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**Abstract**

This manuscript provides novel bounds and estimates, for the first time, on size-dependent properties of composites accounting for generalized interfaces in their microstructure, via analytical homogenization verified by computational analysis. We extend both the composite cylinder assemblage and Mori–Tanaka approaches to account for the general interface model. Our proposed strategy does not only determine the overall response of composites, but also it provides information about the local fields for each phase of the medium including the interface. We present a comprehensive study on a broad range of interface parameters, stiffness ratios and sizes. Our analytical solutions are in excellent agreement with the computational results using the finite element method. Based on the observations throughout our investigations, two notions of *size-dependent bounds* and *ultimate bounds* on the effective response of composites are introduced which yield a significant insight into the size effects, particularly important for the design of nano-composites.

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**Keywords (separated by '-')** General interface - Size effects - Ultimate bounds - Size-dependent bounds - Homogenization - Composites

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# 3 Bounds on size effects in composites via homogenization 4 accounting for general interfaces

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18 **Keywords** General interface · Size effects · Ultimate bounds · Size-dependent bounds · Homogenization ·  
19 Composites

## 20 1 Introduction

21 Interphases between the constituents of heterogeneous materials play a crucial role on the overall material  
22 response and particularly at small scales, due to the large area-to-volume ratio. A common strategy to model  
23 the interphases is to replace them by a zero-thickness general interface [1] characterized by displacement and  
24 traction jumps. This idea was initially proposed by Sanchez-Palencia et al. [2,3] and followed by Hashin [4] for  
25 a thermal problem. Since the area-to-volume ratio is proportional to the inverse of the dimension, accounting  
26 for interfaces in homogenization results in size-dependent properties hence, capturing the size effects, unlike  
27 the classical homogenization [5–7] that lacks a length scale. In this contribution, we present two analytical

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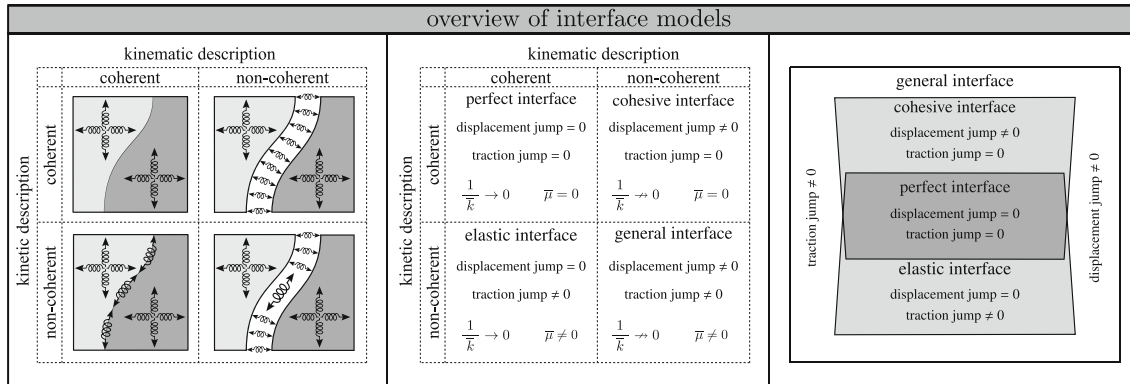
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**Fig. 1** Categorization of the interface models based on their kinetic or kinematic behavior. The perfect interface model does not allow for the displacement jump nor traction jump. The cohesive interface model has continuous traction field, whereas the displacement jump is allowed across the interface. In the elastic interface model, the displacement jump across the interface is zero, whereas the traction jump is permissible. All the models are unified in the general interface model in which both the displacement jump and traction jump across the interface are possible. Two interface properties of  $\bar{\mu}$  and  $\bar{k}$  characterize the interface behavior. The interface stiffness against opening is denoted  $\bar{k}$ , and the interface resistance against stretch is denoted  $\bar{\mu}$

28 solutions to determine the overall behavior of composites via a homogenization framework accounting for  
 29 generalized interfaces. In addition, computational analysis is carried out to evaluate the performance of the  
 30 analytical solutions.

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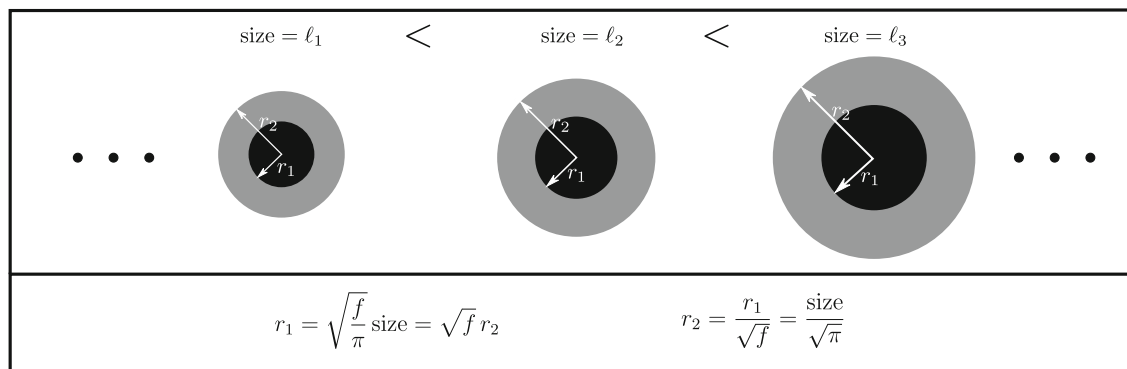
31 Figure 1 categorizes the interface models based on their kinetic (tractions) and kinematic (displacements)  
 32 features. The interface is referred to as perfect if the traction and displacement fields are continuous across the  
 33 interface, and thus, the perfect interface model is coherent both kinetically and kinematically.

34 The elastic interface model is kinematically coherent but kinetically non-coherent and hence semi-perfect.  
 35 The main assumption of the interface elasticity theory [8–15] is that the interface is allowed to have its  
 36 own thermodynamic structure. This assumption could result in a traction jump across the interface due to  
 37 the Young–Laplace equation [16–18]. The subject of surface and interface elasticity has been extensively  
 38 studied in [19–35] among others. The cohesive interface model allows for the displacement jump but not for  
 39 the traction jump. This model is kinetically coherent and kinematically non-coherent. The cohesive interface  
 40 model emerges in a variety of studies dating from the seminal works [36–38] to its extensions and applications  
 41 in [39–57]. The general interface model is a unified version of all the aforementioned interface models where  
 42 both the displacement jump and traction jump are admissible. The general interface has been examined in a  
 43 fundamental contribution by Hashin [58] and further studied in [59–68] among others.

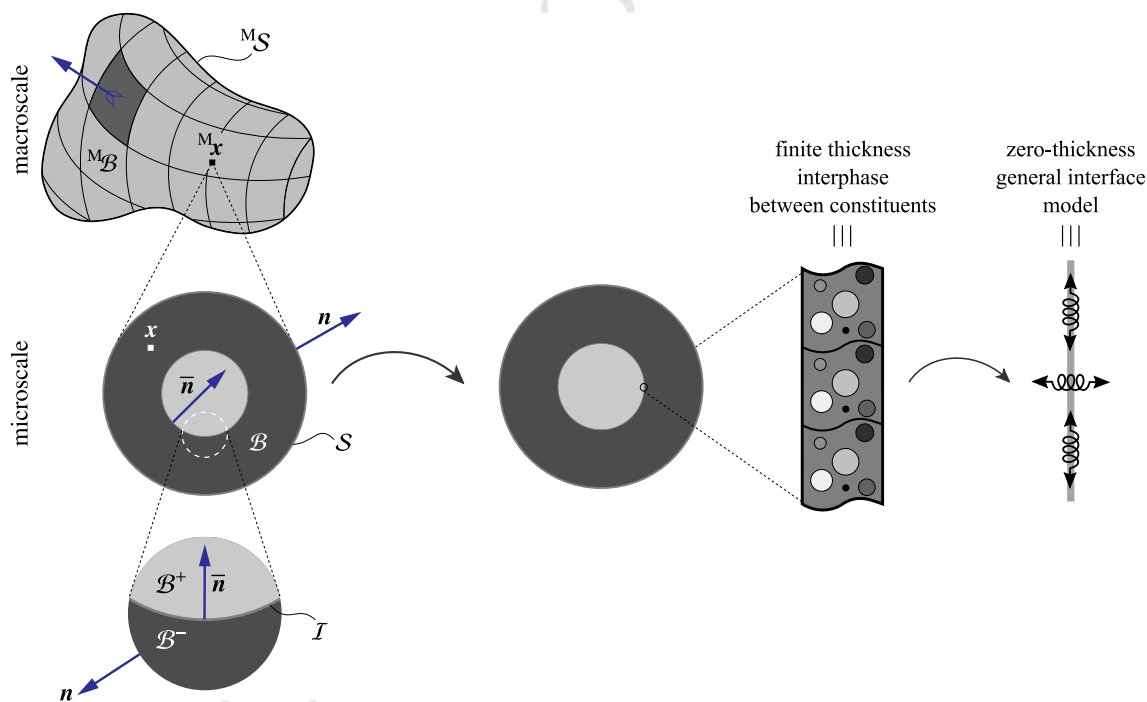
44 In the past decade, scale-dependent macroscopic behavior due to the microscale elasticity has been com-  
 45 prehensively studied from both analytical [69–79] and computational [80–84] perspectives. Comparisons with  
 46 atomistic simulations and experiments in [85–90] justify that the size effects due to interfaces are physically  
 47 meaningful. The underlying assumption in this contribution is that the size effects are only observed due to the  
 48 presence of the interface at the microstructure. While the surface/interface elasticity itself may be explained  
 49 by the tangential contributions of second-gradient continua on the boundary, the full contributions of second-  
 50 gradient continua in the bulk are not taken into account. Obviously, one must eventually develop a complete  
 51 model in which both strain-gradient and surface/interface elasticity are present. Only then, one can claim  
 52 whether or not the size effect due to the interface is correlated with those associated with the strain-gradient  
 53 effects. See [23] for an excellent study on size-dependent effects in nano-materials.

54 The term “size” in this contribution refers to the physical size of a microstructure. Figure 2 illustrates  
 55 schematically the definition of the size. The volume fraction of the inclusion is denoted  $f$ . For a given volume  
 56 fraction and size, the radii of the inclusion and the matrix can be calculated. Throughout this manuscript,  
 57 the macroscopic quantities are distinct from their microscopic counterparts by a left superscript “M.” For  
 58 instance,  $M\{\bullet\}$  is a macroscopic quantity with its counterpart being  $\{\bullet\}$  at the microscale. Interface quantities  
 59 are distinguished from the bulk quantities by a bar placed on top them. That is,  $\{\bar{\bullet}\}$  denotes an interface quantity  
 60 with its bulk counterpart  $\{\bullet\}$ . Moreover, the average and the jump operators across the interface are denoted  
 61 by  $\{\{\bullet\}\}$  and  $[[\{\bullet\}]]$ , respectively.

