Modelling Simul. Mater. Sci. Eng. **7** (1999) 829–840. Printed in the UK PII: S0965-0393(99)03041-7

Estimating the overall properties of heterogeneous Cosserat materials

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Received 6 December 1998, accepted for publication 22 March 1999

Abstract. Classical homogenization methods do not account for size effects in the effective properties of polycrystals: they do not predict the influence of grain size nor the width of shear bands in localization phenomena. The polycrystal can be regarded as an example of a heterogeneous Cosserat material. A method is proposed to estimate the effective properties of aggregates of Cosserat media. A validation of the methodology is given in the case of linear Cosserat elasticity. Some steps towards an extension of the self-consistent scheme to Cosserat materials are then presented.

1. Introduction

1.1. Scope of this work

The modelling of the mechanical behaviour of materials at a mesoscopic scale requires, in some cases, the use of continua having an intrinsic length scale. When the microstructure involves oriented stiffening elements or if directors can be attached to each material point, one may resort to the Cosserat continuum, which, in addition to the usual translational degrees of freedom, admits rotational degrees of freedom [1]. A dislocated single crystal can be regarded as an example of such a continuum, for which lattice curvature is due to so-called geometrically necessary dislocations [3]. The importance of explicitly introducing the influence of lattice curvature on subsequent hardening clearly appears in the analysis of localization phenomena in single crystals [3]. As a result, a polycrystal is an aggregate of Cosserat media and, therefore, is a heterogeneous Cosserat material. The problem is then to work out the effective properties and the resulting characteristic length of an aggregate of Cosserat constituents. The aim of this work is to provide some methods to estimate them. The proposed method may be referred to as an homogenization technique in a broad sense. In particular, we will not restrict ourselves to the usual case for which the typical size d of the heterogeneities is much smaller than the size of the considered structure or, more precisely, than a typical wavelength L_ω of the applied loading conditions (for that purpose, see [4]). Homogenization techniques are now well developed in the case of classical media in the linear regime but also in the nonlinear regime [5]. Some of them have been extended to replace a classical heterogeneous medium under strong mean deformation gradients by an effective Cosserat medium [2]. In [6], we considered discrete and continuous heterogeneous Cosserat materials and generalized some homogenization methods. As in [6], we assume that a representative volume element (RVE), Ω, can be defined, in order to replace the heterogeneous Cosserat medium by a homogeneous

0965-0393/99/050829+12$30.00

equivalent one. 'Equivalent' is meant for a certain limited range of loading conditions that will be explicated in the following, and, under the conditions aforementioned ($d \leqslant L_\omega$), it is not claimed that a unique homogeneous equivalent medium does exist. For that reason, we may simply speak of a homogeneous substitute medium (HSM). The RVE is assumed to have a finite size and its volume is denoted by $|\Omega|$. The geometry of the RVE and the distribution of mechanical properties may be exactly known (periodic case) or known only in a statistical sense (random media). Contrary to the classical case, the absolute size of the RVE plays a significant role and at least the order of magnitude of this characteristic size must be specified. Clearly, it depends on the type of structural problems one wants to solve on a macroscopic level. For simplicity, cracks, voids or rigid particles in Ω are excluded.

In this work, we use a Hill–Mandel-type approach of homogenization, but, in the case of periodic microstructures, we use an asymptotic analysis as proposed in [12]. In particular, the pertinence of different asymptotic processes depending on the ratio l_c/L_ω (where l_c is a characteristic length of the constituents, to be defined) is discussed in [12] and only one of them is developed in the following. The methods are applied to the case of linear elasticity. An expression for the effective properties as a function of the concentration tensors is derived. It is applied to a specific microstructure for which estimated effective properties are determined, using the finite-element method. To assess the quality of this estimation, structural calculations are performed involving a finite number of cells. A reference calculation taking every heterogeneity into account is compared to the response of the substitute medium. The proposed method will turn out to be simple and efficient although improvements are possible.

The last part of this work presents some steps towards a possible extension of the self-consistent scheme to heterogeneous Cosserat materials. In particular, finite-element simulations of a generalized Eshelby problem and of a Cosserat elastic heterogeneity embedded in an infinite Cosserat matrix are provided.

1.2. Notation

Throughout the paper, $\underline{\mathbf{x}}$, $\underset{\sim}{\mathbf{x}}$ and $\underset{\approx}{\mathbf{x}}$ denote a vector, a second-rank and a four-rank tensor, respectively. The third-order permutation tensor will be denoted $\underline{\underset{\sim}{\epsilon}}$ if applied to a second-rank tensor and $\underset{\sim}{\underline{\epsilon}}$ if applied to a vector. $\underline{\nabla}$ is the nabla operator. The divergence of $\underset{\sim}{\mathbf{a}}$ is denoted by $\underset{\sim}{\mathbf{a}} \cdot \underline{\nabla}$. When the notation becomes ambiguous, indices are used.

The deformation of a Cosserat continuum is described by a displacement field $\underline{\mathbf{u}}$ and a microrotation field $\underset{\sim}{\mathbf{R}}$ which accounts for the rotation of the underlying microstructure represented by three orthogonal rigid vectors called directors [7]. The rotation $\underset{\sim}{\mathbf{R}}$ will be represented by the vector $\underline{\mathbf{\Phi}}$ according to $\underset{\sim}{\mathbf{R}} = \underset{\sim}{\mathbf{1}} + \underset{\approx}{\epsilon}\underline{\mathbf{\Phi}}$, in the case of small microrotations. The associated deformation and torsion-curvature tensors are $\underset{\sim}{\mathbf{e}}$ and $\underset{\sim}{\kappa}$

$$\underset{\sim}{\mathbf{e}} = \underline{\mathbf{u}} \otimes \underline{\nabla} + \underset{\approx}{\epsilon}\underline{\mathbf{\Phi}} \qquad \underset{\sim}{\kappa} = \underline{\mathbf{\Phi}} \otimes \underline{\nabla}. \tag{1}$$

The dual quantities associated with the deformation and curvature tensors are the force stress tensor $\underset{\sim}{\sigma}$ and the couple stress tensor $\underset{\sim}{\mu}$. In general, these tensors are not symmetric. The force and couple stress tensors must fulfil the equilibrium equations in the static case

$$\underset{\sim}{\sigma} \cdot \underline{\nabla} = 0 \qquad \underset{\sim}{\mu} \cdot \underline{\nabla} - \underline{\underset{\sim}{\epsilon}}\underset{\sim}{\sigma} = 0. \tag{2}$$

Volume forces and couples are excluded for simplicity. The study is restricted to small deformations, small microrotations and small curvatures.

