline{m})\epsilon^*(\underline{m})^2 = \frac{1}{3}\delta^3(1-\delta^3)\left(\underline{\underline{E}}_1 + \frac{\nu}{1-\nu}\underline{\underline{E}}_2 + \underline{\underline{E}}_3\right) + \frac{\beta(\delta)}{1-\nu}\left(2\underline{\underline{E}}_1 - \underline{\underline{E}}_2 - \underline{\underline{E}}_3\right). \tag{47}$$

6. Effective material properties

The effective material properties $\underline{\underline{C}}^{\text{eff}}$ are given by

$$\underline{\underline{C}}^{\text{eff}} = \underline{\underline{C}} + c(\underline{\underline{C}}_{\text{i}} - \underline{\underline{C}}) : \underline{\underline{P}}, \tag{48}$$

where c is a concentration ratio $c = |\,\Omega_{\text{i}}\,|\,/\,|\,\Omega\,| = \delta^3$ and $\underline{\underline{P}}$ is the concentration tensor which relates the prescribed macrostrain with the averaged inclusion strain, i.e. $\underline{\underline{e}}_{\text{b}} + \left\langle \underline{\underline{e}} \right\rangle_{\Omega_{\text{i}}} = \underline{\underline{P}} : \underline{\underline{e}}_{\text{b}}$. Using (38) it follows that $\underline{\underline{C}}^{\text{eff}} = \underline{\underline{C}} : (\underline{\underline{I}} - c\underline{\underline{Z}})$, where $\underline{\underline{Z}} = \underline{\underline{Z}}(\delta)$ gives solution of (39). Since the cubic symmetry of the problem has been assumed, $\underline{\underline{C}}^{\text{eff}}$ is a cubic tensor. Its material moduli are the bulk modulus κ, the shear modulus μ and the second shear modulus $\hat{\mu} = C_{1111} - C_{1122} - 2C_{1212}$. Their values are, after solving (39) and (48), expressed in a nondimensional form as

$$\begin{aligned}
\kappa &= 1 + \frac{3c(1-\kappa_{\text{r}})(1-\nu)}{(\nu+1)(c(\kappa_{\text{r}}-1)-\kappa_{\text{r}})+4\nu-2}, \\
\mu &= 1 - \frac{96c^2(\mu_{\text{r}}-1)(\nu-1)}{\Delta}, \\
\hat{\mu} &= \frac{192c^2(\mu_{\text{r}}-1)^2(1-\nu)(5\beta(\delta)+64(c-1)c)}{\Delta\left((1-\mu_{\text{r}})\left(3\beta(\delta)+64c^2(2\nu-1)\right)+64c(\mu_{\text{r}}(2\nu-1)+\nu-2)\right)},
\end{aligned} \tag{49}$$

where κ_{r} and μ_{r} are the quotients of the inclusion versus the matrix moduli and

$$\Delta = \left(64c^2(\nu-1) - \beta(\delta)\right)(\mu_{\text{r}}-1) - 32c(2\mu_{\text{r}}+1)(\nu-1). \tag{50}$$

As can be seen the homogeneous eigenstrain approximation gives κ that is independent upon $\beta(\delta)$ and agrees with the well known Hashin (1960) result. One can show that the reason that κ is independent upon $\beta(\delta)$ stems from the fact that whenever the eigenstrain is approximated in such a way that $\underline{\underline{\epsilon}}^*(Q\underline{x}) = \underline{\underline{\epsilon}}^*(\underline{x})$, here Q is a rotation from the cubic symmetry group, the isotropic macro strain $\underline{\underline{e}}_{\text{b}}$ results in the isotropic eigenstrain and this automatically imply Hashin's formula for the bulk modulus.

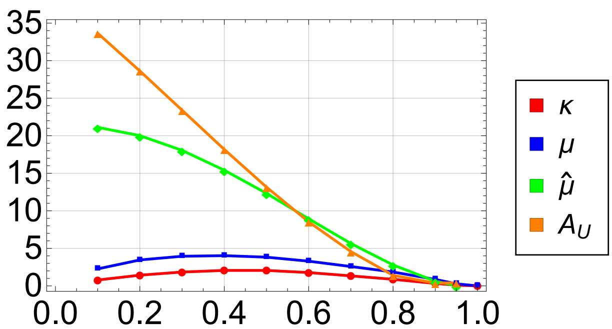


Fig. 2 Relative error in percentage of the effective elasticity coefficients with respect to the concentration ratio of the cubic glass epoxy inclusion