62 The rest of this manuscript is organized as follows. Section 2 elaborates on the problem definition and  
 63 provides the governing equations. In Sect. 3, the analytical approaches accounting for the general interface



**Fig. 2** Illustration of the term “size.” Having the volume fraction, the radius of the inclusion and the matrix can be obtained for each specific size. As a result, size is proportional to the radius of the inclusion or that of the matrix



**Fig. 3** Problem definition for homogenization including the general interface model. The macrostructure is shown as well as the microstructure which is in fact the RVE. It is assumed that the constitutive laws at the microscale are known and by prescribing a macroscopic strain  $M\epsilon$  on the microstructure, the macroscopic stress  $M\sigma$  is obtained via averaging. A finite-thickness interphase is replaced with a zero-thickness interface model. The classical interface models cannot capture heterogeneous material layer, and thus, the general interface model is required

64 model are presented. Numerical examples are provided in Sect. 4 to compare the computational and analytical  
 65 results. Section 5 concludes this work and provides further outlook for future contributions.

## 66 2 Governing equations

67 In this section, the governing equations of continua embedding a general interface are given. For the sake of  
 68 brevity, only the final form of the essential equations are stated. For more details on the derivations, the reader  
 69 is referred to [1, 65, 91]. Consider a continuum body taking the configuration  $M\mathcal{B}$  at the macroscale, as shown  
 70 in Fig. 3, with its corresponding RVE at the microscale denoted as  $\mathcal{B}$ . A general interface model is required to  
 71 replace the finite-thickness interphase between the constituents [92]. It is assumed that the constitutive behavior  
 72 of the material at the microscale is known and the macroscopic overall response of the medium is obtained

73 via averaging over the RVE [see [93–98], among others]. In doing so, a macroscopic strain  ${}^M\boldsymbol{\varepsilon}$  is prescribed  
 74 on the microstructure and the macroscopic stress  ${}^M\boldsymbol{\sigma}$  is obtained. Moreover, to establish a computational  
 75 homogenization framework, an appropriate RVE must be chosen such that (i) it is small enough to guarantee  
 76 scale separation and (ii) it is large enough to be representative of the microstructure. For more details on the  
 77 definition of RVE, see [99–102]. Here, we significantly simplify the RVE to a circular microstructure in order  
 78 to obtain in-plane isotropic effective behavior of the RVE suitable for comparison with the proposed analytical  
 79 estimates.

80 The interface  $\mathcal{I}$  separates the microstructure into two subdomains  $\mathcal{B}^+$  and  $\mathcal{B}^-$ . The outward unit normal  
 81 to the external boundary is denoted as  $\mathbf{n}$ , whereas  $\bar{\mathbf{n}}$  defines the interface unit normal vector pointing from the  
 82 minus side of the interface to its plus side. The displacement field is denoted as  $\mathbf{u}$ , and the interface displacement  
 83  $\bar{\mathbf{u}}$  is defined by the average displacement across the interface conforming to the definition of the mid-surface.  
 84 The displacement average and the displacement jump across the interface read

$$85 \quad \bar{\mathbf{u}} := \{\{\mathbf{u}\}\} = \frac{1}{2} [\mathbf{u}^+ + \mathbf{u}^-] \quad \text{and} \quad \llbracket \mathbf{u} \rrbracket = [\mathbf{u}^+ - \mathbf{u}^-], \quad (1)$$

86 respectively, where  $\mathbf{u}^+$  is the displacement of the plus side of the interface and  $\mathbf{u}^-$  is the displacement of the  
 87 minus side of the interface. The strain field in the bulk and on the interface read

$$88 \quad \boldsymbol{\varepsilon} = \frac{1}{2} [\mathbf{i} \cdot \text{grad} \mathbf{u} + [\text{grad} \mathbf{u}]^t \cdot \mathbf{i}] \quad \text{in } \mathcal{B} \quad \text{and} \quad \bar{\boldsymbol{\varepsilon}} = \frac{1}{2} \left[ \bar{\mathbf{i}} \cdot \overline{\text{grad} \bar{\mathbf{u}}} + [\overline{\text{grad} \bar{\mathbf{u}}}]^t \cdot \bar{\mathbf{i}} \right] \quad \text{on } \mathcal{I}, \quad (2)$$

89 where  $\mathbf{i}$  is the identity tensor. The operator  $\overline{\text{grad}\{\bullet\}}$  characterizes the projection of the gradient onto the interface  
 90 as  $\overline{\text{grad}\{\bullet\}} = \text{grad}\{\bullet\} \cdot \bar{\mathbf{i}}$  with  $\bar{\mathbf{i}} = \mathbf{i} - \bar{\mathbf{n}} \otimes \bar{\mathbf{n}}$ . Note the contraction  $\bar{\mathbf{i}} \cdot \overline{\text{grad} \bar{\mathbf{u}}}$  enforces the projection of the  
 91 interface displacement gradient onto the interface.

92 The total energy density of the medium consists of the bulk free energy density  $\psi$  and the interface free  
 93 energy density  $\bar{\psi}$ . The bulk free energy density is assumed to be only a function of the strain field  $\psi = \psi(\boldsymbol{\varepsilon})$ . The  
 94 interface free energy density is assumed to be a function of both interface strain and interface displacement  
 95 jump as  $\bar{\psi} = \bar{\psi}(\bar{\boldsymbol{\varepsilon}}, \llbracket \mathbf{u} \rrbracket)$ . That is, the contributions of higher gradients of the interface strain or interface  
 96 curvature are not taken into account. Connecting the bulk and interface energy densities to their microscale  
 97 energy conjugates, the constitutive equations read

$$98 \quad \boldsymbol{\sigma} = \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} \quad \text{in } \mathcal{B}, \quad \bar{\boldsymbol{\sigma}} = \frac{\partial \bar{\psi}}{\partial \bar{\boldsymbol{\varepsilon}}} \quad \text{and} \quad \bar{\mathbf{t}} = \frac{\partial \bar{\psi}}{\partial \llbracket \mathbf{u} \rrbracket} \quad \text{on } \mathcal{I}, \quad (3)$$

99 where  $\bar{\mathbf{t}}$  is the interface traction as  $\bar{\mathbf{t}} := \{\{\boldsymbol{\sigma}\}\} \cdot \bar{\mathbf{n}}$ . The balance equations in the absence of external forces read

$$100 \quad \begin{aligned} \text{div} \boldsymbol{\sigma} &= \mathbf{0} \quad \text{in } \mathcal{B}, & \boldsymbol{\sigma} \cdot \mathbf{n} &= \mathbf{t} \quad \text{on } \mathcal{S}, \\ \overline{\text{div}} \bar{\boldsymbol{\sigma}} + \llbracket \boldsymbol{\sigma} \rrbracket \cdot \bar{\mathbf{n}} &= \mathbf{0} \quad \text{on } \mathcal{I} \text{ (along the interface)}, & \{\{\boldsymbol{\sigma}\}\} \cdot \bar{\mathbf{n}} &= \bar{\mathbf{t}} \quad \text{on } \mathcal{I} \text{ (across the interface)}, \end{aligned} \quad (4)$$

101 with  $\mathbf{t}$  being the traction on the boundary  $\mathcal{S}$ . The interface divergence operator  $\overline{\text{div}\{\bullet\}} = \text{grad}\{\bullet\} : \bar{\mathbf{i}}$  embeds  
 102 the interface curvature operator. The constitutive material behavior for the bulk and interface reads

$$103 \quad \boldsymbol{\sigma} = 2\mu \boldsymbol{\varepsilon} + \lambda [\boldsymbol{\varepsilon} : \mathbf{i}] \mathbf{i} \quad \text{in } \mathcal{B}, \quad \bar{\boldsymbol{\sigma}} = 2\bar{\mu} \bar{\boldsymbol{\varepsilon}} + \bar{\lambda} [\bar{\boldsymbol{\varepsilon}} : \bar{\mathbf{i}}] \bar{\mathbf{i}} \quad \text{and} \quad \bar{\mathbf{t}} = \bar{k} \llbracket \mathbf{u} \rrbracket \quad \text{on } \mathcal{I}, \quad (5)$$

104 in which  $\lambda$  and  $\mu$  are the bulk Lamé parameters and  $\bar{\lambda}$  and  $\bar{\mu}$  are the interface Lamé parameters. The interface  
 105 Lamé parameters correspond to the interface in-plane resistance against stretches. The interface orthogonal  
 106 resistance,  $\bar{k}$ , represents the interface resistance against opening. Without loss of generality, it can be shown  
 107 that for the two-dimensional setting here  $\bar{\lambda} = 0$  can be assumed since the resistance along an isotropic interface  
 108 can be sufficiently captured with only one interface parameter.

109 Next, we briefly elaborate on the micro- to macro-transition. The macroscopic strain and stress can be  
 110 obtained through boundary integrals of the microscopic quantities as

$$111 \quad {}^M\boldsymbol{\varepsilon} = \frac{1}{\mathcal{V}} \int_{\mathcal{S}} \frac{1}{2} [\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}] \, dA, \quad {}^M\boldsymbol{\sigma} = \frac{1}{\mathcal{V}} \int_{\mathcal{S}} \mathbf{t} \otimes \mathbf{x} \, dA. \quad (6)$$

112 Exploiting the divergence theorem, the above relations simplify to the averages

$$113 \quad {}^M\boldsymbol{\varepsilon} = \frac{1}{\mathcal{V}} \int_{\mathcal{B}} \boldsymbol{\varepsilon} \, dV + \frac{1}{\mathcal{V}} \int_{\mathcal{I}} \frac{1}{2} [\llbracket \mathbf{u} \rrbracket \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes \llbracket \mathbf{u} \rrbracket] \, dA, \quad {}^M\boldsymbol{\sigma} = \frac{1}{\mathcal{V}} \int_{\mathcal{B}} \boldsymbol{\sigma} \, dV + \frac{1}{\mathcal{V}} \int_{\mathcal{I}} \bar{\boldsymbol{\sigma}} \, dA. \quad (7)$$

**Table 1** The relations between the interface and bulk properties for transversely isotropic composites in terms of the material parameters in Sect. 2 and the commonly accepted notation in analytical homogenization employed in Sect. 3. The parameters in the first row correspond to a generic case but in the second row correspond to a more specific (transversely isotropic) case of interest here