2. On two boundary value problems on the RVE

The determination of the effective properties requires the resolution of an initial boundary value problem (BVP) on Ω. In particular, some boundary conditions must be specified in order to have a well-posed mechanical problem. The field equations of the considered boundary value problem on Ω are given by (1) and (2). Constitutive equations are then necessary but need not be specified yet. In [6], we considered two types of boundary conditions. For the BVP $\mathcal{P}$, Dirichlet boundary conditions have been proposed that read

$$\forall \underline{\mathbf{x}} \in \partial\Omega \qquad \underline{\mathbf{u}} = \underset{\sim}{\mathbf{E}}\underline{\mathbf{x}} \qquad \underline{\mathbf{\Phi}} = \underset{\sim}{\mathbf{K}}\underline{\mathbf{x}} \tag{3}$$

where tensors $\underset{\sim}{\mathbf{E}}$ and $\underset{\sim}{\mathbf{K}}$ are given and constant.

If the material has a periodic microstructure, the geometry of the representative volume element is then completely determined. A unit cell Ω can be defined like in the classical periodic homogenization theory [5]. The BVP $\mathcal{P}^{\text{per}}$ consists in searching the displacement and microrotation fields satisfying the field equations (1) and (2) and having the following form on one unit cell Ω

$$\underline{\mathbf{u}}(\underline{\mathbf{x}}) = \underset{\sim}{\mathbf{E}}\underline{\mathbf{x}} + \underline{\mathbf{v}}(\underline{\mathbf{x}}) \qquad \underline{\mathbf{\Phi}}(\underline{\mathbf{x}}) = \underset{\sim}{\mathbf{K}}\underline{\mathbf{x}} + \underline{\psi}(\underline{\mathbf{x}}) \tag{4}$$

where $\underset{\sim}{\mathbf{E}}$ and $\underset{\sim}{\mathbf{K}}$ are given and constant. The origin of the coordinate system can be taken as the geometric gravity centre of the considered cell (see section 3.3). The vector fields $\underline{\mathbf{v}}$ and $\underline{\psi}$ are assumed to take equal values on opposing sides of $\partial\Omega$. Furthermore, we require the traction and moment vectors to be antiperiodic, which means that they are opposite on opposing sides of $\partial\Omega$ (where the external normal vectors $\underline{\mathbf{n}}$ are opposite).

This problem is defined on a *single* unit cell Ω and if a neighbouring cell is considered, conditions (4) must be applied using the centre of the new cell as the origin of the coordinate system. At the common boundary, deformation, curvature, force and couple stresses may undergo some jumps, so that the solution exhibited on a single cell cannot, in general, be extended to the whole body. The constitutive equations being left unspecified, the existence of a solution to the considered boundary value problem will be assumed. However, we shall prove its uniqueness up to a rigid body motion in the case of elasticity. Let $(\underline{\mathbf{u}}^1, \underline{\mathbf{\Phi}}^1)$ and $(\underline{\mathbf{u}}^2, \underline{\mathbf{\Phi}}^2)$ be two solutions of the considered periodic boundary value problem. Then, it can be shown that

$$\begin{aligned}\int_\Omega ((\underset{\sim}{\boldsymbol{\sigma}}^1 - \underset{\sim}{\boldsymbol{\sigma}}^2) : (\underset{\sim}{\mathbf{e}}^1 - \underset{\sim}{\mathbf{e}}^2) + (\underset{\sim}{\boldsymbol{\mu}}^1 - \underset{\sim}{\boldsymbol{\mu}}^2) : (\underset{\sim}{\boldsymbol{\kappa}}^1 - \underset{\sim}{\boldsymbol{\kappa}}^2))\,\mathrm{d}\Omega \\ = \int_{\partial\Omega} (\sigma_{ij}^1 - \sigma_{ij}^2)(v_i^1 - v_i^2)n_j\,\mathrm{d}\Omega + \int_{\partial\Omega} (\mu_{ij}^1 - \mu_{ij}^2)(\psi_i^1 - \psi_i^2)n_j\,\mathrm{d}\Omega = 0\end{aligned} \tag{5}$$

using the facts that the fields $\underset{\sim}{\boldsymbol{\sigma}}^1$ and $\underset{\sim}{\boldsymbol{\sigma}}^2$ both fulfil the equilibrium equations, and that $\underset{\sim}{\boldsymbol{\sigma}}^i\underline{\mathbf{n}}$ and $\underset{\sim}{\boldsymbol{\mu}}^i\underline{\mathbf{n}}$ (respectively, $\underline{\mathbf{v}}^i$ and $\underline{\psi}^i$) are antiperiodic (respectively, periodic). In the case of linear elasticity, the local constitutive equations are taken to be of the form

$$\underset{\sim}{\boldsymbol{\sigma}} = \underset{\approx}{\mathbf{D}}\underset{\sim}{\mathbf{e}} \qquad \underset{\sim}{\boldsymbol{\mu}} = \underset{\approx}{\mathbf{C}}\underset{\sim}{\boldsymbol{\kappa}} \tag{6}$$

where $\underset{\approx}{\mathbf{D}}$ and $\underset{\approx}{\mathbf{C}}$ are the four-rank Cosserat elasticity tensors. They are such that $D_{ijkl} = D_{klij}$, $C_{ijkl} = C_{klij}$. The expression (5) is then equal to

$$\int_\Omega ((\underset{\sim}{\mathbf{e}}^1 - \underset{\sim}{\mathbf{e}}^2) : \underset{\approx}{\mathbf{D}} : (\underset{\sim}{\mathbf{e}}^1 - \underset{\sim}{\mathbf{e}}^2) + (\underset{\sim}{\boldsymbol{\kappa}}^1 - \underset{\sim}{\boldsymbol{\kappa}}^2) : \underset{\approx}{\mathbf{C}} : (\underset{\sim}{\boldsymbol{\kappa}}^1 - \underset{\sim}{\boldsymbol{\kappa}}^2))\,\mathrm{d}\Omega \tag{7}$$

where both elasticity tensors are definite positive, it follows from (5) and (7) that $\underset{\sim}{\mathbf{e}}^1 = \underset{\sim}{\mathbf{e}}^2$ and $\underset{\sim}{\boldsymbol{\kappa}}^1 = \underset{\sim}{\boldsymbol{\kappa}}^2$. This implies $\exists \underline{\mathbf{\Phi}}^0, \underline{\mathbf{u}}^0$ such that $\underline{\mathbf{\Phi}}^2 = \underline{\mathbf{\Phi}}^1 + \underline{\mathbf{\Phi}}^0$ and $\underline{\mathbf{u}}^2 = \underline{\mathbf{u}}^1 - (\underset{\sim}{\boldsymbol{\epsilon}\mathbf{\Phi}^0})\underline{\mathbf{x}} + \underline{\mathbf{u}}^0$. As a result, the solution of $\mathcal{P}^{per}$ is unique up to a rigid body motion and to a microrotation which is equal to the rotation of the rigid body motion. We note that in the classical case the solution is unique up to a translation. In the finite-element analysis of this problem presented in section 4, we will therefore fix the displacement and the microrotation of one node.

