A multiscale description of particle composites: from lattice microstructures to micropolar continua

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Abstract

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1. Introduction. A three–levels procedure: basics

The mechanical behavior of complex materials, characterized at finer scales by the presence of heterogeneities of significant size and texture, strongly depends on their micro-structural features. By lacking in material internal scale parameters, the classical continuum does not always seem appropriate to describe the macroscopic behavior of these materials taking into account, besides the disposition, the size and the orientation of the micro heterogeneities.

In the modeling of materials with micro-structure, such as particle composites, the discrete and heterogeneous nature of the material must be taken into account, because interfaces and/or material phases dominate the gross mechanical behavior. We want here to highlight the possibility of preserving memory of the microstructure, and in particular of the presence of material length scales, without resorting to the discrete modeling, that can be often cumbersome. This calls for the need of non–classical and non–local continuum descriptions obtained through multi-scale approaches aimed at deducing properties and relations by

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bridging information at proper underlying sub–levels via energy equivalence criteria, as rather acknowledged in literature [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

In the framework of a multi-scale modeling aiming at deriving homogeneous anisotropic continua suitable for this purpose, in order to avoid physical inadequacies and **theoretical computational problems** cosa si intende?, the non–local character of the description is crucial [14]. In particular, this occours in problems in which a characteristic internal length, l, is comparable to the macroscopic (structural) length, L. Among non-local theories, it is useful to distinguish between 'explicit' or 'strong' and 'implicit' or 'weak' non–locality [15, 16, 17] where implicit non–locality concerns continua with extra degrees of freedom, such as in the above mentioned formulations, with particular reference to the micropolar continua [18, 19, 20] here adopted.

Basing on the proved effectiveness of the micropolar continuum modeling for periodic media over years [1, 7, 12, 13], the micropolar multiscale modeling has been here extended for deriving constitutive models of random media such as ceramic/metal/polymer matrix composites, i.e. polycrystals with interfaces (grain boundaries or thin/thick interfaces), or short fiber-reinforced composites, or even masonry-like materials (roman concrete, rocks) that frequently exhibit random microstructure. For these materials a two-step multi-scale procedure has been developed. At the microscopic level the material is described as a lattice system, at a mesoscopic level as a two-phase micropolar continuum and at the macroscopic level as a homogeneous micropolar continuum (Figure 3). The resulting continuum at the highest level is, thus, dependent on the hierarchy of three characteristic lenghts, namely the typical size L of the structure at the macroscopic scale, the size l of the heterogeneities at the mesoscopic level and the micropolar intrinsic lenghts l_μ at the microscopic scale, as described also in [21].

For the transition from the discrete micro-level to the two-phases **continuum** meso-level (i), a coarse graining procedure based on a generalized Cauchy–Born correspondence maps and energy equivalence has been adopted [7, 10, 13]. For the meso-macro level transition (ii), a statistical homogenization procedure

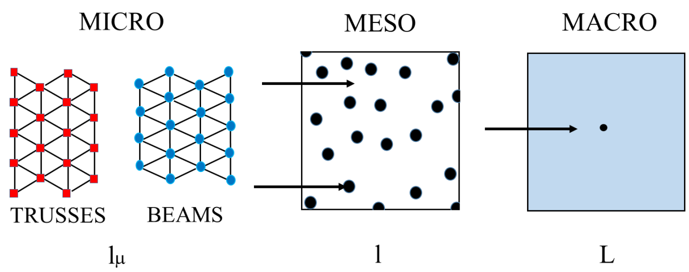

Figure 1: Schematic of the three scales homogenization procedure. Lattice system (micromodel); inhomogeneous continuum (mesomodel); homogenized continuum (macromodel).

has been developed basing on the solution of Boundary Value Problems (BVP), posed on Statistically Representative Elements (SVE) under Boundary Conditions (BC) derived from a generalized macrohomogeneity condition of Hill's type [22]. This procedure provides hierarchies of bonds and aims at estimating the size of the Representative Volume Element (RVE) to adopt for performing homogenization. In this framework, a new criterion of convergence has been introduced and the elastic, classical and micropolar, constitutive moduli have been identified for particular classes of particle composites [23, 24].

As an example of material to which apply such a multiscale approach, let us consider a special case of particulate composite: the cement matrix composites (CMC), comprising micro– or nano–scale metallic particles in a ceramic matrix. In these materials the particles are discrete and they typically provide a toughening increment by plastically deforming and preventing the advance of cracks. Among others, we consider Alumina-Zirconia Ceramic-Matrix Composites of Figure 2, where the SEM images show different assemblies ranging from pure Alumina to pure Zirconia. The Alumina-Zirconia Ceramic-Matrix Composites are very promising as structural materials, combining the properties of the alumina matrix (high hardness and Young's modulus) with additional toughening effects, due to the Zirconia dispersion, see [25]. At the microscopic scale the material exhibits a complex microstructure pertaining both to matrix and inclusions that appear as spatial assemblies of irregular particles seamlessly arranged, as is evident in Figure 3 (a), where a sketch of the micro–structure is shown. A schematic of the meso and micro levels for the aforementioned $Al_2O_3 - ZrO_2$ CMC composite is presented in Figure 3 (b).