Bulk					Interface						
$\mu_{\text{ax}}$	$\mu_{\text{tr}}$	$\kappa_{\text{tr}}$	$l$	$n$	$\bar{\mu}_{\text{ax}}$	$\bar{m}$	$\bar{n}$	$\bar{l}$	$\bar{k}_r$	$\bar{k}_\theta$	$\bar{k}_z$
$\mu$	$\mu$	$\lambda + \mu$	$\lambda$	$\lambda + 2\mu$	$\bar{\mu}$	$2\bar{\mu}$	$2\bar{\mu}$	0	$k$	$k$	$k$
$\mu_{\text{ax}}$ : axial shear modulus	$\mu_{\text{tr}}$ : transverse shear modulus	$\kappa_{\text{tr}}$ : transverse bulk modulus	$l$ : stiffness in $r_z$ and $\theta_z$ directions	$n$ : axial stiffness	$\bar{\mu}_{\text{ax}}$ : interface axial shear modulus	$\bar{m}$ : interface transverse shear parameter	$\bar{n}$ : interface axial stiffness	$\bar{l}$ : interface stiffness in $\theta_z$ direction	$\bar{k}_r$ : interface orthogonal resistance in $r$	$\bar{k}_\theta$ : interface orthogonal resistance in $\theta$	$\bar{k}_z$ : interface orthogonal resistance in $z$
$\mu$ : shear modulus	$\lambda$ : first Lamé parameter				$\bar{\mu}$ : interface in-plane resistance				$k$ : interface orthogonal resistance		

114 Finally, the Hill–Mandel condition must be employed to guarantee the energy equivalence between the two  
115 scales. The interface enhanced Hill–Mandel condition reads

$$116 \quad \delta^{\text{M}}\psi \stackrel{!}{=} \frac{1}{\mathcal{V}} \int_{\mathcal{B}} \delta\psi \, dV + \frac{1}{\mathcal{V}} \int_{\mathcal{I}} \delta\bar{\psi} \, dA, \quad (8)$$

117 where  $\stackrel{!}{=}$  shows the conditional equality. Utilizing the Hill’s lemma, after some steps the Hill–Mandel condi-  
118 tion (8) simplifies to the boundary integral

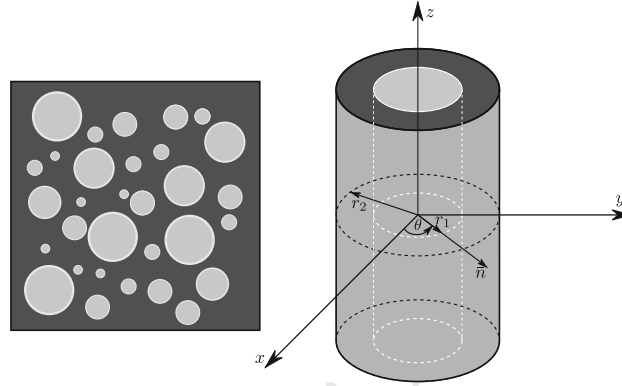
$$119 \quad \int_{\mathcal{S}} [\delta\mathbf{u} - \delta^{\text{M}}\boldsymbol{\varepsilon} \cdot \mathbf{x}] \cdot [\mathbf{t} - \text{M}\boldsymbol{\sigma} \cdot \mathbf{n}] \, dA \stackrel{!}{=} 0, \quad (9)$$

120 identifying appropriate boundary conditions on the RVE. Among various boundary conditions satisfying the  
121 Hill–Mandel condition, the canonical ones of interest here are the linear displacement boundary condition  
122 (DBC) and constant traction boundary condition (TBC). See Firooz et al. [103] for a comprehensive study on  
123 the influences of the boundary condition as well as the RVE type on the overall behavior of composites.

### 124 3 Analytical estimates

125 The aim of this section is to elaborate the analytical methods to determine the overall behavior of fiber  
126 composites embedding general interfaces. First, the preliminaries of the RVE problem for fiber reinforced  
127 composites is provided. Second, we extend the composite cylinder assemblage approach and the generalized  
128 self-consistent method to account for general interfaces resulting in bounds and estimates on the macroscopic  
129 properties of composites. Finally, an interface enhanced Mori–Tanaka method is developed to incorporate  
130 general interfaces which not only provides the overall properties but also determines the state of the stress and  
131 strain in each phase of the medium including the interface. Table 1 gathers the relations between the material  
132 parameters in Sect. 2 and the commonly accepted notation in analytical homogenization employed in this  
133 section as well as the physical meaning of each modulus.

134 In passing, we shall add that the composite cylinders assemblage (CCA) framework has been designed to  
135 account for transversely isotropic constituents at most. Further anisotropy does not allow to identify analytical  
136 solutions in boundary value problems like those presented in this manuscript; at least this cannot be done in a  
137 straightforward manner. Cylindrical orthotropy of the fiber and the interface, however, has been addressed for  
138 similar type of boundary value problems in [104]. To the best of the authors knowledge, no further anisotropy  
139 has been studied so far using the composite cylinders assemblage approach. Considering Eshelby-based mean-  
140 field approaches, one could follow a strategy similar to the one described by Dinzart and Sabar [105] for general  
141 anisotropy of the constituents.



**Fig. 4** Heterogeneous medium and its corresponding appropriate RVE considered in our problem. The inner radius shows the radius of the fiber, whereas the outer one shows the radius of the matrix. The interface lies at  $r = r_1$

### 142 3.1 Preliminaries of the RVE problem for fiber composites

143 Figure 4 demonstrates the heterogeneous medium and its underlying RVE consisting of two concentric cylinders  
 144 corresponding to the fiber (phase 1) and matrix (phase 2) with the interface lying at  $r = r_1$ . The volume fraction  
 145 of the fiber is  $f = r_1^2/r_2^2$ . Obviously, for the problem of interest here, it is more convenient to express the  
 146 equilibrium equations and the constitutive law in cylindrical coordinate system with coordinates  $r$ ,  $\theta$  and  $z$ .

147 For transversely isotropic materials, the constitutive material behavior in Voigt notation reads

$$\begin{aligned}
 & \begin{bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \\ \sigma_{r\theta} \\ \sigma_{rz} \\ \sigma_{\theta z} \end{bmatrix} = \begin{bmatrix} \kappa_{tr} + \mu_{tr} & \kappa_{tr} - \mu_{tr} & l & 0 & 0 & 0 \\ \kappa_{tr} - \mu_{tr} & \kappa_{tr} + \mu_{tr} & l & 0 & 0 & 0 \\ l & l & n & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu_{tr} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu_{ax} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu_{ax} \end{bmatrix} \begin{bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{zz} \\ 2\varepsilon_{r\theta} \\ 2\varepsilon_{rz} \\ 2\varepsilon_{\theta z} \end{bmatrix} \quad \text{with} \quad (10) \\
 & \varepsilon_{rr} = \frac{\partial u_r}{\partial r}, \\
 & \varepsilon_{\theta\theta} = \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{u_r}{r}, \\
 & \varepsilon_{zz} = \frac{\partial u_z}{\partial z}, \\
 & 2\varepsilon_{rz} = \frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z}, \\
 & 2\varepsilon_{\theta z} = \frac{1}{r} \frac{\partial u_z}{\partial \theta} + \frac{\partial u_\theta}{\partial z}, \\
 & 2\varepsilon_{r\theta} = \frac{\partial u_\theta}{\partial r} + \frac{1}{r} \frac{\partial u_r}{\partial \theta} - \frac{u_\theta}{r},
 \end{aligned}$$

149 and the equilibrium equations in the bulk read

$$\begin{cases} \frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0, \\ \frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{\partial \sigma_{\theta z}}{\partial z} + \frac{2}{r} \sigma_{r\theta} = 0, \\ \frac{\partial \sigma_{rz}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta z}}{\partial \theta} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{1}{r} \sigma_{rz} = 0. \end{cases} \quad (11)$$

151 The constitutive relations for the general interface at  $r = r_1$  are characterized by four parameters for the  
 152 traction jump ( $\bar{m}$ ,  $\bar{l}$ ,  $\bar{n}$  and  $\bar{\mu}_{ax}$ ) and three parameters for the displacement jump ( $\bar{k}_r$ ,  $\bar{k}_\theta$  and  $\bar{k}_z$ ) as

$$\begin{aligned}
 \begin{bmatrix} \bar{\sigma}_{\theta\theta} \\ \bar{\sigma}_{zz} \\ \bar{\sigma}_{\theta z} \end{bmatrix} &= \begin{bmatrix} \bar{m} & \bar{l} & 0 \\ \bar{l} & \bar{n} & 0 \\ 0 & 0 & \bar{\mu}_{ax} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_{\theta\theta} \\ \bar{\varepsilon}_{zz} \\ 2\bar{\varepsilon}_{\theta z} \end{bmatrix} \quad \text{with} \quad \begin{aligned} \bar{\varepsilon}_{\theta\theta} &= \frac{1}{r_1} \frac{\partial \bar{u}_\theta}{\partial \theta} + \frac{\bar{u}_r}{r_1} \\ \bar{\varepsilon}_{zz} &= \frac{\partial \bar{u}_z}{\partial z} \\ 2\bar{\varepsilon}_{\theta z} &= \frac{1}{r_1} \frac{\partial \bar{u}_z}{\partial \theta} + \frac{\partial \bar{u}_\theta}{\partial z} \end{aligned} \quad \text{and} \quad \begin{bmatrix} \bar{t}_r \\ \bar{t}_\theta \\ \bar{t}_z \end{bmatrix} = \begin{bmatrix} \bar{k}_r \llbracket u_r \rrbracket \\ \bar{k}_\theta \llbracket u_\theta \rrbracket \\ \bar{k}_z \llbracket u_z \rrbracket \end{bmatrix}. \quad (12)
 \end{aligned}$$

The equilibrium equations at the interface are

$$\begin{cases} -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \llbracket \sigma_{rr} \rrbracket = 0, \\ \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \frac{\partial \bar{\sigma}_{\theta z}}{\partial z} + \llbracket \sigma_{r\theta} \rrbracket = 0, \\ \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta z}}{\partial \theta} + \frac{\partial \bar{\sigma}_{zz}}{\partial z} + \llbracket \sigma_{rz} \rrbracket = 0. \end{cases} \quad (13)$$

The three normal vectors in cylindrical coordinates are

$$\mathbf{n}_r = \begin{bmatrix} \cos \theta \\ \sin \theta \\ 0 \end{bmatrix}, \quad \mathbf{n}_\theta = \begin{bmatrix} -\sin \theta \\ \cos \theta \\ 0 \end{bmatrix}, \quad \mathbf{n}_z = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad (14)$$

and therefore, the displacements and stresses can be represented in tensorial forms as

$$\begin{aligned}
 \mathbf{u} &= u_r \mathbf{n}_r + u_\theta \mathbf{n}_\theta + u_z \mathbf{n}_z, \\
 \boldsymbol{\sigma} &= \sigma_{rr} \mathbf{n}_r \otimes \mathbf{n}_r + \sigma_{\theta\theta} \mathbf{n}_\theta \otimes \mathbf{n}_\theta + \sigma_{zz} \mathbf{n}_z \otimes \mathbf{n}_z + \frac{1}{2} \sigma_{r\theta} [\mathbf{n}_r \otimes \mathbf{n}_\theta + \mathbf{n}_\theta \otimes \mathbf{n}_r] \\
 &\quad + \frac{1}{2} \sigma_{rz} [\mathbf{n}_r \otimes \mathbf{n}_z + \mathbf{n}_z \otimes \mathbf{n}_r] + \frac{1}{2} \sigma_{\theta z} [\mathbf{n}_\theta \otimes \mathbf{n}_z + \mathbf{n}_z \otimes \mathbf{n}_\theta], \\
 \bar{\boldsymbol{\sigma}} &= \bar{\sigma}_{\theta\theta} \mathbf{n}_\theta \otimes \mathbf{n}_\theta + \bar{\sigma}_{zz} \mathbf{n}_z \otimes \mathbf{n}_z + \frac{1}{2} \bar{\sigma}_{\theta z} [\mathbf{n}_\theta \otimes \mathbf{n}_z + \mathbf{n}_z \otimes \mathbf{n}_\theta].
 \end{aligned} \quad (15)$$