In the case of linear elasticity, both $\mathcal{P}$ and $\mathcal{P}^{\rm per}$ admit a solution like in the classical case, as a consequence of the Lax–Milgram theorem.

For the two problems $\mathcal{P}$ and $\mathcal{P}^{\rm per}$, the following average relations are derived using the Gauss theorem

$$\langle \underline{\mathbf{u}} \otimes \underline{\nabla} \rangle = \frac{1}{|\Omega|} \int_\Omega \underline{\mathbf{u}} \otimes \underline{\nabla}\, \mathrm{d}\Omega = \underset{\sim}{\mathbf{E}} \qquad \langle \underset{\sim}{\kappa} \rangle = \underset{\sim}{\mathbf{K}} \tag{8}$$

$$\langle \underset{\sim}{\sigma} : \underset{\sim}{\mathbf{e}} + \underset{\sim}{\mu} : \underset{\sim}{\kappa} \rangle = \langle \underset{\sim}{\sigma} \rangle : \underset{\sim}{\mathbf{E}} + \langle \underset{\sim}{\mu} + (\underline{\underline{\epsilon}}\underset{\sim}{\sigma}) \otimes \underline{\mathbf{x}} \rangle : \underset{\sim}{\mathbf{K}}. \tag{9}$$

As a result, if $\underset{\sim}{\mathbf{E}}$ and $\underset{\sim}{\mathbf{K}}$ are taken as the macroscopic deformation and curvature, the right-hand term of (9) can be interpreted as the expression of the internal work of an effective medium considered as a Cosserat continuum. This leads to the definition of the overall force and couple stress tensors

$$\underset{\sim}{\Sigma} = \langle \underset{\sim}{\sigma} \rangle \qquad \underset{\sim}{\mathbf{M}} = \langle \underset{\sim}{\mu} + (\underline{\underline{\epsilon}}\underset{\sim}{\sigma}) \otimes \underline{\mathbf{x}} \rangle. \tag{10}$$

At this point, a generalized version of Hill–Mandel's condition can be formulated [6]. We let $(\underset{\sim}{\sigma}^\star, \underset{\sim}{\mu}^\star)$ be the self-equilibrated force and couple stress fields on Ω, which means that they fulfil equations (2). Letting $(\underset{\sim}{\mathbf{e}}', \underset{\sim}{\kappa}')$ be two compatible deformation and curvature fields $((\underline{\mathbf{u}}', \underline{\Phi}')$ are the associated displacement and microrotation fields). We note that $(\underset{\sim}{\sigma}^\star, \underset{\sim}{\mu}^\star)$ and $(\underset{\sim}{\mathbf{e}}', \underset{\sim}{\kappa}')$ are not necessarily related to each other by the constitutive relations. Then if $(\underset{\sim}{\mathbf{e}}', \underset{\sim}{\kappa}')$ satisfy the boundary conditions (3) or (4), the following relation holds

$$\langle \underset{\sim}{\sigma}^\star : \underset{\sim}{\mathbf{e}}' + \underset{\sim}{\mu}^\star : \underset{\sim}{\kappa}' \rangle = \langle \underset{\sim}{\sigma}^\star \rangle : \langle \underline{\mathbf{u}}' \otimes \underline{\nabla} \rangle + \langle \underset{\sim}{\mu}^\star + (\underline{\underline{\epsilon}}\underset{\sim}{\sigma}^\star) \otimes \underline{\mathbf{x}} \rangle : \langle \underset{\sim}{\kappa}' \rangle. \tag{11}$$

A wide use of this lemma will be made in the next section.

3. Application to heterogeneous linear Cosserat elasticity

3.1. Direct definition of the overall moduli

In the case of linear elasticity and for each one of the two BVP $\mathcal{P}$ and $\mathcal{P}^{\rm per}$ considered earlier, there exist four concentration tensors such that $\forall \underline{\mathbf{x}} \in \Omega$:

$$\underset{\sim}{\mathbf{e}}(\underline{\mathbf{x}}) = \underset{\approx}{\mathbf{A}}^1(\underline{\mathbf{x}})\underset{\sim}{\mathbf{E}} + \underset{\approx}{\mathbf{A}}^2(\underline{\mathbf{x}})\underset{\sim}{\mathbf{K}} \qquad \underset{\sim}{\kappa}(\underline{\mathbf{x}}) = \underset{\approx}{\mathbf{B}}^1(\underline{\mathbf{x}})\underset{\sim}{\mathbf{E}} + \underset{\approx}{\mathbf{B}}^2(\underline{\mathbf{x}})\underset{\sim}{\mathbf{K}}. \tag{12}$$

There exist also two concentration tensors such that: $\underset{\sim}{\underline{\underline{\epsilon}}\underline{\Phi}}(\underline{\mathbf{x}}) = \underset{\approx}{\mathbf{R}}^1(\underline{\mathbf{x}})\underset{\sim}{\mathbf{E}} + \underset{\approx}{\mathbf{R}}^2(\underline{\mathbf{x}})\underset{\sim}{\mathbf{K}}$. Knowledge of these six concentration tensors assumes that the considered BVP has been solved, which may be very difficult and depends on the special geometry and elastic properties of Ω. As a result we will work on only some properties of these tensors. Note that they generally have no special symmetry. The results (8) and (10), imply

$$\langle \underset{\approx}{\mathbf{A}}^1 - \underset{\approx}{\mathbf{R}}^1 \rangle = \underset{\approx}{\mathbf{1}} \qquad \langle \underset{\approx}{\mathbf{A}}^2 - \underset{\approx}{\mathbf{R}}^2 \rangle = 0 \qquad \langle \underset{\approx}{\mathbf{B}}^1 \rangle = 0 \qquad \langle \underset{\approx}{\mathbf{B}}^2 \rangle = \underset{\approx}{\mathbf{1}}. \tag{13}$$