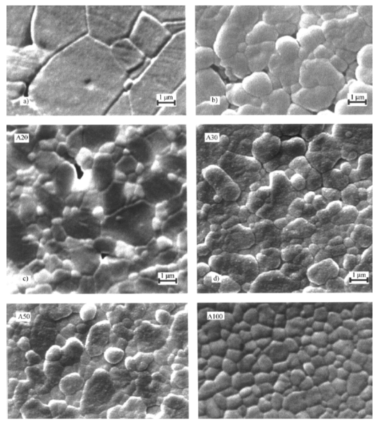

Figure 2: SEM images of different types of Alumina matrix Al_2O_3 and Zirconia ZrO_2 inclusions composites, ranging from pure allumina (first) to pure zirconia (last), [26]

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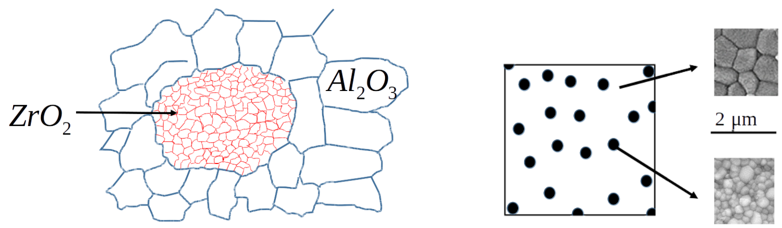
The paper is organized as follows.

- (Section 2, i) We begin with illustrating the discrete–continuum approach adopted to perform the micro/meso transition. Considering the reference material made of particles embedded in a matrix, with different material properties, we assume that each constituent is a material with microstructure that can be described as a lattice system. At this microlevel, due to the high volume fraction of particles (grains) composing each constituent, the microstructure of the two materials is considered deterministic.

  Firstly, focus is on physically–based corpuscular–continuous models, as originated by the molecular models developed in the 19^{th} century to give explanations 'per causas' of elasticity [27, 28]. In particular, the discrete–



(b)

Figure 3: a) Sketch of Alumina-Zirconia Ceramic Matrix Composite. b) MESO and MICRO scales of $Al_2O_3 - ZrO_2$ CMC composite.

continuum deterministic approach, based on a generalization of the so-called Cauchy–Born rule used in crystal elasticity and in classical molecular theory of elasticity [29, 30, 14], is used for deriving a continuum equivalent in terms of energy to lattice models made of interacting particles, that can be perceived as truss–like or a beam–like networks, or even other kind of 'structured' lattice systems, as in [6, 10]. This continuum retains memory of the fine organization of the material by means of additional field descriptors and it is named multifield continuum.

Once defined the lattice system, basing on such a generalized rule and assuming proper response functions for the lattice interactions, the requirement of the preservation of the strain energy in the micro–meso transition, for any admissible deformation field over a REV, allow us to identify the (classical and non-classical) constitutive parameters of the macromodel, in terms of the geometry of the microstructure (shape, size, orientation, texture).

The meso-scale model is then obtained as the result of the above mentioned coarse–graining procedure from the underlying discrete level (microlevel), that in the case of truss–like scheme leads to a classical continuum while in the case of a beam–like scheme leads to a multifield continuum with rigid local structure (micropolar) particularly suitable when microscopic bending deformation mechanisms are predominant, as in the case of polycrystals with stiff particles or fiber-beam networks (fiber reinforced composites, cellular materials, or some kind of ceramic matrix composites Figure 2) [3, 4].

- (Section 3, ii) The second step of the multiscale procedure concerns the transition from a micropolar two–phases continuum to a micropolar homogeneous continum through an average field homogenization procedure. This procedure is based on the solution of BVP, defined at the meso–level, under Dirichlet and Neumann BC derived from a macrohomogeneity condition of Hill's type, here generalized in order to take into account the additional degrees of freedom of the micropolar continuum, namely the relative rotation and curvature [22].

  Due to the generally low-volume fraction at the meso–level the material is perceived as a random aggregate of inclusions embedded in a matrix, either softer or stiffer. As a result of the coarse graining procedure (i), both the inclusions and the matrix are described as isotropic micropolar continua. The macroscopic continuum is also supposed to be micropolar, able to naturally account for scale and skew–symmetric shear effects [31, 7, 13]. In this framework, the adopted generalized macrohomogeneity condition ensures a one–to–one correspondence between the two scales, avoiding the introduction of kind of internal constraints for the deformation mechanisms as occurs in the case of continua of different type [32, 12]. With the aim of investigating the gross mechanical response of this special class of random composites, we adopt a statistically–based multiscale procedure which allow us to detect the size of the RVE, that is unknown in the case of random media [33, 34], and to estimate the constitutive moduli of the energy equivalent homogeneous micropolar continuum [23, 24]. The RVE is obtained by increasing a scale factor representing the ratio between the size of a control window (SVE) and the particle size, until the statistical convergence, defined through an ad hoc conceived criterion, is reached.

- (Section 4) Some results obtained for an ideal material that mimics the internal microstructure of a CMC Composite are presented. The example is representative of different different kind of composites– ranging from metal or ceramic matrix composites up to concrete, masonry-like and geo-materials – highlight the importance of taking into account the spatial randomness of inclusions in identifying the bulk, shear and bending behavior of composites as well as the effectiveness of the micro-polar continuum modeling.

2. Micro/Meso Transition - Coarse Graining

At the first level – the finest one, conventionally defined as micro–level – the reference material is described (see Figure 3) as a lattice system made of rigid particles of hexagonal shape and elastic interfaces (Figure 4).

Since many years it has been shown that in such systems the gross mechanical behavior is strongly influenced by the particle orientation and then if the material has to be treated as a continuum, this continuum **must be** mi pare una osservazione un p troppo forte of the Cosserat type [35**?** , 36, 1]. Here below we adopt the procedure, defined in [1] following the track of [37], and then extended and generalized in [7, 13] for deriving a micropolar continuous model energy equivalent to a lattice system in which particles interact through forces and couples, as in a beam–like network. The micropolar continuum is identified by assuming the maintenance of the power expended in the transition from the micro (discrete) to the meso (continuous) model, for a given a class of regular motions. The constitutive functions for the meso–level continuous materials are then derived in terms of the geometrical and mechanical properties of the rigid particles model. Particular attention is devoted to the evaluation of the characteristic intrinsic lengths $l_{\mu(i)}$ of each micropolar constituent as directly gathered by the underlying microstructure. These parameters, adopted in the constitutive law at the mesoscopic level, are, indeed, difficult to estimate throught experimental tests [38] and the calibration of their values is a very debated issue.