Using the equilibrium equations in the bulk and on the interface, the divergence theorem for our problem can be written as

$$\begin{aligned}
 \int_B \operatorname{div}\{\bullet\} dV + \int_I \llbracket \{\bullet\} \rrbracket \cdot \bar{\mathbf{n}} dA &= \int_S \{\bullet\} \cdot \mathbf{n} dA \quad \text{and} \\
 \int_I \overline{\operatorname{div}\{\bullet\}} dA - \int_I \overline{\operatorname{div}\bar{\mathbf{n}}}\{\bullet\} \cdot \bar{\mathbf{n}} dA &= \int_{\partial I} \{\bullet\} \cdot \tilde{\mathbf{n}} dL,
 \end{aligned} \quad (16)$$

where  $\tilde{\mathbf{n}}$  is the normal at the boundary of the interface but along the interface itself. Using the above theorems, the average mechanical energy in the composite reads

$$\begin{aligned}
 U &= \frac{1}{2\mathcal{V}} \int_B \boldsymbol{\sigma} : \boldsymbol{\varepsilon} dV + \frac{1}{2\mathcal{V}} \int_I \bar{\boldsymbol{\sigma}} : \bar{\boldsymbol{\varepsilon}} dA \\
 &= \frac{1}{2\mathcal{V}} \left[ \underbrace{\int_B \operatorname{div}(\mathbf{u} \cdot \boldsymbol{\sigma}) dV + \int_I \bar{\mathbf{u}} \cdot \llbracket \boldsymbol{\sigma} \rrbracket \cdot \bar{\mathbf{n}} dA}_{\int_{\partial B} [\boldsymbol{\sigma} \cdot \mathbf{n}] \cdot \mathbf{u} dA} \right] + \frac{1}{2\mathcal{V}} \underbrace{\int_I \overline{\operatorname{div}(\bar{\mathbf{u}} \cdot \bar{\boldsymbol{\sigma}})} dA}_{\int_{\partial I} [\bar{\boldsymbol{\sigma}} \cdot \bar{\mathbf{n}}] \cdot \bar{\mathbf{u}} dL},
 \end{aligned} \quad (17)$$

The volume element in the cylindrical coordinates is  $dv = r dr d\theta dz$ , the (vertical) surface element at a constant radius  $r$  is  $ds_r = r d\theta dz$ , the (horizontal) surface element at a constant height  $z$  is  $ds_z = r dr d\theta$  and

169 the line element at a constant radius  $r$  and height  $z$  is  $dl = r d\theta$ . Finally, the average mechanical energy in the  
170 RVE and in equivalent homogeneous medium read

$$\begin{aligned}
 U^{\text{RVE}} &= \frac{1}{2\mathcal{V}} \int_0^{2\pi} \int_0^{r_2} \left[ \left[ \sigma_{rz} u_r + \sigma_{\theta z} u_\theta + \sigma_{zz} u_z \right]_{z=L} - \left[ \sigma_{rz} u_r + \sigma_{\theta z} u_\theta + \sigma_{zz} u_z \right]_{z=-L} \right] r dr d\theta \\
 &\quad + \frac{1}{2\mathcal{V}} \int_{-L}^L \int_0^{2\pi} \left[ \sigma_{rr} u_r + \sigma_{\theta r} u_\theta + \sigma_{zr} u_z \right]_{r=r_2} r_2 d\theta dz \\
 &\quad + \frac{1}{2\mathcal{V}} \int_0^{2\pi} \left[ \left[ \bar{\sigma}_{\theta z} \bar{u}_\theta + \bar{\sigma}_{zz} \bar{u}_z \right]_{z=L} - \left[ \bar{\sigma}_{\theta z} \bar{u}_\theta + \bar{\sigma}_{zz} \bar{u}_z \right]_{z=-L} \right]_{r=r_1} r_1 d\theta, \quad (18) \\
 U^{\text{eq}} &= \frac{1}{2\mathcal{V}} \int_0^{2\pi} \int_0^{r_2} \left[ \left[ \sigma_{rz}^{\text{eq}} u_r^{\text{eq}} + \sigma_{\theta z}^{\text{eq}} u_\theta^{\text{eq}} + \sigma_{zz}^{\text{eq}} u_z^{\text{eq}} \right]_{z=L} - \left[ \sigma_{rz}^{\text{eq}} u_r^{\text{eq}} + \sigma_{\theta z}^{\text{eq}} u_\theta^{\text{eq}} + \sigma_{zz}^{\text{eq}} u_z^{\text{eq}} \right]_{z=-L} \right] r dr d\theta \\
 &\quad + \frac{1}{2\mathcal{V}} \int_{-L}^L \int_0^{2\pi} \left[ \sigma_{rr}^{\text{eq}} u_r^{\text{eq}} + \sigma_{\theta r}^{\text{eq}} u_\theta^{\text{eq}} + \sigma_{zr}^{\text{eq}} u_z^{\text{eq}} \right]_{r=r_2} r_2 d\theta dz.
 \end{aligned}$$

172 As we will see later, for the expansion and the in-plane shear boundary value problems, all the quantities with  
173 index  $z$  vanish and the above relations simplify to

$$\begin{aligned}
 U^{\text{RVE}} &= \frac{1}{4\pi r_2^2 L} \int_{-L}^L \int_0^{2\pi} \left[ \sigma_{rr}^{(2)} u_r^{(2)} + \sigma_{r\theta}^{(2)} u_\theta^{(2)} \right]_{r=r_2} r_2 d\theta dz, \\
 U^{\text{eq}} &= \frac{1}{4\pi r_2^2 L} \int_{-L}^L \int_0^{2\pi} \left[ \sigma_{rr}^{\text{eq}} u_r^{\text{eq}} + \sigma_{r\theta}^{\text{eq}} u_\theta^{\text{eq}} \right]_{r=r_2} r_2 d\theta dz. \quad (19)
 \end{aligned}$$

### 175 3.2 Composite cylinder assemblage (CCA) approach and generalized self-consistent method (GSCM)

176 Recently, Chatzigeorgiou et al. [65] proposed an extension of the generalized self-consistent method  
177 (GSCM) [106] and the composite cylinders assemblage (CCA) approach [107] to determine the effective  
178 shear modulus and bulk modulus of fiber composites embedding general interfaces. Motivated by these obser-  
179 vations, here the original formalism of Hashin and Rosen [107] is extended to account for the general interface  
180 to determine bounds on the overall shear modulus  $^M\mu$ . Note that the same methodology can be employed to  
181 obtain bounds for the effective bulk modulus  $^M\kappa$ . However, the upper and lower bounds on the bulk modulus  
182 coincide. Therefore, the bounds and estimates for the bulk modulus yield identical results. The derivations of  
183 the effective bulk and shear modulus developed in [65] are briefly (and more explicitly) stated here for the  
184 sake of completeness.

#### 185 3.2.1 Effective bulk modulus

186 Assume that the RVE is subject to a radial expansion with its upper and lower surfaces fixed as depicted in  
187 Fig. 5 (left). The displacement field in cylindrical coordinates reads

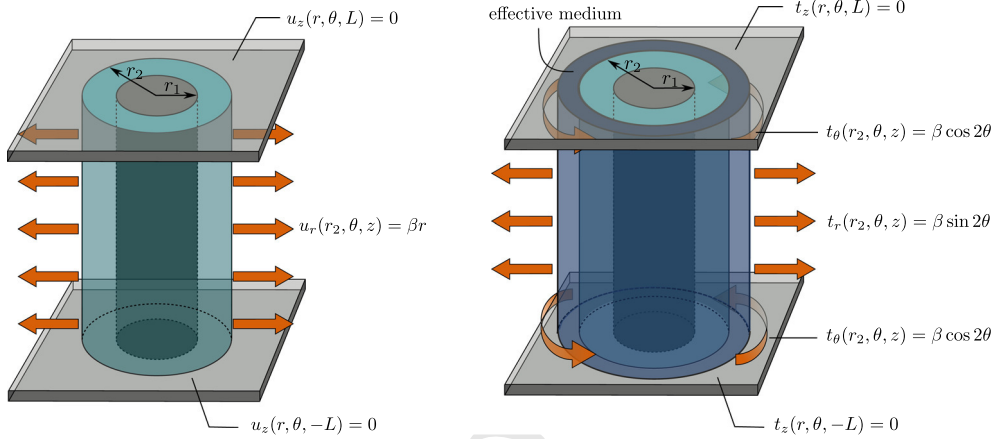
$$\mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta r \\ 0 \\ 0 \end{bmatrix}. \quad (20)$$

189 Hashin and Rosen showed that the displacement field within each constituent reads

$$u_r^{(i)} = \beta \Xi_1^{(i)} r + \beta \Xi_2^{(i)} \frac{1}{r} \quad \text{and} \quad u_\theta^{(i)} = u_z^{(i)} = 0, \quad (21)$$

191 for  $i = 1, 2$  where  $i = 1$  corresponds to the fiber and  $i = 2$  corresponds to the matrix. The unknowns  $\Xi_1^{(1)}$ ,  
192  $\Xi_1^{(2)}$ ,  $\Xi_2^{(1)}$  and  $\Xi_2^{(2)}$  can be calculated using the boundary and interface conditions

$$\begin{aligned}
 u_r^{(1)} \text{ finite at } r = 0 &\rightarrow \Xi_2^{(1)} = 0, && \text{(finite displacement at } r = 0) \\
 \bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket &\rightarrow \frac{\sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1)}{2} = \bar{k} \left[ u_r^{(2)}(r_1) - u_r^{(1)}(r_1) \right], && \text{(traction average at } r = r_1) \\
 \llbracket \text{div } \bar{\sigma} \rrbracket_r + \llbracket t_r \rrbracket = 0 &\rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, && \text{(traction equilibrium at } r = r_1) \\
 u_r^{(2)}(r_2) &= \beta r_2, && \text{(prescribed displacement at } r = r_2)
 \end{aligned} \quad (22)$$



**Fig. 5** Boundary value problems for obtaining the macroscopic bulk modulus (left) and the macroscopic shear modulus (right) developed in [65]