Taking the average of elasticity relations (6) and considering the expression of the overall deformation, curvature, force and couple stress tensors, we get the overall elasticity relations

$$\underset{\sim}{\Sigma} = \langle \underset{\approx}{\mathbf{D}}\underset{\approx}{\mathbf{A}}^1 \rangle \underset{\sim}{\mathbf{E}} + \langle \underset{\approx}{\mathbf{D}}\underset{\approx}{\mathbf{A}}^2 \rangle \underset{\sim}{\mathbf{K}} \tag{14}$$

$$\underset{\sim}{\mathbf{M}} = \langle \underset{\approx}{\mathbf{C}}\underset{\approx}{\mathbf{B}}^1 + (\underline{\underline{\epsilon}}(\underset{\approx}{\mathbf{D}}\underset{\approx}{\mathbf{A}}^1)) \otimes \underline{\mathbf{x}} \rangle \underset{\sim}{\mathbf{E}} + \langle \underset{\approx}{\mathbf{C}}\underset{\approx}{\mathbf{B}}^2 + (\underline{\underline{\epsilon}}(\underset{\approx}{\mathbf{D}}\underset{\approx}{\mathbf{A}}^2)) \otimes \underline{\mathbf{x}} \rangle \underset{\sim}{\mathbf{K}}. \tag{15}$$

This defines the overall elastic moduli, according to the general expression of Cosserat elasticity described in [8]. The short notation in the last equation may be somewhat confusing so that we give the associated index notation

$$((\underline{\underline{\epsilon}}(\underset{\approx}{\mathbf{D}}\underset{\approx}{\mathbf{A}}^1) \otimes \underline{\mathbf{x}})\underset{\sim}{\mathbf{E}})_{ij} = \epsilon_{ikl} D_{klmn} A^1_{mnpq} x_j E_{pq}. \tag{16}$$

3.2. Energy-based definition of the overall moduli

An energy-based definition of the overall moduli is also proposed. The average free energy w reads

$$
\begin{aligned}
2w &= \langle \underset{\sim}{\boldsymbol{\sigma}} : \underset{\sim}{\mathbf{e}} + \underset{\sim}{\boldsymbol{\mu}} : \underset{\sim}{\boldsymbol{\kappa}} \rangle = \langle \underset{\sim}{\mathbf{e}} : \underset{\approx}{\mathbf{D}} : \underset{\sim}{\mathbf{e}} + \underset{\sim}{\boldsymbol{\kappa}} : \underset{\approx}{\mathbf{C}} : \underset{\sim}{\boldsymbol{\kappa}} \rangle \\
&= \underset{\sim}{\mathbf{E}} : \langle \underset{\approx}{\mathbf{A}}^{1\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{1} + \underset{\approx}{\mathbf{B}}^{1\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{1} \rangle : \underset{\sim}{\mathbf{E}} + \underset{\sim}{\mathbf{K}} : \langle \underset{\approx}{\mathbf{A}}^{2\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{2} + \underset{\approx}{\mathbf{B}}^{2\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{2} \rangle : \underset{\sim}{\mathbf{K}} \\
&\quad + \underset{\sim}{\mathbf{E}} : \langle \underset{\approx}{\mathbf{A}}^{1\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{2} + \underset{\approx}{\mathbf{B}}^{1\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{2} \rangle : \underset{\sim}{\mathbf{K}} + \underset{\sim}{\mathbf{K}} : \langle \underset{\approx}{\mathbf{A}}^{2\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{1} + \underset{\approx}{\mathbf{B}}^{2\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{1} \rangle : \underset{\sim}{\mathbf{E}}.
\end{aligned}
\tag{17}
$$

This provides the definition of three overall elastic tensors. The symmetry of the first two elasticity tensors clearly appears in these expressions, which was not the case in the last section. A reduced form can now be obtained by application of Hill–Mandel's lemma.

For this purpose, we look for compatible deformation and curvature fields satisfying the Dirichlet boundary conditions (3) or the periodic ones (4). A set of such fields can be obtained by applying the particular overall deformation and curvature

$$
(E_{ij}^{(mn)} = \delta_{im}\delta_{jn},\, K_{ij} = 0) \qquad (E_{ij} = 0,\, K_{ij}^{(mn)} = \delta_{im}\delta_{jn}) \tag{18}
$$

successively, for each given fixed pair (m, n). According to equations (12), we obtain the compatible deformation-curvature fields

$$
(e_{ij}^{\prime 1(mn)} = A_{ijmn}^{1},\, \kappa_{ij}^{\prime 1(mn)} = B_{ijmn}^{1}) \qquad (e_{ij}^{\prime 2(mn)} = A_{ijmn}^{2},\, \kappa_{ij}^{\prime 2(mn)} = B_{ijmn}^{2}). \tag{19}
$$

This means that the concentration tensors of equations (12) enable us to construct admissible deformation and curvature fields. Similarly, self-equilibrated force and couple stress fields can be worked out using the previous fields $(\underset{\sim}{\mathbf{e}}^{\prime 1(mn)}/\underset{\sim}{\boldsymbol{\kappa}}^{\prime 1(mn)})$ and $(\underset{\sim}{\mathbf{e}}^{\prime 2(mn)}/\underset{\sim}{\boldsymbol{\kappa}}^{\prime 2(mn)})$. For each given pair (m, n)

$$
\begin{aligned}
&(\sigma_{ij}^{\star 1(mn)} = D_{ijkl} A_{klmn}^{1},\, \mu_{ij}^{\star 1(mn)} = C_{ijkl} B_{klmn}^{1}) \\
&(\sigma_{ij}^{\star 2(mn)} = D_{ijkl} A_{klmn}^{2},\, \mu_{ij}^{\star 2(mn)} = C_{ijkl} B_{klmn}^{2})
\end{aligned}
\tag{20}
$$

are self-equilibrated force and couple stress fields. Hill–Mandel's lemma (11) can then be applied to any combination of admissible deformation-curvature fields and self-equilibrated force and couple stress tensors.