2.1. Lattice system

In this paragraph the methodological aspects of the procedure are developed within the framework of linearized elasticity, where velocity and angular velocity stand for infinitesimal displacement and rotations, respectively. It is worth noting, however, that the procedure can be employed in more general contexts, even if the generalization is not trivial.

Let us assume that each particle, $\mathcal{A}$, is a rigid body. The vector $\mathbf{w}^a$ and the skew-symmetric tensor $\mathbf{W}^a$ ($\mathbf{W}^a = -(\mathbf{W}^a)^T$) respectively denote the velocity of the particle center g^a and the particle angular velocity.

Under the rigid body assumption, for any point belonging to the particle $(\cdot)$, it is:

$$\begin{aligned} \mathbf{w}^a(\cdot) &= \mathbf{w}^a + \mathbf{W}^a((\cdot) - g^a) \\ \mathbf{W}^a(\cdot) &= \mathbf{W}^a \,. \end{aligned} \tag{1}$$

Let $\mathcal{A}$ and $\mathcal{B}$ be two interacting particles and select a pair of points ($p^a \in \mathcal{A}$, $p^b \in \mathcal{B}$) that we call a 'test pair'. As strain measures for the test pair (p^a, p^b) we then assume the following quantities:

$$\begin{aligned} \mathbf{w}_p &= \mathbf{w}^a(p^a) - \mathbf{w}^b(p^b) \\ \mathbf{W}_p &= \mathbf{W}^a - \mathbf{W}^b \,, \end{aligned} \tag{2}$$

that, using Equations (2), can be rewritten as follows:

$$\begin{aligned} \mathbf{w}_p &= \mathbf{w}^a - \mathbf{w}^b + \mathbf{W}^a(p^a - g^a) - \mathbf{W}^a(p^b - g^b) \\ \mathbf{W}_p &= \mathbf{W}^a - \mathbf{W}^b \,. \end{aligned} \tag{3}$$

Furthermore, we assume that the contact interaction between the two particles $\mathcal{A}$ and $\mathcal{B}$ is described by a force and a couple through the test pair (p^a, p^b). The vector $\mathbf{t}^a$ ($\mathbf{t}^b$) and the skewsymmetric tensor $\mathbf{C}^a$ ($\mathbf{C}^b$) respectively represent the force and the couple that $\mathcal{B}$ ($\mathcal{A}$) exerts on $\mathcal{A}$ ($\mathcal{B}$).

Let us consider now a representative part $\mathcal{P}$ of the system made of n particles and of volume V. The power of the internal actions acting on $\mathcal{P}$ can be expressed in the form:

$$\pi = \sum_i (\mathbf{t}^i \cdot \dot{\mathbf{w}}^i + \frac{1}{2}\mathbf{C}^i \cdot \dot{\mathbf{W}}^i)\,, \tag{4}$$

with i ranging from from 1 to n.

By taking into account the balance equations for each p^{th} test pair:

$$\begin{aligned} \mathbf{t}^a + \mathbf{t}^b &= \mathbf{0} \\ \mathbf{C}^a + \mathbf{C}^b - \frac{1}{2}\{[(p^a - p^b) \otimes \mathbf{t}^b - \mathbf{t}^b \otimes (p^a - p^b)]\} &= \mathbf{0}\,, \end{aligned} \tag{5}$$

the following mean power formula over $\mathcal{P}$ can be derived in the form:

$$\pi = \frac{1}{V}\sum_p \pi_p, \qquad \pi_p = \mathbf{t}_p \cdot [\mathbf{w}_p - \mathbf{W}_p(p^a - p^b)] + \frac{1}{2}\mathbf{C}_p \cdot \mathbf{W}_p\,, \tag{6}$$

where $\mathbf{t}_p = \mathbf{t}_a = -\mathbf{t}^b$ and $\mathbf{C}_p = \mathbf{C}^a = -\mathbf{C}^b + \frac{1}{2}\{[(p^a - p^b) \otimes \mathbf{t}^b - \mathbf{t}^b \otimes (p^a - p^b)]\}$, the range of p being the number of the test pairs in $\mathcal{P}$.

We finally assume the following linear constitutive functions for each test-pair in $\mathcal{P}$:

$$\begin{aligned} \mathbf{t}_p &= \mathbf{K}_p \mathbf{w}_p\,, \\ \mathbf{C}_p &= \mathbb{K}_p \mathbf{W}_p\,, \end{aligned} \tag{7}$$

where the elastic second order tensor $\mathbf{K}_p$ and the fourth order tensor $\mathbb{K}_p$ have as components the normal, tangential and rotational constants of the joint surfaces.

2.2. Identification of the micropolar continuum

Let us consider a continuum body occupying the region $\mathcal{B}$, a place $x \in \mathcal{B}$, and an open neighbourhood, $\mathcal{M}$, of x. The deformation of any point in $p \in \mathcal{M}$ is assumed homogeneous and approximated by the functions:

$$\begin{aligned} \mathbf{w}(p) &= \mathbf{w}(x) + \mathbf{H}(x)(p - x) \\ \mathbf{W}(p) &= \mathbf{W}(x) + \mathbb{H}(x)(p - x)\,, \end{aligned} \tag{8}$$

with $\mathbf{H} = \partial\mathbf{w}(x)/\partial x = \nabla\mathbf{w}$ and $\mathbb{H} = \partial\mathbf{W}(x)/\partial x = \nabla\mathbb{H}$.

