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DICAM

A MICROPOLAR HOMOGENIZATION APPROACH FOR RANDOM PARTICLE-BASED COMPOSITES

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Abstract. *This study presents a multiscale procedure for determining the size of the Representative Volume Element (RVE) and the homogenized moduli of particle-based composite materials, modeled as micropolar continua. The homogenization, consistent with a generalized Hill-Mandel condition, is adopted in conjunction with a statistical procedure, by which two hierarchies of scale-dependent bounds on classical and micropolar constitutive moduli are obtained using Dirichlet and Neumann BCs. Two different types of inclusion, either stiffer or softer than the matrix, are considered in the numerical applications. The results highlight the importance of accounting for micropolar bending deformation modes, spatial randomness of the medium, and presence of inclusions crossing the edges of the test window used in the homogenization.*

Sommario. *Questo studio presenta una procedura multiscala per la determinazione della dimensione dell'Elemento di Volume Rappresentativo e dei moduli omogeneizzati di materiali compositi particellari, modellati come continui micropolari. Si adotta una tecnica di omogeneizzazione, coerente con una condizione di Hill-Mandel generalizzata, combinata con una procedura statistica, per ottenere due gerarchie di limiti, dipendenti dalla scala, per i moduli costitutivi, sia classici che micropolari, imponendo condizioni al contorno di Dirichlet e Neumann. Nelle applicazioni numeriche, si fa riferimento a due tipi di inclusioni, più soffici o più rigide rispetto alla matrice. I risultati evidenziano l'importanza di considerare i modi di deformazione micropolari, la casualità spaziale del mezzo, oltre che la presenza di inclusioni che intersecano il contorno della finestra di prova utilizzata nell'omogeneizzazione.*

1 INTRODUCTION

Particle-based composites, used in many engineering applications or present in nature, exhibit a microstructure made of randomly distributed inclusions (*particles*) embedded into a dissimilar matrix; examples of such materials are polymer, ceramic, metal, and cement matrix composites. The determination of their overall mechanical response cannot disregard their discontinuous nature at finer scales, but the explicit modeling of all the microscopic features inevitably leads to solve computationally cumbersome problems. An efficient way to circumvent these difficulties consists in adopting multiscale techniques; such methods have been widely applied periodic media, even in the context of micropolar continua, regarded as suitable models for taking into account size effects and nonsymmetrical shear behavior[1–5].

The main issue in the context of random homogenization is that, differently from periodic homogenization, the size of the Representative Volume Element (RVE) is not a-priori known, and must be determined as an additional unknown of the homogenization problem[6]. This problem has been successfully tackled in the literature, by using stochastic approaches based on a finite-size scaling of intermediate control volume elements, referred to as Statistical Volume Elements (SVEs)[7,8]. According to these approaches, the unknown RVE size is found as the convergence value of two hierarchies of constitutive bounds associated with the solutions of Dirichlet and Neumann BVPs consistent with a generalized macro-homogeneity condition.

Such a stochastic approach has been extended to micropolar materials in previous works of some of the Authors[9,10]. Here, this approach, adopted for deriving the overall constitutive tensor of general two-phase (inclusions/matrix) materials, has been applied focusing on the convergence trend of the elastic moduli. Two different inclusions types, either stiffer or softer than the matrix, have been considered. By increasing the scale factor between SVEs and inclusions sizes, two series of BVPs have been solved. The overall constitutive relations are found to be isotropic and thus, represented in terms of bulk, shear and micropolar bending moduli. Moreover, a special attention has been devoted to investigate the differences in the predicted overall response in the presence or not of inclusions crossing the SVE's boundary.

2 MICROPOLAR HOMOGENIZATION

The particle-based composite under consideration is described at two levels: a *fine-scale* level, where the material is modeled as a two-phase composite made of randomly distributed particles of finite size d and given elastic parameters embedded in a continuous matrix with different material properties; and a *gross-scale* level, where the actual nonhomogeneous material is replaced by an equivalent homogeneous material, with characteristic dimension L.

Both the fine and gross levels are here modeled as micropolar continua. At the gross, macroscopic, level, the adoption of a micropolar model is relevant when the principle of separation of scales is not valid; i.e. when d is not negligible with respect to L. At the fine level, here called mesoscopic level, each constituent is assumed as a microstructured material associated with at least a further characteristic length, l_c; this level may be regarded as the result of a homogenization from a third level, i.e. the conventionally defined microscopic level. In the following, this further homogenization step will be implicitly assumed, allowing to focus the attention on the transition from the mesoscopic to the macroscopic level.