The application of Hill–Mandel's lemma (11) to $(\underset{\sim}{\mathbf{e}}^{\prime 1(mn)}, \underset{\sim}{\boldsymbol{\kappa}}^{\prime 1(mn)})/(\underset{\sim}{\boldsymbol{\sigma}}^{\star 1(pq)}, \underset{\sim}{\boldsymbol{\mu}}^{\star 1(pq)})$ and the use of relations (13) lead to

$$
\begin{aligned}
\langle \underset{\approx}{\mathbf{A}}^{1\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{1} + \underset{\approx}{\mathbf{B}}^{1\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{1} \rangle_{mnpq} &= \langle \underset{\sim}{\mathbf{e}}^{\prime 1(mn)} : \underset{\sim}{\boldsymbol{\sigma}}^{\star 1(pq)} + \underset{\sim}{\boldsymbol{\kappa}}^{\prime 1(mn)} : \underset{\sim}{\boldsymbol{\mu}}^{\star 1(pq)} \rangle \\
&= \langle \underline{\mathbf{u}}^{\prime 1(mn)} \otimes \underline{\boldsymbol{\nabla}} \rangle : \langle \underset{\sim}{\boldsymbol{\sigma}}^{\star 1(pq)} \rangle + \langle \underset{\sim}{\boldsymbol{\kappa}}^{\prime 1(mn)} \rangle : \langle \underset{\sim}{\boldsymbol{\mu}}^{\star 1(pq)} + (\underline{\underset{\sim}{\boldsymbol{\epsilon}}} \underset{\sim}{\boldsymbol{\sigma}}^{\star 1(pq)}) \otimes \underline{\mathbf{x}} \rangle \\
&= \langle A_{ijmn}^{1} - R_{ijmn}^{1} \rangle : \langle D_{ijkl} A_{klpq}^{1} \rangle + \langle B_{ijmn}^{1} \rangle : \langle C_{ijkl} B_{klpq}^{1} + \epsilon_{irs} D_{rsuv} A_{uvpq}^{1} x_j \rangle
\end{aligned}
\tag{21}
$$

hence $\langle \underset{\approx}{\mathbf{A}}^{1\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{1} + \underset{\approx}{\mathbf{B}}^{1\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{1} \rangle = \langle \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{1} \rangle$.

Similarly, the application of Hill–Mandel's lemma (11) to $(\underset{\sim}{\mathbf{e}}^{\prime 2(mn)}, \underset{\sim}{\boldsymbol{\kappa}}^{\prime 2(mn)})/(\underset{\sim}{\boldsymbol{\sigma}}^{\star 2(pq)}, \underset{\sim}{\boldsymbol{\mu}}^{\star 2(pq)})$ and the use of relations (13) lead to

$$
\begin{aligned}
\langle \underset{\approx}{\mathbf{A}}^{2\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{2} + \underset{\approx}{\mathbf{B}}^{2\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{2} \rangle &= \langle \underset{\approx}{\mathbf{A}}^{2} - \underset{\approx}{\mathbf{R}}^{2} \rangle : \langle \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{2} \rangle + \langle \underset{\approx}{\mathbf{B}}^{2} \rangle : \langle \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{2} + (\underline{\underset{\sim}{\boldsymbol{\epsilon}}} (\underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{2})) \otimes \underline{\mathbf{x}} \rangle \\
&= \langle \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{2} + (\underline{\underset{\sim}{\boldsymbol{\epsilon}}} (\underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{2})) \otimes \underline{\mathbf{x}} \rangle.
\end{aligned}
\tag{22}
$$

The successive application of Hill–Mandel's lemma to $(\underset{\sim}{\mathbf{e}}^{\prime 1(mn)}, \underset{\sim}{\boldsymbol{\kappa}}^{\prime 1(mn)})/(\underset{\sim}{\boldsymbol{\sigma}}^{\star 2(pq)}, \underset{\sim}{\boldsymbol{\mu}}^{\star 2(pq)})$ and $(\underset{\sim}{\mathbf{e}}^{\prime 2(mn)}, \underset{\sim}{\boldsymbol{\kappa}}^{\prime 2(mn)})/(\underset{\sim}{\boldsymbol{\sigma}}^{\star 1(pq)}, \underset{\sim}{\boldsymbol{\mu}}^{\star 1(pq)})$ and the use of relations (13) leads to

$$
\langle \underset{\approx}{\mathbf{A}}^{1\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{2} + \underset{\approx}{\mathbf{B}}^{1\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^{2} \rangle = \langle \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^{2} \rangle \tag{23}
$$

and

$$\langle \underset{\approx}{\mathbf{A}}^{2\mathrm{T}} \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^1 + \underset{\approx}{\mathbf{B}}^{2\mathrm{T}} \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^1 \rangle = \langle \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^1 + (\underline{\boldsymbol{\epsilon}}(\underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^1)) \otimes \underline{\mathbf{x}} \rangle. \tag{24}$$

Since the local elasticity tensors are symmetric, we get the non-trivial equality, which could not be proved in the last section

$$\langle \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^2 \rangle = \langle \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^1 + (\underline{\boldsymbol{\epsilon}}(\underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^1)) \otimes \underline{\mathbf{x}} \rangle^{\mathrm{T}}. \tag{25}$$

The previous relations prove that the direct definition of the overall elastic moduli (section 3.1) and the energy-based definition are equivalent.

3.3. Microstructures with point symmetry

The RVE is said to have point symmetry if $\underset{\approx}{\mathbf{D}}(-\underline{\mathbf{x}}) = \underset{\approx}{\mathbf{D}}(\underline{\mathbf{x}})$ and $\underset{\approx}{\mathbf{C}}(-\underline{\mathbf{x}}) = \underset{\approx}{\mathbf{C}}(\underline{\mathbf{x}})$, $\forall \underline{\mathbf{x}} \in \Omega$. We consider now the BVPs $\mathcal{P}$ and $\mathcal{P}^{\mathrm{per}}$ with $\underset{\sim}{\mathbf{E}} = 0$ and prescribed $\underset{\sim}{\mathbf{K}}$. The solution of the problem then fulfils the conditions

$$\underline{\mathbf{v}}(-\underline{\mathbf{x}}) = \underline{\mathbf{v}}(\underline{\mathbf{x}}) \qquad \underline{\psi}(-\underline{\mathbf{x}}) = -\underline{\psi}(\underline{\mathbf{x}}) \qquad \underset{\sim}{\mathbf{e}}(-\underline{\mathbf{x}}) = -\underset{\sim}{\mathbf{e}}(\underline{\mathbf{x}}) \qquad \underset{\sim}{\boldsymbol{\kappa}}(-\underline{\mathbf{x}}) = \underset{\sim}{\boldsymbol{\kappa}}(\underline{\mathbf{x}})$$

from which we deduce $\underset{\approx}{\mathbf{A}}^2(-\underline{\mathbf{x}}) = -\underset{\approx}{\mathbf{A}}^2(\underline{\mathbf{x}})$ and $\langle \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^2 \rangle = 0$. As a result the overall constitutive equations are

$$\underset{\sim}{\boldsymbol{\Sigma}} = \langle \underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^1 \rangle \underset{\sim}{\mathbf{E}} \qquad \underset{\sim}{\mathbf{M}} = \langle \underset{\approx}{\mathbf{C}} \underset{\approx}{\mathbf{B}}^2 + (\underline{\boldsymbol{\epsilon}}(\underset{\approx}{\mathbf{D}} \underset{\approx}{\mathbf{A}}^2)) \otimes \underline{\mathbf{x}} \rangle \underset{\sim}{\mathbf{K}} \tag{26}$$

that define the effective elasticity tensors $\underset{\approx}{\mathbf{D}}^h$ and $\underset{\approx}{\mathbf{C}}^h$. These results hold only if the geometric centre of gravity $\underline{\mathbf{x}}_{\mathrm{G}}$ used to formulate the boundary conditions (4) is a centre of symmetry of Ω. If not, a coupling may appear between force and couple stresses as in (14) and (15). This is similar to the coupling terms that arise in the theory of composite beams for a general choice of the neutral fibre. An analogous problem in the case of second gradient models has been treated in [9].