If we assume that the lattice system has a modular structure, the deformation of a representative element (*module*) can be related to the deformation of $\mathcal{M}$ by postulating that:

$$\begin{aligned}\mathbf{w}^a &= \mathbf{w}(x) + \mathbf{H}(x)(g^a - x) \\ \mathbf{W}^a &= \mathbf{W}(x) + \mathbb{H}(x)(g^a - x)\end{aligned} \tag{9}$$

Finally, by using Equations (8) and (9), the expressions (3) can be rewritten as:

$$\begin{aligned}\mathbf{w}_p &= \mathbf{H}(x)(g^b - g^a) - \mathbf{W}(x)(g^b - g^a) \\ &\quad +[\mathbb{H}(x)(g^b - x)](p^b - g^b) - [\mathbb{H}(x)(g^a - x)](p^a - g^a)\,, \\ \mathbf{W}_p &= \mathbb{H}(x)(g^b - g^a)\,.\end{aligned} \tag{10}$$

Using the deformation correspondence proposed above (9), it is possible to obtain an expression of the power of the contact actions in the discrete model in terms of the kinematic quantities pertaining to the continuum ones. With regard to a generic test pair (p^a, p^b), from (6) and using Equations (10) we obtain the test–pair power as function of continuous kinematic fields $\mathbf{H}(x)$, $\mathbf{W}(x)$, $\mathbb{H}(x)$:

$$\begin{aligned}\pi_p &= \mathbf{t}_p \cdot \{[\mathbf{H}(x) - \mathbf{W}(x)](g^b - g^a) \\ &\quad +[\mathbb{H}(x)(g^b - x)](p^b - g^b) - [\mathbb{H}(x)(g^a - x)](p^a - g^a)\} \\ &\quad +\frac{1}{2}\mathbf{C}_p \cdot \mathbb{H}(x)(g^b - g^a)\,.\end{aligned} \tag{11}$$

By performing simple algebra, the above expression can be rewritten in the form:

$$\begin{aligned}\pi_p &= (\mathbf{H} - \mathbf{W}) \cdot \left[\mathbf{t}_p \otimes (g^b - g^a)\right] \\ &\quad +\frac{1}{2}\mathbb{H} \cdot \left\{2\mathbf{t}_p \otimes [(p^b - g^b) \otimes (g^b - x) - (p^a - g^a) \otimes (g^a - x)]\right. \\ &\quad \left. +\mathbf{C}_p \otimes (g^b - g^a)\ \right\}\,.\end{aligned} \tag{12}$$

where the dependence on x of the kinematic fields has been understood. The constitutive functions for the contact actions of the equivalent continuum can thus be obtained by requiring that the stress power density at x is equal to the mean power of the lattice system over the module:

$$\frac{1}{V}\sum_p \pi_p = \pi[(\mathbf{H}-\mathbf{W}),\, \mathbb{H}]\,, \qquad \forall\ (\mathbf{H}-\mathbf{W}),\, \mathbb{H}\,, \tag{13}$$

where V denotes the volume of the module, and the summation is extended to all the 'test pairs' appearing in the selected module supposed as centred in x. From the above expression, we obtain:

$$\pi[(\mathbf{H}-\mathbf{W}),\, \mathbb{H}] = (\mathbf{H}-\mathbf{W})\cdot\mathbf{S} + \frac{1}{2}\mathbb{S}\cdot\mathbb{H}\,, \tag{14}$$

where:

$$\begin{aligned}
\mathbf{S} &= \frac{1}{V}\sum_p \mathbf{t}_p \otimes (g^b - g^a)\\
\mathbb{S} &= \frac{1}{V}\sum_p \{\ 2\mathbf{t}_p \otimes [(p^b - g^b)\otimes(g^b - x) - (p^a - g^a)\otimes(g^a - x)]\\
&\quad +\mathbf{C}_p \otimes (g^b - g^a)\ \}
\end{aligned} \tag{15}$$

with

$$\begin{aligned}
\mathbf{t}_p &= \mathbf{K}_p\,\{\ [\mathbf{H}(x) - \mathbf{W}(x)](g^b - g^a)\\
&\quad +[\mathbb{H}(x)(g^b - x)](p^b - g^b) - [\mathbb{H}(x)(g^a - x)](p^a - g^a)\ \}\\
\mathbf{C}_p &= \mathbb{K}_p\ [\mathbb{H}(x)(g^b - g^a)]
\end{aligned} \tag{16}$$

3. Meso/Macro Transition - Homogenization

As a result of the coarse graining procedure presented in Section 2, both the inclusions and the matrix are described as micropolar continua which deterministic structure is encoded in the power density formula (12). The macroscopic continuum is also supposed to be micropolar, which in the case of periodic media have been proved to be able to naturally account for scale and skew-symmetric shear effects [13].

The kind of composites here considered have particles embedded in a matrix, randomly distributed according to a so-called dilute concentration (low volume fraction of max 40%) – such as polycrystals with thick interfaces, fiber reinforced composites, and even masonry materials (Roman concrete, tuffaceous rock, rubble masonry fills, etc.) – cannot be treated as periodic at the meso–level.

The transition from the mesoscopic to the macroscopic scale is then performed resorting to a statistical homogenization approach applied to a material with randomly distributed inclusions, either stiffer or softer than the matrix. Namely, a numerical homogenization based on the solution of properly defined BVP set at the meso–level and derived consistently with a generalized macrohomogeneity condition of Hills type [23].