At the mesoscopic level, the heterogeneous material is composed of two constituents, both described as linearly elastic and isotropic micropolar materials. Within a linearized theory, the kinematics of such a continuum model is governed by the compatibility equations:

$$\gamma_{ij} = u_{i,j} + e_{kij}\varphi_k , \qquad \kappa_{ij} = \varphi_{i,j} , \tag{1}$$

where (u_i) and (φ_i) are the displacement and rotation vectors of each material point, (γ_{ij}) and (κ_{ij}) are the strain and curvature tensors, respectively, and (e_{ijk}) is the Levi-Civita tensor, with i,j,k = 1,2,3.

The balance equations, derived by neglecting body forces and couples, are:

$$\tau_{ij,j}=0\,,\qquad \mu_{ij,j}+e_{kji}\tau_{ij}=0\,, \tag{2}$$

where (τ_{ij}) and (μ_{ij}) are the stress and couple stress tensors, respectively. After defining the tractions and surface couples on the boundary of a control volume with outward normal (n_i), denoted as (t_i) and (m_i), respectively, we have:

$$t_i=\tau_{ij}n_j\,,\qquad m_i=\mu_{ij}n_j\,. \tag{3}$$

We decompose the classical and micropolar strain and stress measures in order to separately investigate their effects into their symmetric and skew-symmetric parts:

$$\gamma_{ij}=\varepsilon_{ij}+\alpha_{ij}\,,\qquad \tau_{ij}=\sigma_{ij}+\beta_{ij}\,, \tag{4}$$

where (ε_{ij} = ½($u_{i,j}$ + $u_{j,i}$)) and (σ_{ij}= ½(τ_{ij} + τ_{ji})) are the classical symmetric strain and stress tensors, whereas (α_{ij}= ½($u_{i,j}$ − $u_{j,i}$) + $e_{kij}\varphi_k$) and (β_{ij}= ½(τ_{ij} −τ_{ji})) are the skew-symmetric strain and stress tensors, characterizing, together with the curvature and couple stress tensors, a micropolar medium. The quantity α_{ij} represents the relative rotation between the local rigid rotation and the macro-rotation and the micro-rotation.

By restricting our attention to a 2D setting, the stress-strain relations for a linearly elastic and isotropic micropolar material can be written as:

$$\begin{aligned}\sigma_{ij}&=\lambda\varepsilon_{kk}\delta_{ij}+2\mu\varepsilon_{ij}\,,\\ \beta_{12}&=-2\mu_c\alpha_{12}\,,\\ \mu_{3j}&=2\mu l_c^2\kappa_{3j}\,,\end{aligned} \tag{5}$$

with i,j = 1,2; these constitutive relations involve four independent constitutive parameters: the Lamé constants λ and μ, the Cosserat shear modulus μ_c, and the characteristic length l_c, which is responsible for the bending stiffness.

At the macroscopic level, no assumptions about the material symmetries are formulated, and the homogenized moduli are obtained using the homogenization procedure, according to the following macro-homogeneity condition generalized for micropolar continua:

$$\frac{1}{A_\delta}\int_{\mathcal{B}_\delta}\left(\sigma_{ij}\varepsilon_{ij}+\beta_{ij}\alpha_{ij}+\mu_{ij}\kappa_{ij}\right)dA=\bar{\sigma}_{ij}\bar{\varepsilon}_{ij}+\bar{\beta}_{ij}\bar{\alpha}_{ij}+\bar{\mu}_{ij}\bar{\kappa}_{ij}\,, \tag{6}$$

written for a mesoscale window $\mathcal{B}_\delta$ of size L, occupying the region of area A_δ, where $\delta = L/d$, is the scale factor, d being the averaged inclusion size, and where overbars denote surface average of the introduced variables.