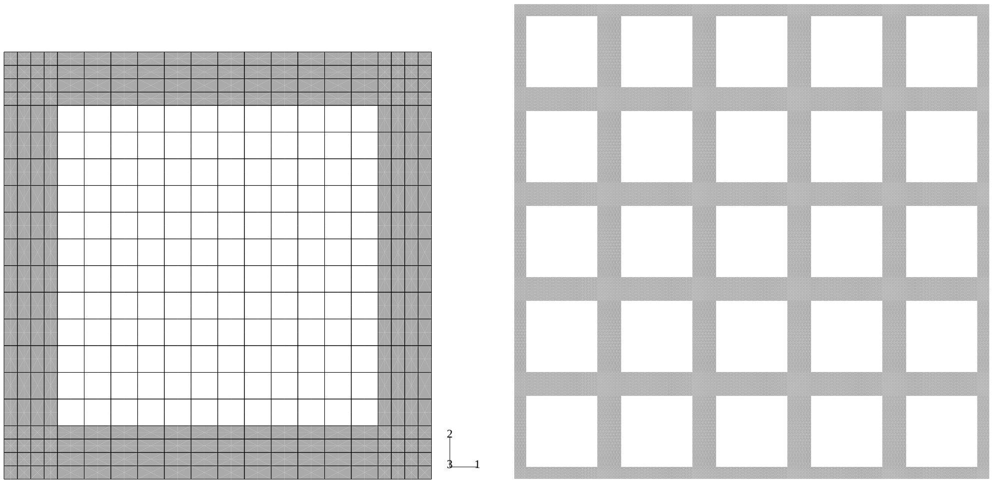
4. Assessing the quality of the proposed estimation

We propose to determine numerically the effective properties of a heterogeneous linear elastic Cosserat material in two dimensions (plane strain) according to (26). To quantify the pertinence of these overall properties, we consider structural calculations. In each case an expensive reference calculation is carried out for which every heterogeneity is taken into account. Then, we investigate whether the homogeneous medium with the derived overall properties is able to give a precise account of the deformation of the structure. The calculations have been performed with the object-oriented finite-element code ZéBuLoN [10]. The Dirichlet boundary conditions (3) and the periodic boundary conditions (4) have been implemented. The elements used are quadratic two-dimensional plane strain Cosserat elements with full integration. A numerical treatment of the unconstrained Cosserat medium has already been proposed in [11].

4.1. Effective properties of a two-phase periodic material

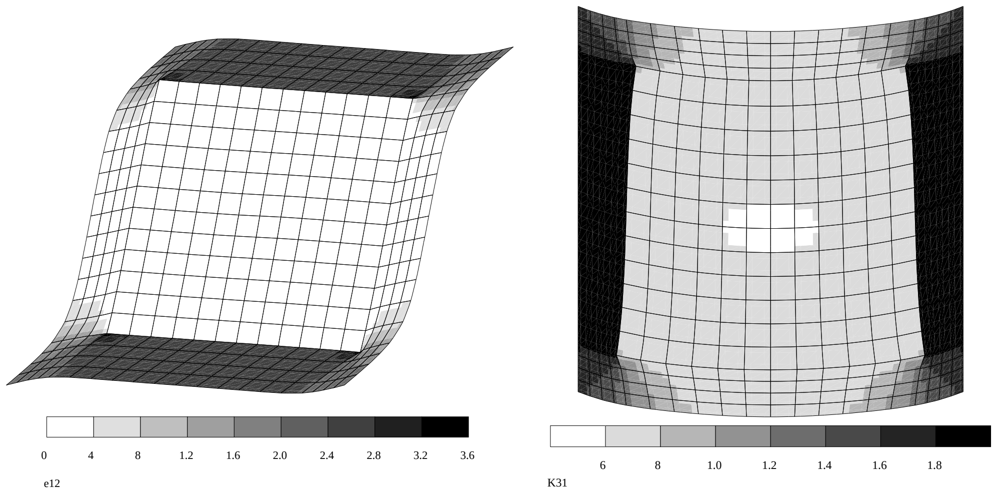
We now consider a plane cubic assemblage of cubic heterogeneities. The RVE is chosen as a single square in its matrix (figure 1(a)). The cell is a square of size 1 mm. The volume fraction of inclusions is $f = 60\%$. The elastic properties of the constituents are isotropic and the constitutive equations read

$$\underset{\sim}{\boldsymbol{\sigma}} = \lambda \underset{\sim}{\mathbf{1}} \,\mathrm{Tr}\, \underset{\sim}{\mathbf{e}} + 2\mu \,\{\underset{\sim}{\mathbf{e}}\} + 2\mu_c \,\}\underset{\sim}{\mathbf{e}}\{ \qquad \underset{\sim}{\boldsymbol{\mu}} = \alpha \underset{\sim}{\mathbf{1}} \,\mathrm{Tr}\, \underset{\sim}{\boldsymbol{\kappa}} + 2\beta \,\{\underset{\sim}{\boldsymbol{\kappa}}\} + 2\gamma \,\}\underset{\sim}{\boldsymbol{\kappa}}\{ \tag{27}$$



(*a*) (*b*)

Figure 1. Unit cell (*a*) and structure with 25 heterogenities (*b*).