3.1. The micropolar model

In the context of the linearized theory, each material point is characterized by the velocity vector $\mathbf{w}$ and the angular velocity skew–symmetric tensor $\mathbf{W}$. The strains measures are the strain, $\mathbf{U}$, and curvature tensor, $\mathbb{U}$, which are derived according to the compatibility equations:

$$\begin{aligned} \mathbf{U} &= \mathbf{H} - \mathbf{W} = \mathbf{E} + \boldsymbol{\Theta} - \mathbf{W}\,, && (17)\\ \mathbb{U} &= \mathbb{H}\,, && (18) \end{aligned}$$

where $\mathbf{E} = (\mathbf{H} + \mathbf{H}^T)/2$ and $\boldsymbol{\Theta} = (\mathbf{H} - \mathbf{H}^T)/2$ are, respectively, the symmetric and the skewsymmetric part of $\mathbf{H} = \nabla \mathbf{w}$

The power conjugated stress measures, respectively are: the stress tensor $\mathbf{S}$ and the couple stress tensor $\mathbb{S}$. If we decompose the stress tensor into its symmetric, $\mathbf{T} = (\mathbf{S} + \mathbf{S}^T)/2$, and skew-symmetric, $\mathbf{A} = (\mathbf{S} - \mathbf{S}^T)/2$, part as: $\mathbf{S} = \mathbf{T} + \mathbf{A}$, the stress density formula (12) becomes

$$\pi = \mathbf{S} \cdot \mathbf{U} + \frac{1}{2}\mathbb{S} \cdot \mathbb{U} \; = \mathbf{T} \cdot \mathbf{E} + \mathbf{A} \cdot (\boldsymbol{\Theta} - \mathbf{W}) + \frac{1}{2}\mathbb{S} \cdot \mathbb{U} \qquad (19)$$

The balance equations for the continuum, occupying an Euclidean region $\mathcal{B}$, with no external body forces and couples can be derived from a generalized formulation of the virtual power theorem as:

$$\begin{aligned} div\, \mathbf{S} &= \mathbf{0}\,, \\ div\, \mathbb{S} + 2\mathbf{A} &= \mathsf{0}\,, && (20) \end{aligned}$$

while the boundary conditions, on $\partial\mathcal{B}$, for the surface tractions and couples respectively represented by the vector $\mathbf{t}$ and the skew-symmetric tensor $\mathbf{C}$, ($\mathbf{C} = -\mathbf{C}^T$), accounting for a generalized version of the Cauchy theorem, are:

$$\begin{aligned} \mathbf{S}\mathbf{n} &= \mathbf{t}\,, \\ \mathbb{S}\mathbf{n} &= \mathbf{M}\,, \end{aligned} \tag{21}$$

$\mathbf{n}$ being the outward normal to the boundary $\partial\mathcal{B}$.

The stress-strain relations for the linear elastic anisotropic micropolar material writes:

$$\begin{aligned} \mathbf{S} &= \underline{\mathbb{A}}\,\mathbf{U} + \underline{\mathbb{B}}\,\mathbb{U}\,, \\ \mathbb{S} &= \underline{\mathbb{C}}\,\mathbf{U} + \underline{\mathbb{D}}\,\mathbb{U}\,, \end{aligned} \tag{22}$$

where $\underline{\mathbb{A}}$ and $\underline{\mathbb{D}}$ are fourth, and sixth order constitutive tensors with the major symmetries, respectively, while $\underline{\mathbb{B}}$ and $\underline{\mathbb{C}}$, are fifth order constitutive tensors respecting the symmetry relation: $\underline{\mathbb{B}}\mathbb{V}\cdot\mathbf{V} = \underline{\mathbb{C}}\mathbf{V}\cdot\mathbb{V}$, $\forall\mathbf{V},\mathbb{V}$.

It is worth noting that in the presence of central symmetries the tensors $\underline{\mathbb{B}}$ and $\underline{\mathbb{C}}$ are null and Equations (22) reduces to:

$$\begin{aligned} \mathbf{S} &= \underline{\mathbb{A}}\mathbf{U}\,, \\ \mathbb{S} &= \underline{\mathbb{D}}\mathbb{U}\,. \end{aligned} \tag{23}$$

Taking into account the decomposition in the symmetric and skewsymmetric part of the stress and strain tensors, Equations (23) can be also written:

$$\begin{aligned} \mathbf{T} &= \underline{\mathbb{A}}^{YY}\mathbf{E} + \underline{\mathbb{A}}^{YK}(\mathbf{\Theta} - \mathbf{W})\,, \\ \mathbf{A} &= \underline{\mathbb{A}}^{KY}\mathbf{E} + \underline{\mathbb{A}}^{KK}(\mathbf{\Theta} - \mathbf{W})\,, \\ \mathbb{S} &= \underline{\mathbb{D}}\,\mathbb{U}\,, \end{aligned} \tag{24}$$

where the components of the tensors $\underline{\mathbb{A}}^{\alpha,\beta}$ ($\alpha,\ \beta = Y,\ K$) are obtained as linear combination of the constitutive tensors in (22).

3.2. The meso-level micropolar model

The constitutive equations for the two–phase elastic materials (inclusions and matrix) are identified, using Equations (15, 16), in the form (22).

Let us consider a two–dimensional portion of the material of the material in the case in which the result of the coarse–graining procedure identifies two linear elastic isotropic phases.