194 leading to the system

$$195 \begin{bmatrix} 0 & 1 & \frac{1}{r_2^2} \\ -\lambda_1 - \mu_1 - \frac{\bar{\mu}}{2r_1} & \lambda_2 + \mu_2 - \frac{\bar{\mu}}{2r_1} & -\frac{2\mu_2 r_1 + \bar{\mu}}{2r_1^3} \\ \frac{\lambda_1 + \mu_1}{\bar{k}} + r_1 & \frac{\lambda_2 + \mu_2}{\bar{k}} - r_1 & -\frac{\mu_2 + \bar{k}r_1}{\bar{k}r_1^2} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}. \quad (23)$$

196 If the RVE is substituted by an equivalent homogeneous medium, applying the boundary condition (20) yields  
 197 the displacement field  $u_r^{\text{eq}} = \beta r$  and  $u_\theta^{\text{eq}} = u_z^{\text{eq}} = 0$ . Using Eq. (19), the overall energy in the RVE and in the  
 198 equivalent homogeneous medium reads

$$199 U^{\text{RVE}} = 2\beta^2 \left[ \Xi_1^{(2)} [\lambda_2 + \mu_2] - \frac{\Xi_2^{(2)} \mu_2}{r_2^2} \right] \quad \text{and} \quad U^{\text{eq}} = 2\beta^2 M_k, \quad (24)$$

200 where  $\Xi_1^{(2)}$  and  $\Xi_2^{(2)}$  are the solutions of the system (23). The above energies should be equal according to  
 201 Hill–Mandel condition. Therefore, we can obtain an explicit expression for the overall bulk modulus  $M_k$  of  
 202 fiber composites embedding general interfaces

$$203 M_k = \lambda_2 + \mu_2 + \frac{f}{1 + \frac{1-f}{\lambda_2 + 2\mu_2} \frac{[2r_1\lambda_1 + 2r_1\mu_1 + \bar{\mu}][2\bar{k}r_1^2 - \bar{\mu}]}{4r_1^2[2\lambda_1 + 2\mu_1 + \bar{k}r_1] + 2r_1\bar{\mu}} - [\lambda_2 + \mu_2] + \frac{\bar{\mu}}{2r_1}}}. \quad (25)$$

### 204 3.2.2 Effective shear modulus

205 In order to determine the effective shear modulus of fiber composites, Christensen and Lo [106] proposed to  
 206 consider an infinite effective medium surrounding the matrix whose properties are indeed, the unknowns of the  
 207 problem. Therefore, the composite cylinder assemblage approach is transformed to generalized self-consistent  
 208 method (GSCM). To obtain the effective shear modulus, the deviatoric traction is applied to the RVE as depicted  
 209 in Fig. 5 (right). The traction field in cylindrical coordinates reads

$$210 \mathbf{t}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta \sin 2\theta \\ \beta \cos 2\theta \\ 0 \end{bmatrix}. \quad (26)$$

211 Considering the above boundary value problem and following the procedures in [106], the developed displace-  
212 ment fields in the medium read

$$\begin{aligned}
 u_r^{(i)} &= \sum_{j=1}^4 a_j^{(i)} \Xi_j^{(i)} r^{n_j^{(i)}} \sin(2\theta), & u_\theta^{(i)} &= \sum_{j=1}^4 \Xi_j^{(i)} r^{n_j^{(i)}} \cos(2\theta), \\
 u_r^{(\text{eff})} &= \beta \frac{r_2}{4M\mu} \left[ \frac{2r}{r_2} + \Xi_3^{(\text{eff})} \frac{r_2^3}{r^3} + 2 \left[ 1 + \frac{M\mu}{M_k} \right] \Xi_4^{(\text{eff})} \frac{r_2}{r} \right] \sin(2\theta), \\
 u_\theta^{(\text{eff})} &= \beta \frac{r_2}{4M\mu} \left[ \frac{2r}{r_2} - \Xi_3^{(\text{eff})} \frac{r_2^3}{r^3} + 2 \frac{M\mu}{M_k} \Xi_4^{(\text{eff})} \frac{r_2}{r} \right] \cos(2\theta),
 \end{aligned} \tag{27}$$

214 for  $i = 1, 2$  where  $i = 1$  corresponds to the fiber and  $i = 2$  corresponds to the matrix. The constants  $a_j^{(i)}$  read

$$a_j^{(i)} = \frac{2\lambda^{(i)} + 6\mu^{(i)} - 2n_j^{(i)}[\lambda^{(i)} + \mu^{(i)}]}{\lambda^{(i)} + 6\mu^{(i)} + [n_j^{(i)}]^2[\lambda^{(i)} + 2\mu^{(i)}]}, \tag{28}$$

216 with  $n_j^{(i)}$  being the solutions of the polynomial  $n^4 - 10n^2 + 9 = 0$ . The constants  $n_1^{(i)}$  and  $n_2^{(i)}$  are taken to be the  
217 positive solutions, and  $n_3^{(i)}$  and  $n_4^{(i)}$  are taken to be the negative solutions as  $n_1^{(i)} = 3, n_2^{(i)} = 1, n_3^{(i)} = -3$  and  
218  $n_4^{(i)} = -1$ . The ten unknowns  $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_3^{(1)}, \Xi_4^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}, \Xi_3^{(2)}, \Xi_4^{(2)}, \Xi_3^{(\text{eff})}$  and  $\Xi_4^{(\text{eff})}$  can be determined  
219 via applying the interface and boundary conditions. The boundary and interface conditions that hold for the  
220 RVE in this problem are

$$\begin{aligned}
 u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 &\rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, && \text{(finite displacement at } r = 0) \\
 \bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket &\rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r \left[ u_r^{(2)}(r_1) - u_r^{(1)}(r_1) \right], && \text{(traction average at } r = r_1) \\
 \bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket &\rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta \left[ u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1) \right], && \text{(traction average at } r = r_1) \\
 \overline{[\text{div } \bar{\sigma}]}_r + \llbracket t_r \rrbracket = 0 &\rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, && \text{(traction equilibrium at } r = r_1) \tag{29} \\
 \overline{[\text{div } \bar{\sigma}]}_\theta + \llbracket t_\theta \rrbracket = 0 &\rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, && \text{(traction equilibrium at } r = r_1) \\
 \sigma_{rr}^{(2)}(r_2) = \sigma_{rr}^{(\text{eff})}(r_2) &\text{ and } \sigma_{r\theta}^{(2)}(r_2) = \sigma_{r\theta}^{(\text{eff})}(r_2), && \text{(traction continuity at } r = r_2) \\
 u_r^{(2)}(r_2) = u_r^{(\text{eff})}(r_2) &\text{ and } u_\theta^{(2)}(r_2) = u_\theta^{(\text{eff})}(r_2). && \text{(displacement continuity at } r = r_2).
 \end{aligned}$$

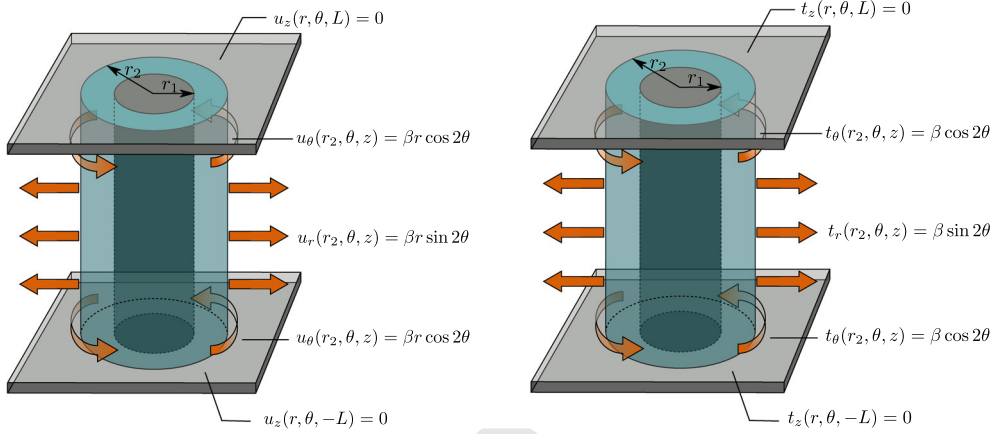
222 In order to find the unknowns using the above system of equations, an additional energetic criterion expressed  
223 in [106] must be imposed which is deduced from the Eshelby's energy principle

$$\int_0^{2\pi} \left[ \sigma_{rr}^{(\text{eff})} u_r^{\text{eq}} + \sigma_{r\theta}^{(\text{eff})} u_\theta^{\text{eq}} - \sigma_{rr}^{\text{eq}} u_r^{(\text{eff})} - \sigma_{r\theta}^{\text{eq}} u_\theta^{(\text{eff})} \right]_{r=r_2} d\theta = 0, \tag{30}$$

225 which yields  $\Xi_4^{(\text{eff})} = 0$ . The remaining unknowns are calculated by solving the system (29). Further details  
226 regarding the solution of the system are available in Appendix A.1. Unlike the effective bulk modulus, it is  
227 not possible to furnish an explicit expression for the effective shear modulus. Nevertheless, a semi-explicit  
228 expression is attainable which reads

$$[a_6 b_5 - a_5 b_6]^M \mu^2 - [b_5 c_5 - b_6 c_5 + a_5 c_6 + a_6 c_6]^M \mu + 2c_5 c_6 = 0.$$

230 Between the two roots obtained from the above relation, the positive one is the effective shear modulus. The  
231 parameters  $a_5, a_6, b_5, b_6, c_5$  and  $c_6$  are obtained from Eq. (A.5), see Appendix A.1 for more details.



**Fig. 6** Boundary value problems for obtaining bounds on the macroscopic shear modulus of a fiber composite. Strain boundary condition (left) and stress boundary condition (right)

### 3.2.3 Strain bound on the shear modulus

To obtain the strain bound on the overall in-plane shear modulus, shear displacement is applied on the boundary of the RVE as shown in Fig. 6 (left) which reads

$$\mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta r \sin 2\theta \\ \beta r \cos 2\theta \\ 0 \end{bmatrix}. \quad (31)$$

Similar to the previous case, the developed displacement fields in the medium result in the analytical form

$$u_r^{(i)} = \sum_{j=1}^4 a_j^{(i)} \Xi_j^{(i)} r^{n_j^{(i)}} \sin(2\theta), \quad u_\theta^{(i)} = \sum_{j=1}^4 \Xi_j^{(i)} r^{n_j^{(i)}} \cos(2\theta), \quad (32)$$

where the superscripts  $i = 1, 2$  correspond to the fiber and matrix, respectively. The constants  $a_j^{(i)}$  are obtained similar to Eq. (28).