By using Eq. (6), it is possible to derive the coupling conditions for both localization and homogenization steps. The localization step, consists in enforcing Dirichlet and Neumann boundary conditions at the mesoscale. With reference to a square-shaped mesoscopic domain $\mathcal{B}_\delta$, by fixing the coordinate system at its center, the derived Dirichlet boundary conditions are:

$$u_i=\bar{\varepsilon}_{ij}\chi_j\,,\qquad \varphi_3=\tfrac{1}{2}e_{ij3}\bar{\alpha}_{ij}+\bar{\kappa}_{3i}x_i\qquad \text{on } \partial\mathcal{B}_\delta, \tag{7}$$

with i,j = 1,2. While the derived Neumann boundary conditions are:

$$t_i=\left(\bar{\sigma}_{ij}+\bar{\beta}_{ij}\right)n_j\,,\qquad m_3=m_3^0+\bar{\mu}_{3i}n_i\qquad \text{on } \partial\mathcal{B}_\delta, \tag{8}$$

where m_3^0 is the moment imposed to ensure the moment balance when $\bar{\beta}_{ij}$ is applied. The homogenization step then consists in evaluating the effective moduli at the macroscale as:

$$\begin{aligned}
\sigma_{ij} &= \bar{\mathbb{A}}_{ijhk}\varepsilon_{hk}\,, \\
\beta_{12} &= \bar{\mathbb{B}}_{1212}\alpha_{12}\,, \\
\mu_{3j} &= \bar{\mathbb{C}}_{3i3j}\kappa_{3j}\,,
\end{aligned} \tag{9}$$

with i,j = 1,2. The structure of Eq. (9) reflects the symmetry class of anisotropic non-chiral materials; the components $\bar{\mathbb{A}}_{ijhk}$ are the classical moduli, while $\bar{\mathbb{B}}_{1212}$, $\bar{\mathbb{C}}_{3i3j}$ are the micropolar moduli.

3 STATISTICAL HOMOGENIZATION FOR RANDOM COMPOSITES

3.1 Description of the computational multiscale procedure

We are interested in deriving the scale-dependent effective response of random particle-based composites described as two-phase materials, assuming that statistical homogeneity and mean-ergodicity hold. Here, a simplified microstructure is considered, made of a matrix with randomly distributed disk-shaped inclusions of diameter d. The inclusion volume fraction is kept fixed, while both number and position of inclusions randomly vary. The constitutive response of a random heterogeneous medium requires the definition of the RVE size, L_{RVE}, much larger than the fine-scale characteristic length, d, so that the influence of the BCs on the RVE is negligible. In accordance with the approach presented in[6–8], we propose a stochastic strategy for obtaining the statistics of scale-dependent upper and lower bounds of the overall moduli, and approaching the RVE size for micropolar continua, based on the definition of several realizations of the microstructure (sampled in a Monte Carlo sense)[10].

In detail, for a fixed value of the scale parameter $\delta = L/d$, a number of square test windows of side L, called Statistical Volume Elements (SVEs), are identified. For each realization of the microstructure $\mathcal{B}_\delta(\omega)$, ω being an elementary event over a sample space, the number and position of inclusions within the window are generated by a hard-core Poisson's point field (i.e. preventing the overlapping between disks). Subsequently, for any $\mathcal{B}_\delta(\omega)$, Dirichlet and Neumann BVPs are solved, accounting for classical and micropolar deformation modes, and the relevant homogenized constitutive moduli are numerically determined. The estimation of an overall modulus is found when its average value falls within the interval corresponding to a confidence level set at 95% over a normal distribution. If the number of realizations needed for ensuring this requirement is greater than a properly fixed value, also depending on the data dispersion[10], the procedure is repeated for an increased value of δ. Finally, the overall moduli are estimated as the mean converged values between the Dirichlet and Neumann bounds. All the BVPs have been solved by using COMSOL Multiphysics® simulation environment.

3.2 Numerical results

Two cases of particle-based composites are considered: (a) a material with stiff inclusions in a soft matrix (high contrast material), and (b) a material with soft inclusions in a stiff matrix (low contrast material). The adopted material parameters are listed in Table 1, presented in a dimensionless form in terms of ratios between corresponding quantities of inclusions and matrix. Both the materials have a nominal area fraction ρ set at 40%. The two-dimensional BVPs are numerically solved considering increasing values of the window size, $\delta = L/d$, in the range between 5 and 25. In the finite element discretization, unstructured meshes of quadratic Lagrangian triangular elements are adopted.