By reordering the components of the symmetric and skew-symmetric stress ($\mathbf{T}$, $\mathbf{A}$) and strains ($\mathbf{E}$, $\boldsymbol{\Theta}$) tensors, as well as the sole independent components of the couple–stress $\mathbb{S}$ (denoted as $\mathbf{s}_1$, $\mathbf{s}_2$) and curvature $\mathbb{U}$ (denoted as $\mathbf{u}_1$, $\mathbf{u}_2$) tensors, into vectors and adopting the Voigt notation these equations can be written as:

$$\begin{bmatrix} \mathbf{S}_{11} \\ \mathbf{S}_{22} \\ \mathbf{S}_{12} \\ \mathbf{S}_{12} \\ \mathbf{s}_1 \\ \mathbf{s}_2 \end{bmatrix} = \begin{bmatrix} \lambda+2\mu & \lambda & 0 & 0 & 0 & 0 \\ \lambda & \lambda+2\mu & 0 & 0 & 0 & 0 \\ 0 & 0 & 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\mu_c & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\mu l_c^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\mu l_c^2 \end{bmatrix} \begin{bmatrix} \mathbf{E}_{11} \\ \mathbf{E}_{22} \\ \mathbf{E}_{12} \\ \boldsymbol{\Theta}_{12} - \mathbf{W}_{12} \\ \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix} \tag{25}$$

Equations (25) show that the non–null constitutive tensors $\underline{\mathbb{A}}$ and $\underline{\mathbb{D}}$ have components depending on four independent elastic constitutive parameters: the Lamé constants λ and μ, the Cosserat shear modulus μ_c, and the so–called characteristic length l_c, which is responsible for the bending stiffness.

3.3. The macro-level micropolar model

The effective elastic components of the micropolar macro–level continuum are directly obtained from the homogenization procedure, consistent with a properly defined generalized macrohomogeneity condition, which establishes an energetic equivalence between a portion of heterogeneous material at the mesoscopic level and the material point at the macroscopic level.

In this respect, let us consider a representative portion of the heterogeneous material at the meso–scale, i.e. a region $\mathcal{B}_\delta$ of volume V_δ and size L (where $\delta = L/d$ is the scale factor, with d being the average inclusion size). The adopted generalized macrohomogeneity condition writes:

$$\overline{\mathbf{T}\cdot\mathbf{E}}+\overline{\mathbf{A}\cdot(\Theta-\mathbf{W})}=\frac{1}{V_\delta}\int_{\mathcal{B}_\delta}(\mathbf{T}\cdot\mathbf{E}+\mathbf{A}\cdot(\Theta-\mathbf{W})+\frac{1}{2}\,\mathbb{S}\cdot\mathbb{U}\,)\,dV\,. \tag{26}$$

This equation ensures a one–to–one correspondence between the two scales, avoiding the introduction of kind of internal constraints for the deformation mechanisms as occurs in the case of continua of different type [12]. In Equation (26) overbars denote macroscopic quantities obtained as volume averages of the corresponding mesoscopic variables, i.e. $\overline{(\cdot)}=\frac{1}{V_\delta}\int_{\mathcal{B}_\delta}(\cdot)\,dV$.

The generalized macrohomogeneity condition (26) requires that the power expended by the stress at the mesoscopic level in the strain (at the same level) equals the power of the macrostress. This condition is verified providing that the following BC hold.

- Dirichlet's boundary conditions (D–BC):

$$\begin{aligned}&\mathbf{w}^Y|_{\partial\mathcal{B}}=\overline{\mathbf{E}}\,\mathbf{x},\\ &\mathbf{\Theta}|_{\partial\mathcal{B}}=\overline{\mathbf{\Theta}}-\overline{\mathbf{W}}\,,\qquad \mathbf{W}|_{\partial\mathcal{B}}=\overline{\mathbb{U}}\,\mathbf{x}\,.\end{aligned} \tag{27}$$

where $\mathbf{x}$ is the vector collecting the coordinates of the points on the boundary. Alternatively:

- Neumann's boundary conditions (N–BC):

$$\begin{aligned}&\mathbf{T}\,\mathbf{n}|_{\partial\mathcal{B}}=\overline{\mathbf{T}}\mathbf{n}\,,\\ &\mathbf{M}|_{\partial\mathcal{B}}=\frac{1}{2}[(\mathbf{x}\otimes\mathbf{A}\,\mathbf{n}-\mathbf{A}\,\mathbf{n}\otimes\mathbf{x})+\overline{\mathbb{S}}\,\mathbf{n}]\,.\end{aligned} \tag{28}$$

Consistently with the above, the effective macroscopic stress–strain relations result as:

$$\begin{aligned}\overline{\mathbf{S}}&=\underline{\overline{\mathbb{A}}}\quad\overline{\mathbf{U}}+\underline{\overline{\mathbb{B}}}\quad\overline{\mathbb{U}}\,,\\ \overline{\mathbb{S}}&=\underline{\overline{\mathbb{C}}}\quad\overline{\mathbf{U}}+\underline{\overline{\mathbb{D}}}\quad\overline{\mathbb{U}}\,,\end{aligned} \tag{29}$$

Considering two dimensional assemblies for which the central symmetry holds it is $\mathbb{B}=\mathbb{C}=\mathsf{0}$, and the constitutive equations can be written as:

$$\overline{\mathbf{T}}\;=\;\underline{\overline{\mathbb{A}}}^{YY}\overline{\mathbf{E}}+\underline{\overline{\mathbb{A}}}^{YK}(\overline{\mathbf{\Theta}}-\overline{\mathbf{W}})\,,$$

$$
\begin{aligned}
\overline{\mathbf{A}} &= \overline{\underline{\mathbb{A}}}^{KY}\overline{\mathbf{E}} + \overline{\underline{\mathbb{A}}}^{KK}(\overline{\boldsymbol{\Theta}} - \overline{\mathbf{W}})\,, \\
\bar{\mathbf{s}} &= \overline{\underline{\mathbf{D}}}\,\bar{\mathbf{u}}\,,
\end{aligned} \tag{30}
$$