The eight unknowns  $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_3^{(1)}, \Xi_4^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}, \Xi_3^{(2)}$  and  $\Xi_4^{(2)}$  can be determined via applying the boundary and interface conditions which read

$$\begin{aligned} u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 &\rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, && \text{(finite displacement at } r = 0) \\ \bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket &\rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r \left[ u_r^{(2)}(r_1) - u_r^{(1)}(r_1) \right], && \text{(traction average at } r = r_1) \\ \bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket &\rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta \left[ u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1) \right], && \text{(traction average at } r = r_1) \\ \llbracket \text{div } \bar{\sigma} \rrbracket_r + \llbracket t_r \rrbracket = 0 &\rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, && \text{(traction equilibrium at } r = r_1) \\ \llbracket \text{div } \bar{\sigma} \rrbracket_\theta + \llbracket t_\theta \rrbracket = 0 &\rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, && \text{(traction equilibrium at } r = r_1) \\ u_r^{(2)}(r_2) = \beta r_2 \sin(2\theta) \quad \text{and} \quad u_\theta^{(2)}(r_2) = \beta r_2 \cos(2\theta). &&& \text{(boundary condition at } r = r_2). \end{aligned} \quad (33)$$

Further details regarding the construction of the system of equations are available in Appendix A.2. For an equivalent homogeneous medium with the same boundary conditions, the displacement field reads  $u_r^{\text{cd}}(r) = \beta r \sin(2\theta)$  and  $u_\theta^{\text{cd}}(r) = \beta r \cos(2\theta)$ . Having the stress and displacement fields, using Eq. (19), one can

246 calculate the average mechanical energy in the RVE and in the equivalent homogeneous medium

$$247 \quad U^{\text{RVE}} = \frac{\beta^2}{2} \left[ \frac{6\mu_2[\lambda_2 + \mu_2]r_2^2}{2\lambda_2 + 3\mu_2} \Xi_1^{(2)} + 4\mu_2 \Xi_2^{(2)} - \frac{2[\lambda_2 + \mu_2]}{r_2^2} \Xi_4^{(2)} \right], \quad (34)$$

$$248 \quad U^{\text{eq}} = 2\beta^2 M \mu.$$

248 Considering  $U^{\text{RVE}} = U^{\text{eq}}$  results in a semi-explicit expression for the strain bound on the effective in-plane  
249 shear modulus

$$250 \quad M \mu_{\text{strain}} = \frac{1}{4} \left[ \frac{6\mu_2[\lambda_2 + \mu_2]r_2^2}{2\lambda_2 + 3\mu_2} \Xi_1^{(2)} + 4\mu_2 \Xi_2^{(2)} - \frac{2[\lambda_2 + \mu_2]}{r_2^2} \Xi_4^{(2)} \right]. \quad (35)$$

251 where  $\Xi_1^{(2)}$ ,  $\Xi_2^{(2)}$ ,  $\Xi_3^{(2)}$  and  $\Xi_4^{(2)}$  are the solution of the system of equations (A.6).

### 252 3.2.4 Stress bound on the shear modulus

253 Following the same methodology for the boundary value problem of Fig. 6 (right), the stress bound on the  
254 macroscopic in-plane shear modulus can be obtained. Consider an RVE subject to the traction field

$$255 \quad \mathbf{t}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta \sin 2\theta \\ \beta \cos 2\theta \\ 0 \end{bmatrix}. \quad (36)$$

256 The displacement fields in the constituents due to this boundary conditions are similar to Eq. (32). The eight  
257 unknowns  $\Xi_1^{(1)}$ ,  $\Xi_2^{(1)}$ ,  $\Xi_3^{(1)}$ ,  $\Xi_4^{(1)}$ ,  $\Xi_1^{(2)}$ ,  $\Xi_2^{(2)}$ ,  $\Xi_3^{(2)}$  and  $\Xi_4^{(2)}$  can be determined via applying the boundary and  
258 interface conditions which read

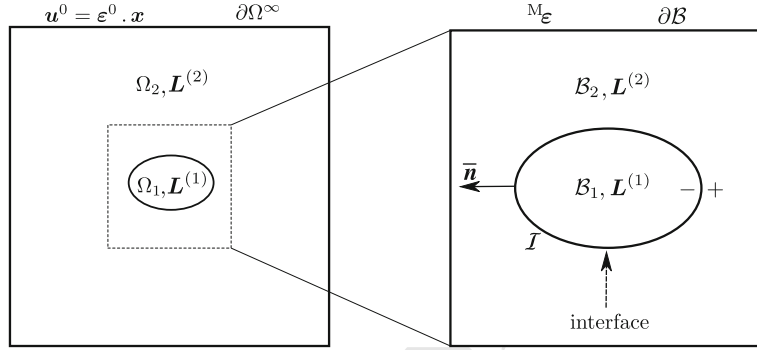
$$259 \quad \begin{aligned} u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 &\rightarrow \Xi_3^{(1)} = \Xi_4^{(1)} = 0, && \text{(finite displacement at } r = 0) \\ \bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket &\rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r \left[ u_r^{(2)}(r_1) - u_r^{(1)}(r_1) \right], && \text{(traction average at } r = r_1) \\ \bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket &\rightarrow \sigma_{r\theta}^{(2)}(r_1) + \sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta \left[ u_\theta^{(2)}(r_1) - u_\theta^{(1)}(r_1) \right], && \text{(traction average at } r = r_1) \\ \llbracket \text{div } \bar{\sigma} \rrbracket_r + \llbracket t_r \rrbracket = 0 &\rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, && \text{(traction equilibrium at } r = r_1) \\ \llbracket \text{div } \bar{\sigma} \rrbracket_\theta + \llbracket t_\theta \rrbracket = 0 &\rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}}{\partial \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0, && \text{(traction equilibrium at } r = r_1) \\ \sigma_{rr}^{(2)}(r_2) = \beta \sin(2\theta) \quad \text{and} \quad \sigma_{r\theta}^{(2)}(r_2) = \beta \cos(2\theta). &&& \text{(boundary condition at } r = r_2). \end{aligned} \quad (37)$$

260 Further details regarding the construction of the system of equations are available in Appendix A.3. For an  
261 equivalent homogeneous medium with the same boundary conditions, the displacement field reads

$$262 \quad u_r^{\text{eq}}(r) = \frac{\beta}{2M\mu} r \sin(2\theta), \quad u_\theta^{\text{eq}}(r) = \frac{\beta}{2M\mu} r \cos(2\theta), \quad u_z^{\text{eq}}(r) = 0. \quad (38)$$

263 Using Eq. (19), the same strategy can be employed to define the energy stored in the RVE and the equivalent  
264 homogeneous medium.

$$265 \quad \begin{aligned} U^{\text{RVE}} &= \frac{\beta^2}{2} \left[ \frac{3[\lambda_2 + \mu_2]r_2^2}{2\lambda_2 + 3\mu_2} \Xi_1^{(2)} + 2\Xi_2^{(2)} + \frac{\lambda_2 + 3\mu_2}{\mu_2 r_2^2} \Xi_4^{(2)} \right], && (39) \\ U^{\text{eq}} &= \frac{\beta^2}{2M\mu}. \end{aligned}$$



**Fig. 7** Illustration of inhomogeneity with general interface inside an infinite matrix (left) and RVE of fiber composite with general interface (right)

266 Considering  $U^{\text{RVE}} = U^{\text{eq}}$  results in a semi-explicit expression for the stress bound on the effective in-plane  
 267 shear modulus

$$268 \quad M_{\mu_{\text{stress}}} = \left[ \frac{3[\lambda_2 + \mu_2]r_2^2}{2\lambda_2 + 3\mu_2} \Xi_1^{(2)} + 2\Xi_2^{(2)} + \frac{\lambda_2 + 3\mu_2}{\mu_2 r_2^2} \Xi_4^{(2)} \right]^{-1}. \quad (40)$$

269 where  $\Xi_1^{(2)}$ ,  $\Xi_2^{(2)}$ ,  $\Xi_3^{(2)}$  and  $\Xi_4^{(2)}$  are the solution of the system of equations (A.7).

### 270 3.3 Modified Mori–Tanaka method

271 Analytical estimates for the effective properties of fiber composites with general interfaces have been developed  
 272 in [65]. Using energy principles, Duan et al. [108] proposed to substitute the fiber/interface system with  
 273 an equivalent fiber to predict the overall behavior of the medium. Both methodologies provide reasonable  
 274 estimates compared to full field homogenization strategies, like the periodic homogenization framework, but  
 275 they cannot provide information about the local fields that are developed in various phases of the medium,  
 276 including the interface. *Our new methodology here not only obtains the effective properties, but also defines*  
 277 *the concentration tensors in each phase.* The primary advantage of the concentration tensors is that they  
 278 link the macroscopic fields with the average fields in the matrix, fiber and interface hence, furnishing better  
 279 insights into the microstructural response of composites. For composites with interfaces, the main idea is to  
 280 identify the global interaction tensors for the fiber/interface system by solving the Eshelby’s inhomogeneity  
 281 problem [109]. Such investigation is motivated by similar techniques in the literature for coated particles or  
 282 fibers [98, 110–112]. Note the Mori–Tanaka estimates can lose major symmetry and thus results in physically  
 283 meaningless estimates. However, the loss of symmetry in the Mori–Tanaka estimates appears in composites  
 284 with different shapes of fibers, or fibers of the same shape but different orientation (non-uniform orientation  
 285 distribution function). For aligned long fiber composites, it has been shown analytically that Mori–Tanaka  
 286 continues to produce effective properties that respect the major symmetry [113]. This limitation of the Mori–  
 287 Tanaka estimates holds regardless of interfaces.

#### 288 3.3.1 General framework

289 Figure 7 (left) illustrates an inhomogeneity with general ellipsoidal shape occupying the space  $\Omega_1$  with elasticity  
 290 modulus  $\mathbf{L}^{(1)}$  surrounded by a general interface  $\mathcal{I}$ . An infinite matrix occupying the space  $\Omega_2$  with elasticity  
 291 tensor  $\mathbf{L}^{(2)}$  is embedding the inhomogeneity/interface system. The matrix is subjected to a far field linear  
 292 displacement condition  $\mathbf{u}^0 = \boldsymbol{\varepsilon}^0 \cdot \mathbf{x}$ . The equilibrium equations throughout the medium are given in Eq. (4)  
 293 and further detailed in [65].