To find out how good is the homogeneous eigenstrain approximation, comparison between it and the results computed by the FEM solution of the periodic homogenization is made. Figure 2 shows the relative error of the comparison in percentage with respect to c for the glass epoxy composite, $E_{\mathrm{i}} = 3$GPa, $\nu_{\mathrm{i}} = 0.35$, $E_{\mathrm{m}} = 70$GPa, $\nu_{\mathrm{m}} = 0.2$, ($\kappa_{\mathrm{r}} = 11.67$ and $\mu_{\mathrm{r}} = 26.25$). Results are given for the effective κ, μ, $\hat{\mu}$ and the anisotropy index $A_{\mathrm{U}} = \frac{6}{5}\left(\sqrt{Z} - 1/\sqrt{Z}\right)^2$, where $Z = 2C_{1212}/(C_{1111} - C_{1122})$ is the Zener anisotropy index. For definition and importance of A_{U} see Ranganathan *et al.* (2008). Note that the relative error for $\hat{\mu}$ and A_{U} is large for small values of c since their values are small. Their values $\hat{\mu}$ and A_{U} are shown in Fig. 3.

As can be seen, the relative error is rather large for $\hat{\mu}$ and A_{U} for small concentrations but it is reasonably small for $c > 0.8$. This is true not only for the particular glass epoxy composite but also for the whole range of materials having a simple cubic microstructure with a cubic inclusion. The equivalent eigenstrain approximation worst performs in the case of voids where strictly speaking theory of variational eigenstrain approximation does not apply, see Mejak (2014). Nevertheless the approximation is again good, see Figure 4 and thus the approximation is also valid for thin walled structures. In particular, it is valid for cubic foam and thus in conjunction with the forthcoming Taylor series approximation of $\beta(\delta)$ its effective elastic properties in a closed form have been obtained.

Since equivalent eigenstrain approximation gives good results for $c > 0.8$, a Taylor series expansion of $\beta(\delta)$ around $\delta = 1$ is proposed as a good approximation of the material properties. Hence, $\beta(\delta)$ is approximated as

$$\beta(\delta) \doteq \beta_1(1-\delta)^2 + \beta_2(1-\delta)^3, \qquad \beta_1 = 21, \quad \beta_2 = -39. \tag{51}$$

Putting (51) into (49-50) an asymptotic expansion of the effective material properties is obtained. For $c \in [0.7, 1]$ it is practically indistinguishable from the original approximation (49) and thus it gives reasonable approximation of the effective properties.

We note that the asymptotic expansion at $\delta = 0$ is not of interest as the homogeneous eigenstrain approximation is of pure quality for small concentration ratios c for a cubical inclusion. The reason that the homogeneous eigenstrain approximation is good approximation for an ellipsoidal inclusion and bad for a cubical inclusion at small c is that only an ellipsoidal inclusion results in homogeneous eigenstress within the inclusion, see for example Liu (2008), and thus in this case the homogeneous

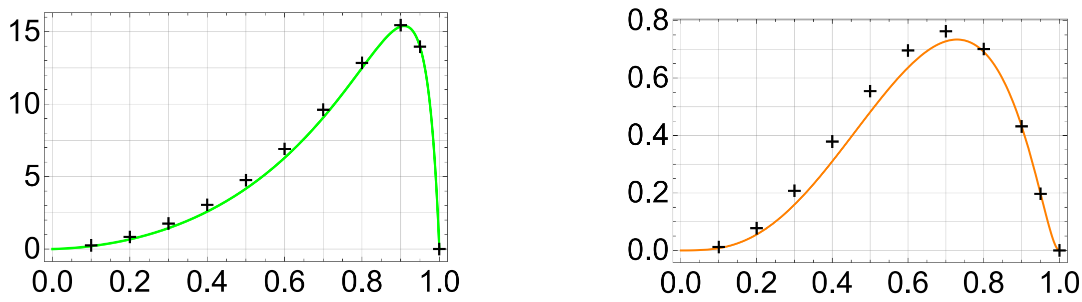


Fig. 3 The effective second shear modulus $\hat{\mu}$ and the anisotropy index A_{U} for the glass epoxy composite. Solid curves are computed by (49-50) while the crosses are obtained by the finite element computation

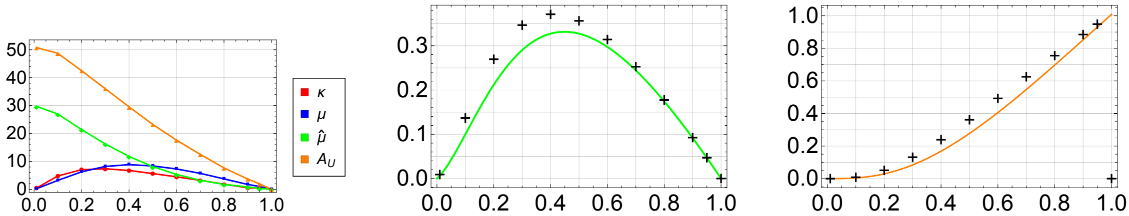


Fig. 4 Relative error, $\hat{\mu}$ and A_{U} for the cubic foam with $\nu = 0.3$.

eigenstrain is a good approximation at low concentration ratio where interactions between inclusions are of minor importance. Using a piecewise homogeneous eigenstrain approximation a better agreement can be obtained. However, it this case formulae (49) as well as the asymptotic expansions are more involved. Note also that (49-50) is valid only for a cubic inclusion and not, for example, for a spherical inclusion or any other inclusion.