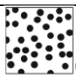
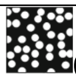
Material	Parameters			
	λ_i/λ_m	μ_i/μ_m	μ_{ci}/μ_{cm}	l_{ci}/l_{cm}
(a)	46	4.93	4.93	10^{1}
(b)	0.021	0.202	0.202	10^{-1}

Table 1: Ratios between material parameters of inclusions and matrix.

The homogenized behavior has been found to be approximately isotropic; therefore, only the classical bulk, $\bar{K}_\delta$, and shear, $\bar{G}_\delta$, moduli, as well as the bending modulus $\bar{l}_{c_\delta}$ have been computed. In order to investigate the convergence trend of these elastic moduli, the following scaling measures, functions of the scale parameter δ, have been defined:

$$f_\delta^K = \frac{\bar{K}_\delta^D}{\bar{K}_\delta^N} - \frac{\bar{K}_{hom}^D}{\bar{K}_{hom}^N}, \qquad f_\delta^G = \frac{\bar{G}_\delta^D}{\bar{G}_\delta^N} - \frac{\bar{G}_{hom}^D}{\bar{G}_{hom}^N}, \qquad f_\delta^C = \frac{\bar{l}_{c\,\delta}^{\,D}}{\bar{l}_{c\,\delta}^{\,N}} - \frac{\bar{l}_{c\,hom}^{\,D}}{\bar{l}_{c\,hom}^{\,N}} \tag{10}$$

where $\bar{K}_{hom}$, $\bar{G}_{hom}$ and $\bar{l}_{c\,hom}$ are the moduli obtained for the equivalent homogeneous material; the superscripts D and N stand for Dirichlet and Neumann BCs, respectively. Note that in the homogeneous case the moduli obtained using Dirichlet and Neumann BC's are equal.

Figures 1, 2 and 3 show the convergence trend of the bulk, shear and micropolar bending moduli for the two considered values of the contrast; these results also highlight the influence of considering inclusions that intersect or do not insersect the windows' edges on the overall behavior. For the classical constitutive scaling measures f_δ^K and f_δ^G, there is no significant deviation in the overall response between the cases of crossing and non-crossing inclusions; the different trends are more evident for the micropolar value f_δ^C. Moreover, it can be noted that f_δ^C tends to zero for both materials when the inclusions do not cross the boundaries.

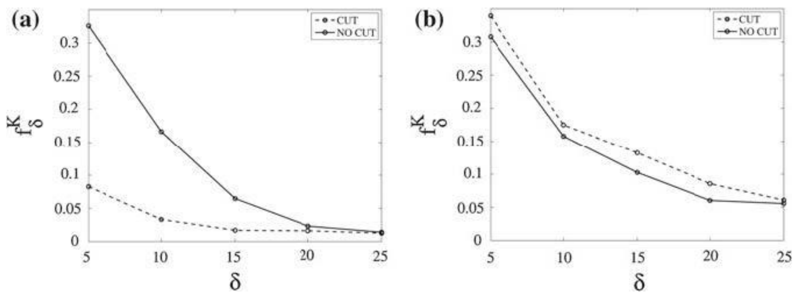


Figure 1: Convergence trend of the classical bulk modulus with inclusions crossing (dash lines) and non-crossing (solid lines) the windows' edges: a) high contrast material; b) low contrast material.

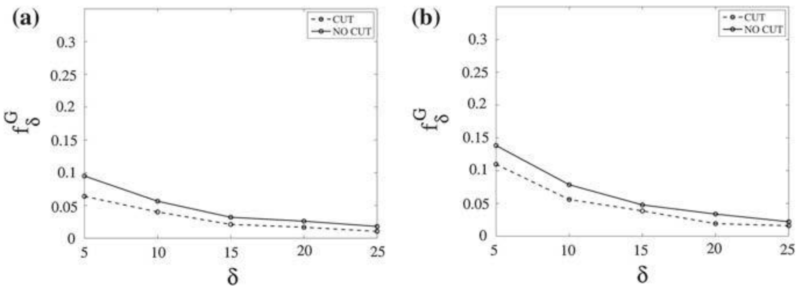


Figure 2: Convergence trend of the classical shear modulus with inclusions crossing (dash lines) and non-crossing (solid lines) the windows' edges: a) high contrast material; b) low contrast material.