294 In this contribution, similar to [108] we propose to treat the fiber/interface system as a unique phase, but  
 295 instead of identifying the response, we identify a strain interaction tensor  $\mathbf{T}$  and a stress–strain interaction  
 296 tensor  $\mathbf{H}$  as

$$297 \quad \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+ = \mathbf{T} : \boldsymbol{\varepsilon}^0 = \frac{1}{2|\Omega_1|} \int_{\mathcal{I}} [\mathbf{u}^+ \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes \mathbf{u}^+] dA \quad \text{and}$$

$$\langle \boldsymbol{\sigma} \rangle_{\Omega_1}^+ = \mathbf{H} : \boldsymbol{\varepsilon}^0 = \frac{1}{|\Omega_1|} \int_{\Omega_1} \boldsymbol{\sigma}^- dV + \frac{1}{|\Omega_1|} \int_{\mathcal{I}} \bar{\boldsymbol{\sigma}} dA. \quad (41)$$

In addition, one can identify the pure fiber's concentration tensor as

$$\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^- = \mathbf{T}^{(1)} : \boldsymbol{\varepsilon}^0 = \frac{1}{2|\Omega_1|} \int_{\mathcal{I}} [\mathbf{u}^- \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes \mathbf{u}^-] dA. \quad (42)$$

More precisely,  $\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^-$  corresponds to the strain field in the fiber itself, whereas  $\langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+$  corresponds to the strain field in the fiber/interface system. This case study is an extension of the Eshelby's inhomogeneity problem, and the tensors  $\mathbf{T}$  and  $\mathbf{H}$  are extremely useful to develop the mean-field theories for composites [98]. Consider a RVE of fiber composite with the volume of  $\mathcal{V}$  and the boundary of  $\partial\mathcal{B}$  occupying the space  $\mathcal{B}$  shown in Fig. 7 (right). The RVE is subjected to a macroscopic strain  ${}^M\boldsymbol{\varepsilon}$ . The fiber with the volume of  $\mathcal{V}_1$  occupies the space  $\mathcal{B}_1$ , and the matrix with the volume of  $\mathcal{V}_2$  occupies the space  $\mathcal{B}_2$ . Obviously,  $\mathcal{B} = \mathcal{B}_1 \cup \mathcal{B}_2$  and  $\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2$ . The fiber volume fraction is  $f = \mathcal{V}_1/\mathcal{V}$ , and accordingly, Eq. (7) can be rewritten as

$$\begin{aligned} {}^M\boldsymbol{\varepsilon} &= \frac{1}{\mathcal{V}} \int_{\mathcal{B}} \boldsymbol{\varepsilon} dV + \frac{1}{2\mathcal{V}} \int_{\mathcal{I}} [[\mathbf{u}] \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes [\mathbf{u}]] dA = [1-f]\boldsymbol{\varepsilon}^{(2)} + f\boldsymbol{\varepsilon}^{(1)} + \hat{\boldsymbol{\varepsilon}}, \\ {}^M\boldsymbol{\sigma} &= \frac{1}{\mathcal{V}} \int_{\mathcal{B}} \boldsymbol{\sigma} dV + \frac{1}{\mathcal{V}} \int_{\mathcal{I}} \bar{\boldsymbol{\sigma}} dA = [1-f]\mathbf{L}^{(2)} : \boldsymbol{\varepsilon}^{(2)} + f\mathbf{L}^{(1)} : \boldsymbol{\varepsilon}^{(1)} + \hat{\boldsymbol{\sigma}}, \end{aligned} \quad (43)$$

in which

$$\boldsymbol{\varepsilon}^{(1)} = \frac{1}{\mathcal{V}_1} \int_{\mathcal{B}_1} \boldsymbol{\varepsilon} dV, \quad \boldsymbol{\varepsilon}^{(2)} = \frac{1}{\mathcal{V}_2} \int_{\mathcal{B}_2} \boldsymbol{\varepsilon} dV \quad \text{and} \quad \hat{\boldsymbol{\varepsilon}} = \frac{1}{2\mathcal{V}} \int_{\mathcal{I}} [[\mathbf{u}] \otimes \bar{\mathbf{n}} + \bar{\mathbf{n}} \otimes [\mathbf{u}]] dA, \quad (44)$$

are the average strains in the fiber, matrix and interface, respectively. The average stress on the interface reads

$$\hat{\boldsymbol{\sigma}} = \frac{1}{\mathcal{V}} \int_{\mathcal{I}} \bar{\boldsymbol{\sigma}} dA. \quad (45)$$

Exploiting the interaction tensors (41) and (42), the Mori–Tanaka scheme reads

$$\boldsymbol{\varepsilon}^{(1)} = \mathbf{T}^{(1)} : \boldsymbol{\varepsilon}^{(2)}, \quad \boldsymbol{\varepsilon}^{(1)} + \frac{1}{f}\hat{\boldsymbol{\varepsilon}} = \mathbf{T} : \boldsymbol{\varepsilon}^{(2)}, \quad \mathbf{L}^{(1)} : \boldsymbol{\varepsilon}^{(1)} + \frac{1}{f}\hat{\boldsymbol{\sigma}} = \mathbf{H} : \boldsymbol{\varepsilon}^{(2)}. \quad (46)$$

Thus, Eq. (43)<sub>1</sub> yields

$${}^M\boldsymbol{\varepsilon} = \left[ [1-f]\mathbb{I} + f\mathbf{T} \right] : \boldsymbol{\varepsilon}^{(2)} \quad \text{or} \quad \boldsymbol{\varepsilon}^{(2)} = \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}, \quad (47)$$

where  $\mathbb{I}$  is the fourth-order identity tensor and  $\mathbf{A}^{(2)} = [[1-f]\mathbb{I} + f\mathbf{T}]^{-1}$ . On the other hand, Eq. (43)<sub>2</sub> yields

$${}^M\boldsymbol{\sigma} = \left[ [1-f]\mathbf{L}^{(2)} + f\mathbf{H} \right] : \boldsymbol{\varepsilon}^{(2)} = \left[ [1-f]\mathbf{L}^{(2)} + f\mathbf{H} \right] : \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}. \quad (48)$$

Thus, the macroscopic stiffness tensor is given by the expression

$${}^M\mathbf{L} = \left[ [1-f]\mathbf{L}^{(2)} + f\mathbf{H} \right] : \mathbf{A}^{(2)}. \quad (49)$$

The properties of the equivalent fiber employed in [66] can be recovered according to

$$\mathbf{L}^{\text{eq}} = \mathbf{H} : \mathbf{T}^{-1}. \quad (50)$$

The macroscopic elasticity tensors obtained by our proposed method are formally identical to those given in [108]. The conceptual difference is that instead of seeking the properties of the equivalent fiber, the target is to identify the global strain and stress tensors of the fiber/interface system. For a given macroscopic strain  ${}^M\boldsymbol{\varepsilon}$ , the average strain and stress in the fiber and matrix read

$$\begin{aligned} \boldsymbol{\varepsilon}^{(1)} &= \mathbf{T}^{(1)} : \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}, & \boldsymbol{\sigma}^{(1)} &= \mathbf{L}^{(1)} : \boldsymbol{\varepsilon}^{(1)} = \mathbf{L}^{(1)} : \mathbf{T}^{(1)} : \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}, \\ \boldsymbol{\varepsilon}^{(2)} &= \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}, & \boldsymbol{\sigma}^{(2)} &= \mathbf{L}^{(2)} : \boldsymbol{\varepsilon}^{(2)} = \mathbf{L}^{(2)} : \mathbf{A}^{(2)} : {}^M\boldsymbol{\varepsilon}. \end{aligned} \quad (51)$$

329 Using Eq. (46), the average strain and stress on the interface read

$$330 \quad \widehat{\boldsymbol{\varepsilon}} = f \left[ \mathbf{T} - \mathbf{T}^{(1)} \right] : \mathbf{A}^{(2)} : \mathbf{M} \boldsymbol{\varepsilon}, \quad \widehat{\boldsymbol{\sigma}} = f \left[ \mathbf{H} - \mathbf{L}^{(1)} : \mathbf{T}^{(1)} \right] : \mathbf{A}^{(2)} : \mathbf{M} \boldsymbol{\varepsilon}. \quad (52)$$

331 So far, the only missing parts to complete the homogenization framework are the interaction tensors  $\mathbf{T}$ ,  $\mathbf{H}$  and  
 332  $\mathbf{T}^{(1)}$ . To this end, the extended Eshelby's problem is solved analytically for three boundary value problems  
 333 similar to those described by Hashin [114] in the composite cylinders assemblage approach. In fiber composites  
 334 with isotropic or transversely isotropic phases, the strain and stress–strain interaction tensors present transverse  
 335 isotropy. In Voigt notation, they take the forms

$$336 \quad \mathbf{T} = \begin{bmatrix} T_{11} & T_{11} - T_{44} & T_{13} & 0 & 0 & 0 \\ T_{11} - T_{44} & T_{11} & T_{13} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & T_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & T_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & T_{55} \end{bmatrix},$$

$$337 \quad \mathbf{H} = \begin{bmatrix} H_{11} & H_{11} - 2H_{44} & H_{13} & 0 & 0 & 0 \\ H_{11} - 2H_{44} & H_{11} & H_{13} & 0 & 0 & 0 \\ H_{31} & H_{31} & H_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & H_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & H_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & H_{55} \end{bmatrix}, \quad (53)$$

338 see [112] for more details on  $\mathbf{T}$ . Note that  $\mathbf{T}^{(1)}$  has similar structure with  $\mathbf{T}$ . Using this general representation,  
 339 the three boundary value problems to identify the interaction tensors will be introduced.

340 *3.3.1.1 Axial shear conditions* For this case, the far field displacement and strain fields applied to the RVE in  
 341 cylindrical coordinates read

$$342 \quad \mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} 0 \\ 0 \\ \beta r \cos \theta \end{bmatrix}, \quad \boldsymbol{\varepsilon}_{(r,\theta,z)}^0 = \begin{bmatrix} 0 & 0 & \frac{\beta}{2} \cos \theta \\ 0 & 0 & -\frac{\beta}{2} \sin \theta \\ \frac{\beta}{2} \cos \theta & -\frac{\beta}{2} \sin \theta & 0 \end{bmatrix}. \quad (54)$$

343 For these boundary conditions, the important displacements and stresses in the matrix, fiber and interface are  
 344 given by

$$345 \quad u_z^{(i)}(r, \theta) = \beta r U_z^{(i)}(r) \cos \theta \quad \text{with} \quad U_z^{(i)}(r) = \Xi_1^{(i)} + \Xi_2^{(i)} \frac{1}{[r/r_1]^2},$$

$$\sigma_{rz}^{(i)}(r, \theta) = \beta \Sigma_{rz}^{(i)}(r) \cos \theta \quad \text{with} \quad \Sigma_{rz}^{(i)}(r) = \mu_{\text{ax}}^{(i)} \left[ \Xi_1^{(i)} - \Xi_2^{(i)} \frac{1}{[r/r_1]^2} \right], \quad (55)$$

$$\bar{\sigma}_{\theta z}(\theta) = \beta \bar{\Sigma}_{\theta z} \sin \theta \quad \text{with} \quad \bar{\Sigma}_{\theta z} = -\frac{\bar{\mu}_{\text{ax}}}{2} \left[ \Xi_1^{(1)} + \Xi_1^{(2)} + \Xi_2^{(1)} + \Xi_2^{(2)} \right],$$