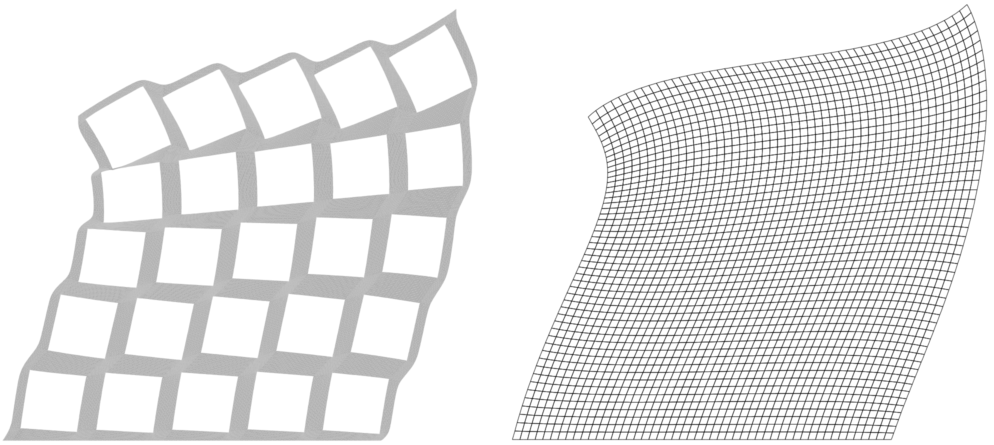
(*a*) (*b*)

Figure 2. Prescribed deformation E_{12} (*a*) and curvature K_{31} (*b*) on a unit cell.

where six elastic constants are involved. The closed braces denote the symmetric part whereas the open braces denote the skew-symmetric part. In two dimensions, α does not intervene and one usually takes $\beta = \gamma$ [11]. A characteristic length can then be defined: $l_c = \sqrt{\beta/\mu}$. The chosen properties of the heterogeneous material are:

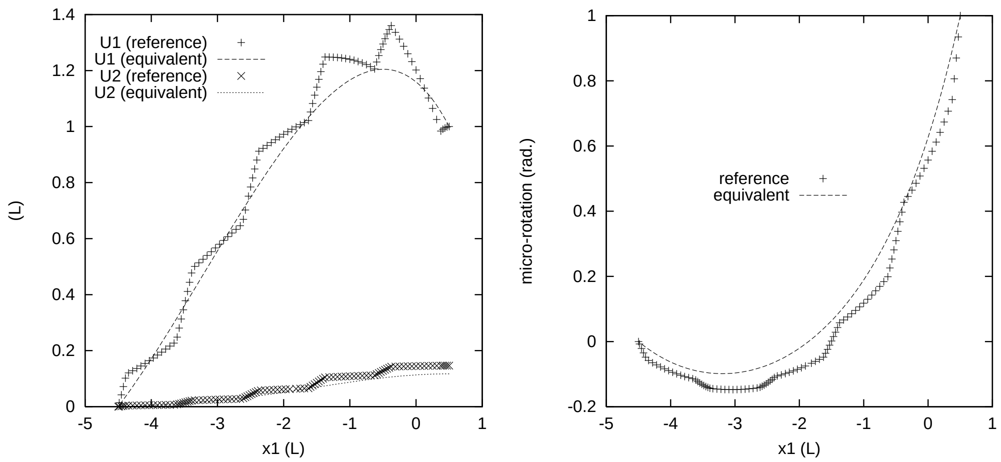
constituent 1 (inclusions): $E = 600\,000$ MPa; $\nu = 0.4$; $\mu_c = 200\,000$ MPa; $l_c = 0.6$ mm;
constituent 2 (matrix): $E = 40\,000$ MPa; $\nu = 0.3$; $\mu_c = 10\,000$ MPa; $l_c = 1.2$ mm.

The resulting properties have plane cubic symmetry. These overall constants are determined by considering successively three individual problems: prescribed $E_{11} = 1$, $E_{12} = 1$ and $K_{31} = 1$. The deformed states of the cell for the two last conditions are given on figures 2(a) and (b)



(*a*) (*b*)

Figure 3. Deformed states of an actual heterogeneous structure (*a*) and of the corresponding homogeneous structure (*b*).



(*a*) (*b*)

Figure 4. Displacements (*a*) and microrotation along a vertical line crossing the inclusions of the fourth row starting from the bottom (*b*).

(see also [6]). The effective properties found are, respectively,

$$D^h_{1111} = 159\,930 \text{ MPa} \qquad D^h_{1122} = 44\,640 \text{ MPa} \qquad D^h_{1212} = 64\,780 \text{ MPa}$$
$$D^h_{1221} = 19\,950 \text{ MPa} \qquad C^h_{3131} = 88\,810 \text{ MPa mm}^2.$$

In a definition similar to that of l_c, an effective length scale can be written as

$$l^h_c = \sqrt{\frac{C^h_{3131}}{2\mu^h_{12}}} \qquad \mu^h_{12} = (D^h_{1212} + D^h_{1221})/2. \tag{28}$$

This effective length is found to be 1.05 mm.

We note that in the case of prescribed curvature, the actual deformed state of the heterogeneous material should not be reconstructed by tessellating the plane with the deformed

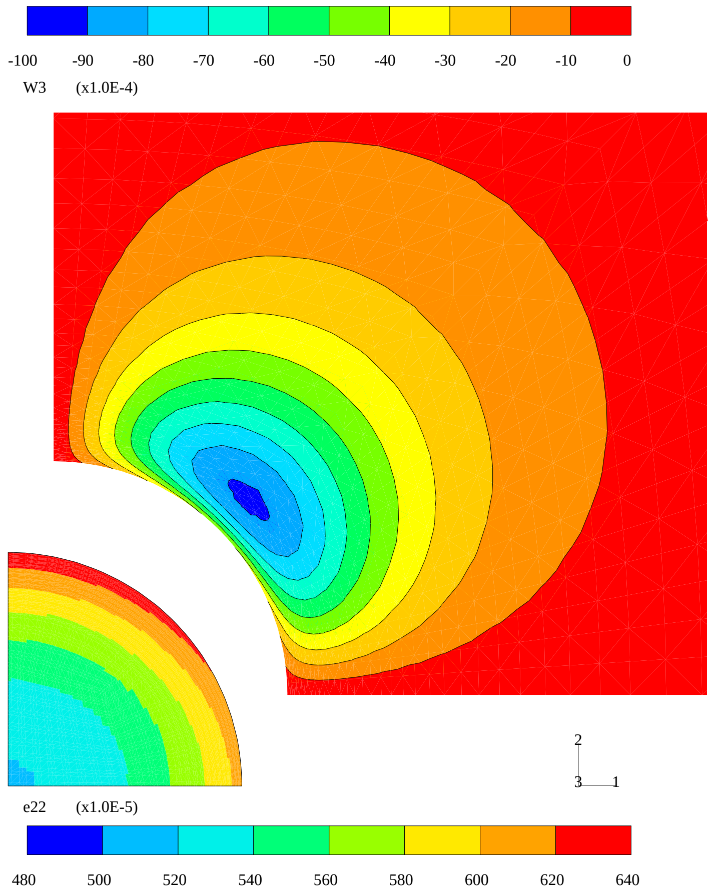


Figure 5. The inhomogeneous Cosserat inclusion problem; the deformation e_{22} is heterogenous inside the inclusion; for the illustration, the matrix has been separated from the inclusion; the microrotation field Φ_3 is given in the matrix; only a part of the matrix surrounding the inclusion is shown.

unit cell although curvature and couple stresses would be continuous at the boundary. Rather, the deformed unit cell of figure 2(b) should be regarded as an approximate representation of an excerpt, i.e. the corresponding cell extracted from the actual material.