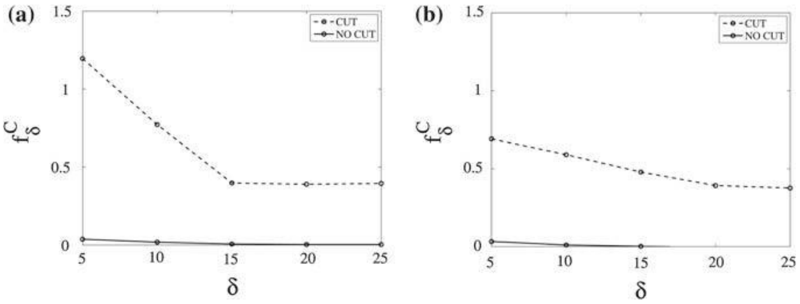


Figure 3: Convergence trend of micropolar bending modulus with inclusions crossing (dash lines) and non-crossing (solid lines) the windows' edges: a) high contrast material; b) low contrast material.

With regard to classical moduli, these results show that the presence of particles softer than the matrix leads to slow down the convergence to the RVE with respect to the opposite case; this means that for composites with soft particles in a stiffer matrix, very large scales for the RVE should be employed, thus compromising the possibility of homogenizing through upper (Dirichlet) and lower (Neumann) bounds for the constitutive moduli. These results seem to highlight the need of resorting to different boundary conditions, e.g. periodic BCs[11,12]. It is worth noting that in the case of inclusions not crossing the windows' edges, the values of effective moduli obtained here are comparable to the values achieved using periodic BCs[10].

Nevertheless, the statistical criterion adopted[8,10] allow us to detect the RVE size and the corresponding material moduli, independently from the material contrast. In Figure 4, the average of the bulk modulus $\bar{K}_{\delta}$ versus the scale parameter δ is displayed for both materials (a) and (b). Such a value is normalized with respect to the corresponding modulus $\bar{K}_{RVE}$, determined as the average of the coefficients evaluated at the convergence window in the case of crossing inclusions. The convergence trend to the RVE depends on whether inclusions cross or do not cross the windows' boundaries. It is worth noting that material (b) shows a slower convergence than material (a); moreover, if crossing inclusions are stiffer than the matrix, the bulk modulus is higher with respect to the case of non-crossing inclusions, whereas in the case of crossing inclusions softer than the matrix, the bulk modulus is lower than in the case of non-crossing inclusions. The occurrence of horizontal trend indicates that the RVE is reached and the corresponding homogenized modulus is obtained as an average value between the Dirichlet and Neumann values. In Figure 5, the average of the shear modulus $\bar{G}_{\delta}$ versus the scale parameter δ is displayed for both materials (a) and (b). Such a value is normalized with respect to the corresponding modulus $\bar{G}_{RVE}$ determined as below. The convergence and the RVE size are comparable to those obtained for the bulk modulus.

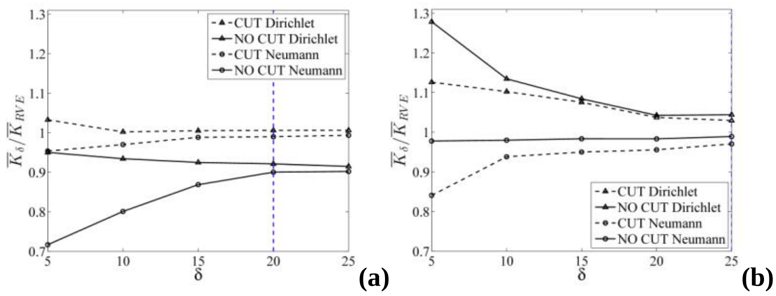


Figure 4: Average of the normalized effective bulk modulus versus the scale parameter, under Dirichlet (D-BC) and Neumann (N-BC) boundary conditions, with inclusions crossing (dash lines) and non-crossing (solid lines) the windows' edges: a) high contrast material; b) low contrast material. The vertical lines indicate the RVE in the case of crossing inclusions.