By reordering the stress and strain tensors into vectors and taking into account the decomposition into symmetric and skewsymmetric parts Equations (29) specialize in:

$$
\begin{bmatrix} \overline{\mathbf{T}}_{11} \\ \overline{\mathbf{T}}_{22} \\ \overline{\mathbf{T}}_{12} \\ \overline{\mathbf{A}}_{12} \\ \bar{\mathbf{s}}_1 \\ \bar{\mathbf{s}}_2 \end{bmatrix}
=
\begin{bmatrix}
\overline{\underline{\mathbb{A}}}^{YY}_{1111} & \overline{\underline{\mathbb{A}}}^{YY}_{1122} & \overline{\underline{\mathbb{A}}}^{YY}_{1112} & \overline{\underline{\mathbb{A}}}^{YK}_{1121} & 0 & 0 \\
\overline{\underline{\mathbb{A}}}^{YY}_{2211} & \overline{\underline{\mathbb{A}}}^{YY}_{2222} & \overline{\underline{\mathbb{A}}}^{YY}_{2212} & \overline{\underline{\mathbb{A}}}^{YK}_{2221} & 0 & 0 \\
\overline{\underline{\mathbb{A}}}^{YK}_{1211} & \overline{\underline{\mathbb{A}}}^{YK}_{1222} & \overline{\underline{\mathbb{A}}}^{YK}_{1212} & \overline{\underline{\mathbb{A}}}^{YK}_{1221} & 0 & 0 \\
\overline{\underline{\mathbb{A}}}^{KY}_{1211} & \overline{\underline{\mathbb{A}}}^{KY}_{1222} & \overline{\underline{\mathbb{A}}}^{KY}_{1212} & \overline{\underline{\mathbb{A}}}^{KK}_{1212} & 0 & 0 \\
0 & 0 & 0 & 0 & \overline{\underline{\mathbf{D}}}_{11} & \overline{\underline{\mathbf{D}}}_{22} \\
0 & 0 & 0 & 0 & \overline{\underline{\mathbf{D}}}_{21} & \overline{\underline{\mathbf{D}}}_{22}
\end{bmatrix}
\begin{bmatrix} \overline{\mathbf{E}}_{11} \\ \overline{\mathbf{E}}_{22} \\ \overline{\mathbf{E}}_{12} \\ \overline{\boldsymbol{\Theta}}_{12} - \overline{\mathbf{W}}_{12} \\ \bar{\mathbf{u}}_1 \\ \bar{\mathbf{u}}_2 \end{bmatrix} \tag{31}
$$

In the special case of orthotropy the components ...are: *QUI si possono inserire I VALORI OTTENUTI NELLA FORMULA (28) DI PAU-TROVALUSCI ActaMech14*

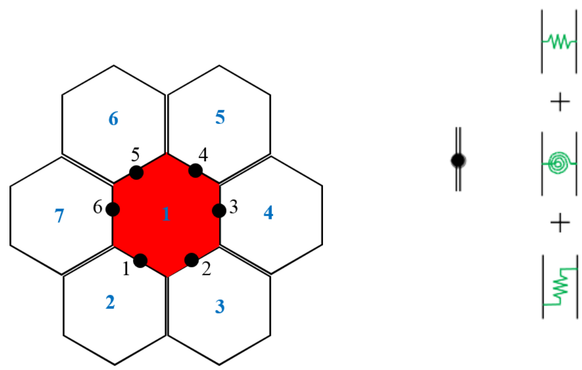
The independent strain and stress components of the 2D micropolar model can be conveniently ordered into the following vectors:

$$
\begin{aligned}
&\{\overline{\mathbf{E}}\} = \{\overline{\mathbf{E}}_{11} \quad \overline{\mathbf{E}}_{22} \quad \overline{\mathbf{E}}_{12}\}^T && \{\overline{\mathbf{T}}\} = \{\overline{\mathbf{T}}_{11} \quad \overline{\mathbf{T}}_{22} \quad \overline{\mathbf{T}}_{12}\}^T \\
&\{\overline{\beta}\} = \{\overline{\boldsymbol{\Theta}}_{12} - \overline{\mathbf{W}}_{12}\} && \{\overline{\alpha}\} = \{\overline{\mathbf{A}}_{12}\} \\
&\{\bar{\mathbf{u}}\} = \{\bar{\mathbf{u}}_{31} \quad \bar{\mathbf{u}}_{32}\}^T && \{\bar{\mathbf{s}}\} = \{\bar{\mathbf{s}}_1 \quad \bar{\mathbf{s}}_2\}^T\,,
\end{aligned} \tag{32}
$$

4. Numerical simulations

The three-scale procedure described in Sections 2 and 3 has been implemented and adopted to evaluate the equivalent micropolar elastic response of an ideal material that mimics the internal microstructure of a Ceramic Matrix Composite, as the Alumina-Zirconia qualitatively described in Section 1.

Going from the micro– up to the meso– and then the macro–scale in this illustrative example the material is described as follows. At the micro–scale



(a) (b)

Figure 4: (a)Hexagonal periodic cell: assemblage of rigid particles connected by axial, rotational and translational springs. (b)Schematic of a single spring characterized by axial, rotational and translational behavior.

the microstructure of both matrix and inclusions is made of periodic assemblages of hexagonal rigid particles, regularly arranged and connected by axial, translational and rotational springs.

****

sono arrivata qui (sotto va modificato)

ATTENZIONE CHE LA SIMBOLOGIA E' CAMBIATA (per semplificare i nomi sono definiti in testa all'articolo)

****

In Figure 4(a) a schematic of a periodic cell (module) is shown in red color: each cell is a hexagon, surrounded by six hexagons, and includes six springs (black circles) located at the center of each side of the hexagons. In Figure 4(b) the axial, rotational and translational stiffnesses of a single spring are graphically shown.