4.2. Application to structural calculations

We consider a rectangular structure made of 5×5 cells (figure 1(b)) and perform the following test: at the bottom, displacement and microrotations are fixed to zero, at the top, a displacement of magnitude 1 mm in direction one and a microrotation of magnitude one (rad) are prescribed. The computation is performed using first, a fine mesh taking every inclusion into account and with the actual properties of the constituents, and second, with a coarser mesh endowed with the previously determined homogeneous properties. The two deformed states are compared in figure 3. A quantitative comparison is given in figure 4. The displacements and microrotations are plotted along a vertical line crossing the cubes (fourth row). The response of the estimated homogeneous equivalent medium appears to be in good agreement with the actual one. The microrotations, however, are predicted with less accuracy than the

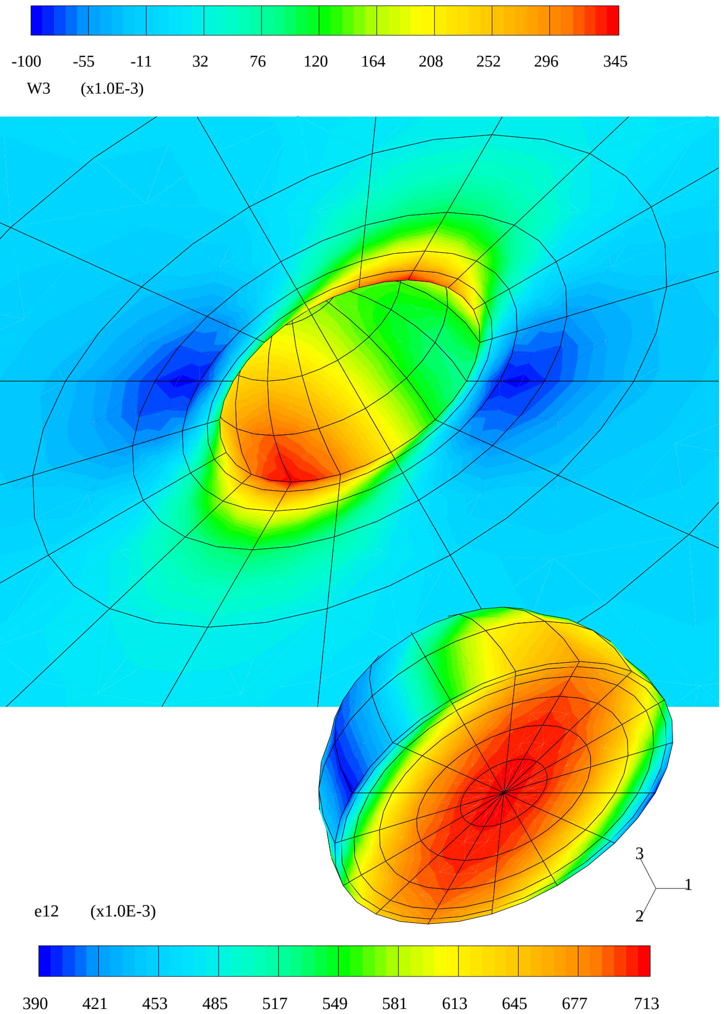


Figure 6. The Eshelby problem for a Cosserat material; three-dimensional case: an eigenstrain e_{12} has been prescribed to the inclusion; for the illustration, it has been extracted from its surrounding matrix; microrotations are given in the matrix and deformation e_{12} in the inclusion.

displacements. Improvements may be achieved using the asymptotic methods proposed in [12].

Boundary effects may play a significant role in the deformation of structures made up of a rather small number of cells as in figure 1(b). Corrections to the classical periodic homogenization procedure exist to take boundary effects into account. This has not been undertaken yet in the case of heterogeneous Cosserat materials.

5. Towards a self-consistent scheme

In the case of polycrystals, the proposed model must be able to account for the influence of grain size on the overall behaviour. This is possible since each grain is made of a Cosserat crystal and has an intrinsic length [3]. In the meantime, it should also be able to account for shear banding in polycrystals, and to provide a finite shear band width (usually a small number of grains). This explains why we have dropped the hypothesis of slowly varying mean fields $d \ll L_\omega$.

With a view to polycrystal modelling, the question can be raised as to whether there exists an extension of the self-consistent scheme [13] to the case of heterogeneous Cosserat materials. In this case, the Dirichlet boundary conditions (3) can be used. The first step consists in solving a generalized Eshelby problem and the problem of an elastic Cosserat heterogeneity in a Cosserat matrix.

5.1. On the problem of the Cosserat elastic heterogeneity

An explicit expression of the mean strain and curvature in a Cosserat spherical inclusion embedded in a matrix made of the same material, and having an eigenstrain $\underset{\sim}{\mathbf{e}}^\star$ and eigencurvature $\underset{\sim}{\kappa}^\star$ can be derived [14]. The same authors propose an estimation of the mean strain and curvature in an inclusion of Cosserat material A embedded in an infinite matrix made of Cosserat material B and submitted to condition (3) at infinity. We have performed a finite-element analysis of these two problems. Two major results must be mentioned here. When the size of the inclusion becomes comparable to the Cosserat characteristic sizes of A and B (supposed to be of the same order), the deformation within the spherical inclusion is no longer homogeneous (figures 5 and 6), contrary to the classical case. On the other hand, we have studied the limiting case for which the material surrounding the Cosserat elastic heterogeneity is made of a classical material: no Cosserat effect arises within the inclusion and the solution is the same as in the classical case for an inclusion endowed with the classical moduli of the Cosserat material.

5.2. Pertinence of a self-consistent scheme

Two questions arise when one thinks of a straightforward extension of the self-consistent scheme to heterogeneous Cosserat media. Each individual problem is that of a Cosserat material embedded in a matrix regarded as an homogeneous equivalent medium. If this matrix is taken as a Cosserat material as suggested by this work, both deformation and curvature must be prescribed at infinity. Since the matrix is infinite, the prescribed curvature will affect only a boundary layer of finite size and not the state of the inclusion. That is why it may be sufficient to consider a classical HSM. However, in the latter case, the final result of the previous section stated that no Cosserat effect will appear in the inclusion! This argues for the use of a finite matrix made of the searched HSM. Such an analysis could be carried out numerically. The finite size of the matrix would, of course, be related to the actual size of the retained representative volume element.

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