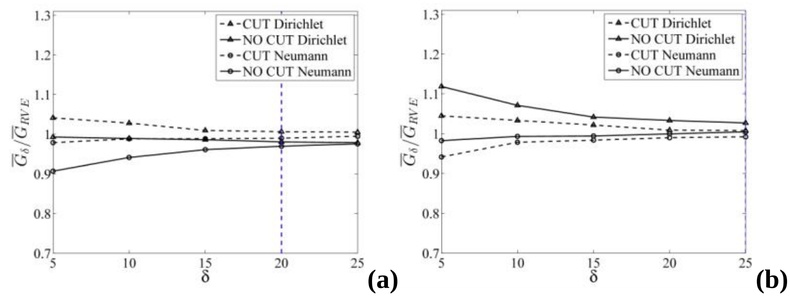


Figure 5: Average of the normalized effective shear modulus versus the scale parameter, under Dirichlet (D-BC) and Neumann (N-BC) boundary conditions, with inclusions crossing (dash lines) and non-crossing (solid lines) the windows' edges: a) high contrast material; b) low contrast material. The vertical lines indicate the RVE in the case of crossing inclusions.

Finally, in Figure 6, the average of the bending modulus $\bar{l}_{c_\delta}$ versus the scale parameter δ is shown for both materials (a) and (b). Such a value is normalized with respect to the corresponding modulus $\bar{l}_{c_{RVE}}$ determined as in the previous cases. The convergence trend and the RVE size are comparable to those obtained for the bulk modulus. The RVE for the material (a) is achieved for δ_{RVE} = 15 in the case of crossing inclusions, while δ_{RVE} = 20 in the case of non-crossing inclusions. Also in this case the occurrence of horizontal trend indicates that the RVE is reached with averaged overall moduli.

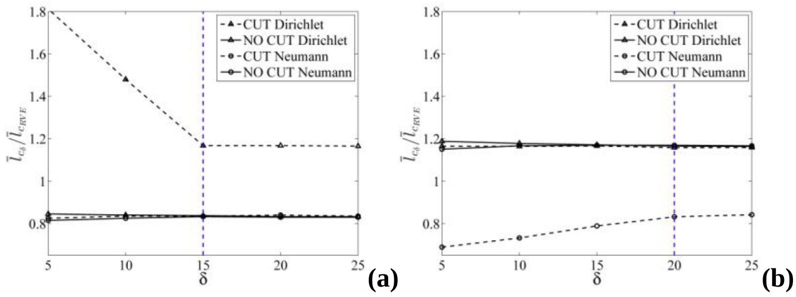


Figure 6: Average of the normalized effective bending modulus versus the scale parameter, under Dirichlet (D-BC) and Neumann (N-BC) boundary conditions, with inclusions crossing (dash lines) and non-crossing (solid lines) the windows' edges: a) high contrast material; b) low contrast material. The vertical lines indicate the RVE in the case of crossing inclusions.

In summary, the results show that the influence of crossing inclusions is important, in both cases of material contrast (a) and (b). This influence is more significant for the micropolar moduli, leading to a stiffer homogenized behavior for material (a) and a softer behavior for material (b) in the presence of inclusions which cross the windows' boundaries.

4 CONCLUDING REMARKS

A scale-dependent multiscale procedure has been proposed for estimating the constitutive moduli of particle-based composites described as micropolar continua. Specifically developed to deal with non-periodic media, it is based on the derivation of hierarchies of upper and lower bounds. By this procedure, the RVE size and the related classical and micropolar overall moduli have been statistically detected for two materials with different contrast between elastic moduli of inclusions and matrix. The reported convergence trend for the considered moduli has been shown that, regardless of the scaling behavior depending on the phase contrast in elastic moduli, the proposed stochastic approach enabled us to determine the RVE size as well as the homogenized moduli. Overall, the numerical results have shown that the RVE size found for the micropolar response is smaller than that for the classical response.

Inclusions both intersecting and not intersecting the edges of mesoscale windows have been considered in the simulations. We have found that the higher contrast medium (a) is slightly more sensitive than the medium (b) to the presence of inclusions crossing the windows' edges, but this is relevant also for the latter medium. Furthermore, the differences in terms of average effective moduli and RVE sizes achieved in the presence of crossing or non-crossing inclusions decrease but remain non-negligible for increasing values of the window size; such differences are more significant when the micropolar moduli are evaluated.

In conclusion, by the proposed stochastic procedure, we have shown that the presence of crossing inclusions cannot be neglected for obtaining a correct estimate of both classical and micropolar effective moduli, even if the RVE size is large enough. In this regard, a subject of future research with the aim of accelerating the convergence could be the development of an enhanced scale-dependent statistical homogenization procedure based on properly conceived periodized BCs[12], without forsaking the realistic hypothesis of crossing inclusions.

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