The MICRO/MESO transition, described in Section 2, is thus performed by adopting, for the matrix and inclusions, respectively, the values for the geomet-

	Edge dimension	Elastic tensor of springs
Matrix	L=7	$\mathbf{K}_p = \begin{pmatrix} 2000 & 0 \\ 0 & 3450 \end{pmatrix}$; $\mathbb{K}_p = 6125$
Inclusions	L=0.6	$\mathbf{K}_p = \begin{pmatrix} 785 & 0 \\ 0 & 780 \end{pmatrix}$; $\mathbb{K}_p = 17.66$

Table 1: Elastic stiffness of the springs

ric and mechanical parameters of the discrete systems shown in Table 1. L is the side length of the rigid hexagonal block, $\mathbf{K}_p$ is the stiffness tensor in Equation (7a), collecting the axial and shear stiffness of the springs, while $\mathbb{K}_p$ is the sole independent component of the stiffness tensor in (7b), i.e. the rotational stiffness of the spring.

The resulting homogenized values adopted as material parameters at the mesoscopic level are thus evaluated. In particular, our interest is here restricted to evaluate the Cosserat shear modulus μ_c and the characteristic length l_c that are difficult to obtain resorting to standard experimental results. It is worth noting that the adopted constitutive functions are strictly diagonal due to the chosen module in Table 1, as a consequence no Poisson's effects can be predicted. More general assumptions are, however, possible as illustrated in [39].

The ratios between the micropolar constants for matrix and inclusions are $\mu_i/\mu_m = 4.93$ and $l_{c_i}/l_{c_m} = 10$.

The meso/macro transition, described in Section 3 is thus carried out, in turn. We exploit the statistically–based multi–scale procedure developed and detailed in [23], and briefly recalled in paragraph 3.3, to achieve the twofold purpose of detecting the RVE size, L_{RVE}, and estimating the constitutive moduli of the energy equivalent homogeneous micropolar continuum.

The considered ideal material exhibits a nearly isotropic homogenized behavior at the macroscopic scale. In this case the micropolar shear stress is a scalar term related to the relative rotation through the constitutive component $\overline{\mathbb{A}}^{KK}_{1212}$, while the couple stress and the curvature tensors are related through the modulus tr$\overline{\mathbf{D}}$, thus the following relations hold:

$$\{\overline{\alpha}\} = \overline{\mathbb{A}}^{KK}_{1212}\{\overline{\beta}\} \tag{33}$$

$$\{\overline{\mathbf{s}}\} = \frac{1}{2}\mathrm{tr}\,\overline{\mathbf{D}}\{\overline{\mathbf{u}}\}\,, \tag{34}$$

We consider the bending modulus $\overline{l_C} = \sqrt{\mathrm{tr}\,\overline{\mathbf{D}}/\overline{\mathbb{A}}^{KK}_{1212}}$, for representing the convergence trend of the micropolar material response.

In Figure 5 the average of the bending modulus $\overline{l_{c\delta}}$ versus the scale parameter δ, normalized with respect to the RVE value $\overline{l_{cRVE}}$ is reported. The RVE is achieved for $\delta_{RVE} = 15$.

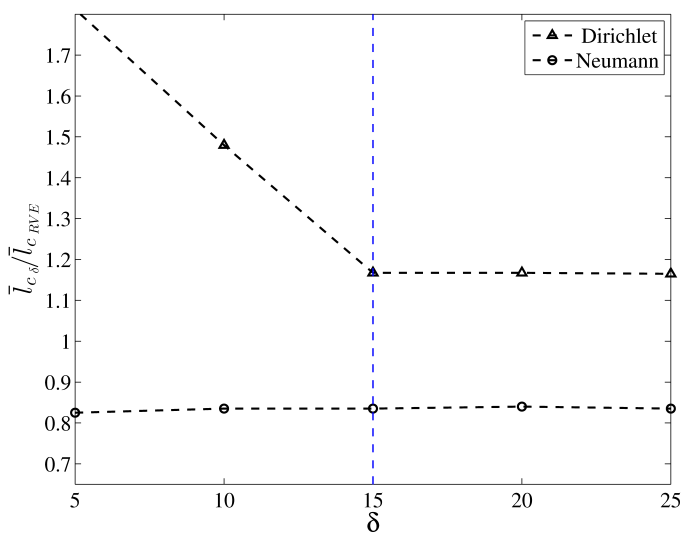


Figure 5: Average of effective bending modulus $\bar{l}_c$ (normalized to the RVE modulus $\bar{l}_{cRVE}$)versus scale parameter δ,solutions of BVPs under Dirichlet and Neumann BCs.

5. Final remarks

We have developed a multi-scale homogenization approach for the study of composite materials characterized by microstructural length scales not negligible with respect to the mesoscopic and macroscopic characteristic lengths. The material is modeled at three scale: the MICRO-scale, characterized by the length scale l_c, where each constituent is described as a discrete system; the MESO-scale, where a material sample d is considered and modeled as a multi-phase micropolar linear elastic material and the MACRO-scale, where an equivalent homogeneous micropolar material is obtained as final result of the multi-scale procedure.

The MICRO-MESO transition is performed via a coarse graining procedure based on a generalized Cauchy-Born correspondence map and energy equivalence between the microscopic lattice system, describing each constituent, and the equivalent micropolar material. The MESO-MACRO transition, instead, a statistical homogenization procedure has been developed, basing on the solution of Boundary Value Problems (BVP), posed on Statistically Representative Elements (SVE), with Boundary Conditions (BC) derived from a generalized macrohomogeneity condition of Hill's type.

The paper extends two previous contributions [40] and [23] independently developed for describing the MICRO-MESO and the MESO-MACRO transition, respectively. The two approaches are here organically combined into an integrated multi-scale approach and the proposed procedure is able to describe the material behaviour following a complete hierarchy of scales from the microscopic up to the macroscopic scale.

An illustrative numerical example is finally provided to assess the capabilities of the procedure. An ideal material that mimics the internal microstructure of a Ceramic Matrix Composite is studied starting from its hexagonal discrete microstructure. At the mesoscopic scale the random nature of the material (concerning the spatial distribution of the particles) is taken into account and the overall homogenizaed macroscopic micropolar elastic moduli are finally obtained.

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