Having obtained the closed form solution a brief parametric study of Poisson's ratio is presented as an illustration of applicability of the closed form solution. Poisson's ratio $\nu = \nu(\underline{n}, \underline{m})$ is defined as the ratio of the lateral contraction in the direction $\underline{m}$ to the axial extension in the direction $\underline{n}$ due to a uniaxial tension in the direction $\underline{n}$. For cubic symmetry one usually apply tension in $[110]$ direction and measures lateral contraction for $[1\bar{1}0]$ and $[001]$ directions, see Baughman *et al.* (1998), although it is known (Ting *et al.* (2005)) that in certain directions, which depend on material moduli, Poisson's ratio can be unbounded. Here we used crystallography notation $[\ldots]$ for giving directions. Using formulae (1-2) from Baughman *et al.* (1998) it turns out that $\nu([110],[1\bar{1}0])$ and $\nu([110],[001])$ depend upon ν_{m}, ν_{i}, κ_{r} and the concentration ratio c. Figure 5 gives results for $\nu_{\mathrm{m}} = 0.4$ and $\nu_{\mathrm{i}} = 0.3$. As expected, $\nu([110],[001])$ is much smaller than $\nu([110],[1\bar{1}0])$. In the limit $\kappa_{\mathrm{r}} \to 0$ or $\kappa_{\mathrm{r}} \to \infty$, the Poisson's ratios are independent upon ν_{i}. For the incompressible matrix $\kappa_{\mathrm{r}} = 0$ and

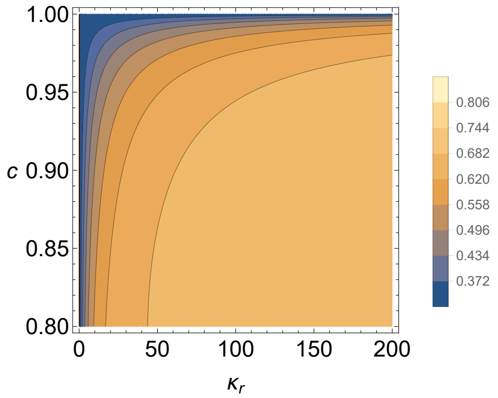
$$\lim_{c \to 1} \nu([110],[1\bar{1}0]) = \frac{7}{11} \quad \text{and} \quad \lim_{c \to 1} \nu([110],[001]) = \frac{1}{11}. \tag{52}$$

Fig. 5 demonstrates that Poisson's ratio can be grater that $1/2$. However, if the inclusion and matrix are isotropic, it is always bounded between $0 \leq \nu \leq 1$ for any directions $\underline{n}$ and $\underline{m}$.

7. Conclusions

A viable approximation in a closed form of effective elasticity moduli of composites with cubic inclusions with a high volume ratio was established. This is of potential great interest as many composite structures are thin walled or are made of plate reinforcements. In particular, the octet foam and their combination Isomax have nearly uniform strain energy distribution (Berger *et al.* (2017)) what guarantee good homogeneous eigenstrain approximation that allows, as demonstrated in the paper, a closed form approximation of the effective properties. In the cases where the homogeneous eigenstrain approximation fails, piecewise homogeneous eigenstrain approximation is a good alternative which is again capable of giving a closed form approximation.

In the future work, the approximation can be extended to structures with orthotropic microstructure. The first part of the paper actually already applies, while the equivalent eigenstrain approxima-



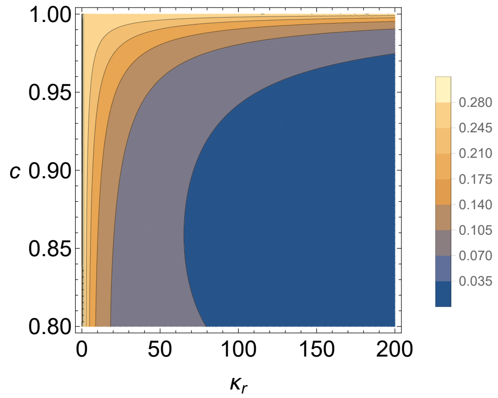


Fig. 5 Density plot of Poisson's ratio $\nu([110],[1\bar{1}0])$ at left and $\nu([110],[001])$ at right with respect to κ_r and concentration ratio c

tion can be readily extended to the orthotropic case. With combination of piecewise homogeneous eigenstrain approximation effective properties of many interesting structures, for example infilled frame structures (Senthil *et al.* (2016)), can be analysed.

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