346 for  $i = 1, 2$  where  $i = 1$  corresponds to the fiber and  $i = 2$  corresponds to the matrix. The unknowns that  
 347 need to be defined are  $\Xi_1^{(1)}$ ,  $\Xi_2^{(1)}$ ,  $\Xi_1^{(2)}$  and  $\Xi_2^{(2)}$ . The boundary and interface conditions lead to the following  
 348 equations

$$349 \quad \begin{aligned} u_z^{(1)} \text{ finite at } r = 0 & \quad \rightarrow \Xi_2^{(1)} = 0, \\ \bar{t}_z = \bar{k}_z \llbracket u_z \rrbracket & \quad \rightarrow \Sigma_{rz}^{(2)}(r_1) + \Sigma_{rz}^{(1)}(r_1) = 2\bar{k}_z r_1 \left[ U_z^{(2)}(r_1) - U_z^{(1)}(r_1) \right], \\ \llbracket \text{div } \bar{\boldsymbol{\sigma}} \rrbracket_z + \llbracket t_z \rrbracket = 0 & \quad \rightarrow \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta z}(\theta)}{\partial \theta} + \sigma_{rz}^{(2)}(r_1) - \sigma_{rz}^{(1)}(r_1) = 0 \rightarrow \frac{\bar{\Sigma}_{\theta z}}{r_1} + \Sigma_{rz}^{(2)}(r_1) - \Sigma_{rz}^{(1)}(r_1) = 0, \\ u_z^{(2)}(r \rightarrow \infty) = \beta r \cos \theta & \quad \rightarrow \Xi_1^{(2)} = 1. \end{aligned} \quad (56)$$

350 Solving the above linear system, the average strain and stress in the fiber/interface system read

$$351 \quad \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^- = U_z^{(1)}(r_1) \boldsymbol{\varepsilon}^0, \quad \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+ = U_z^{(2)}(r_1) \boldsymbol{\varepsilon}^0, \quad \langle \boldsymbol{\sigma} \rangle_{\Omega_1}^+ = \Sigma_{r_z}^{(2)}(r_1) \boldsymbol{\varepsilon}^0. \quad (57)$$

352 Since  $\mathbf{H}$  is a stress-type tensor and the applied shear angle is  $\beta$ , the term  $H_{55}$  must be equal to the generated  
353 stress on the fiber/interface system. Consequently, the axial shear interaction terms are

$$354 \quad T_{55}^{(1)} = \Xi_1^{(1)}, \quad T_{55} = 1 + \Xi_2^{(2)}, \quad H_{55} = \mu_{\text{ax}}^{(2)} \left[ 1 - \Xi_2^{(2)} \right]. \quad (58)$$

355 *3.3.1.2 Transverse shear conditions* For this case, the far field displacement and strain fields applied to the RVE  
356 in the cylindrical coordinates read

$$357 \quad \mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta r \sin 2\theta \\ \beta r \cos 2\theta \\ 0 \end{bmatrix}, \quad \boldsymbol{\varepsilon}_{(r,\theta,z)}^0 = \begin{bmatrix} \beta \sin 2\theta & \beta \cos 2\theta & 0 \\ \beta \cos 2\theta & -\beta \sin 2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (59)$$

358 For these boundary conditions, the important displacements and stresses at each phase are given by the general  
359 expressions

$$\begin{aligned} u_r^{(i)}(r, \theta) &= \beta r U_r^{(i)}(r) \sin 2\theta & \text{with } U_r^{(i)}(r) &= \frac{\kappa_{\text{tr}}^{(i)} - \mu_{\text{tr}}^{(i)}}{2\kappa_{\text{tr}}^{(i)} + \mu_{\text{tr}}^{(i)}} [r/r_1]^2 \Xi_1^{(i)} + \Xi_2^{(i)} \\ &\quad - \frac{1}{[r/r_1]^4} \Xi_3^{(i)} + \frac{\kappa_{\text{tr}}^{(i)} + \mu_{\text{tr}}^{(i)}}{\mu_{\text{tr}}^{(i)}} \frac{1}{[r/r_1]^2} \Xi_4^{(i)}, \\ u_\theta^{(i)}(r, \theta) &= \beta r U_\theta^{(i)}(r) \cos 2\theta & \text{with } U_\theta^{(i)}(r) &= [r/r_1]^2 \Xi_1^{(i)} + \Xi_2^{(i)} + \frac{1}{[r/r_1]^4} \Xi_3^{(i)} + \frac{1}{[r/r_1]^2} \Xi_4^{(i)}, \\ \sigma_{rr}^{(i)}(r, \theta) &= \beta \Sigma_{rr}^{(i)}(r) \sin 2\theta & \text{with } \Sigma_{rr}^{(i)}(r) &= 2\mu_{\text{tr}}^{(i)} \Xi_2^{(i)} + 6\mu_{\text{tr}}^{(i)} \frac{1}{[r/r_1]^4} \Xi_3^{(i)} - 4\kappa_{\text{tr}}^{(i)} \frac{1}{[r/r_1]^2} \Xi_4^{(i)}, \\ \sigma_{r\theta}^{(i)}(r, \theta) &= \beta \Sigma_{r\theta}^{(i)}(r) \cos 2\theta & \text{with } \Sigma_{r\theta}^{(i)}(r) &= \frac{6\kappa_{\text{tr}}^{(i)} \mu_{\text{tr}}^{(i)}}{2\kappa_{\text{tr}}^{(i)} + \mu_{\text{tr}}^{(i)}} [r/r_1]^2 \Xi_1^{(i)} + 2\mu_{\text{tr}}^{(i)} \Xi_2^{(i)} \\ &\quad - 6\mu_{\text{tr}}^{(i)} \frac{1}{[r/r_1]^4} \Xi_3^{(i)} + 2\kappa_{\text{tr}}^{(i)} \frac{1}{[r/r_1]^2} \Xi_4^{(i)}, \\ \bar{u}_r(\theta) &= \beta r_1 \bar{U}_r \sin 2\theta & \text{with } \bar{U}_r &= \frac{U_r^{(1)}(r_1) + U_r^{(2)}(r_1)}{2}, \\ \bar{u}_\theta(\theta) &= \beta r_1 \bar{U}_\theta \cos 2\theta & \text{with } \bar{U}_\theta &= \frac{U_\theta^{(1)}(r_1) + U_\theta^{(2)}(r_1)}{2}, \\ \bar{\sigma}_{\theta\theta}(\theta) &= \beta \bar{\Sigma}_{\theta\theta} \sin 2\theta & \text{with } \bar{\Sigma}_{\theta\theta} &= \bar{m} [\bar{U}_r - 2\bar{U}_\theta], \end{aligned} \quad (60)$$

361 for  $i = 1, 2$  where  $i = 1$  corresponds to the fiber and  $i = 2$  corresponds to the matrix. The unknowns that  
362 need to be defined are  $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_3^{(1)}, \Xi_4^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}, \Xi_3^{(2)}$  and  $\Xi_4^{(2)}$ . The boundary and interface conditions  
363 necessitate the following equations

$$\begin{aligned} u_r^{(1)}, u_\theta^{(1)} \text{ finite at } r = 0 &\quad \rightarrow \quad \Xi_3^{(1)} = \Xi_4^{(1)} = 0, \\ \bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket &\quad \rightarrow \quad \Sigma_{rr}^{(2)}(r_1) + \Sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r r_1 \left[ U_r^{(2)}(r_1) - U_r^{(1)}(r_1) \right], \\ \bar{t}_\theta = \bar{k}_\theta \llbracket u_\theta \rrbracket &\quad \rightarrow \quad \Sigma_{r\theta}^{(2)}(r_1) + \Sigma_{r\theta}^{(1)}(r_1) = 2\bar{k}_\theta r_1 \left[ U_\theta^{(2)}(r_1) - U_\theta^{(1)}(r_1) \right], \\ \llbracket \text{div } \bar{\boldsymbol{\sigma}} \rrbracket_r + \llbracket t_r \rrbracket = 0 &\quad \rightarrow \quad -\frac{\bar{\sigma}_{\theta\theta}(\theta)}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0 \rightarrow -\frac{\bar{\Sigma}_{\theta\theta}}{r_1} + \Sigma_{rr}^{(2)}(r_1) - \Sigma_{rr}^{(1)}(r_1) = 0, \\ \llbracket \text{div } \bar{\boldsymbol{\sigma}} \rrbracket_\theta + \llbracket t_\theta \rrbracket = 0 &\quad \rightarrow \quad \frac{1}{r_1} \frac{\partial \bar{\sigma}_{\theta\theta}(\theta)}{\partial \theta} + \sigma_{r\theta}^{(2)}(r_1) - \sigma_{r\theta}^{(1)}(r_1) = 0 \rightarrow \frac{2\bar{\Sigma}_{\theta\theta}}{r_1} + \Sigma_{r\theta}^{(2)}(r_1) - \Sigma_{r\theta}^{(1)}(r_1) = 0, \\ u_r^{(2)}(r \rightarrow \infty) = \beta r \sin 2\theta \quad \text{and} \quad u_\theta^{(2)}(r \rightarrow \infty) = \beta r \cos 2\theta &\quad \rightarrow \quad \Xi_1^{(2)} = 0 \quad \text{and} \quad \Xi_2^{(2)} = 1. \end{aligned} \quad (61)$$

365

366 Solving the above linear system, the average strain and stress in the fiber/interface system are

$$\begin{aligned}
 \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^- &= \frac{1}{2} \left[ U_r^{(1)}(r_1) + U_\theta^{(1)}(r_1) \right] \boldsymbol{\varepsilon}^0, & \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+ &= \frac{1}{2} \left[ U_r^{(2)}(r_1) + U_\theta^{(2)}(r_1) \right] \boldsymbol{\varepsilon}^0, \\
 \langle \boldsymbol{\sigma} \rangle_{\Omega_1}^+ &= \frac{1}{2} \left[ \Sigma_{rr}^{(2)}(r_1) + \Sigma_{r\theta}^{(2)}(r_1) \right] \boldsymbol{\varepsilon}^0.
 \end{aligned} \tag{62}$$

369 Again, since  $\mathbf{H}$  is a stress-type tensor and the applied shear angle is  $2\beta$ , the term  $H_{44}$  must be equal to the half  
 370 of the generated stress on the fiber/interface system. Consequently, the transverse shear interaction terms are

$$\begin{aligned}
 T_{44}^{(1)} &= \frac{3\kappa_{tr}^{(1)}}{4\kappa_{tr}^{(1)} + 2\mu_{tr}^{(1)}} \Xi_1^{(1)} + \Xi_2^{(1)}, & T_{44} &= 1 + \frac{\kappa_{tr}^{(2)} + 2\mu_{tr}^{(2)}}{2\mu_{tr}^{(2)}} \Xi_4^{(2)}, \\
 H_{44} &= \mu_{tr}^{(2)} - \frac{\kappa_{tr}^{(2)}}{2} \Xi_4^{(2)}.
 \end{aligned} \tag{63}$$

373 *3.3.1.3 Axisymmetric conditions* For this case, the far field displacement and strain fields applied to the RVE in  
 374 the cylindrical coordinates read

$$\mathbf{u}_{(r,\theta,z)}^0 = \begin{bmatrix} e^T r \\ 0 \\ e^A z \end{bmatrix}, \quad \boldsymbol{\varepsilon}_{(r,\theta,z)}^0 = \begin{bmatrix} e^T & 0 & 0 \\ 0 & e^T & 0 \\ 0 & 0 & e^A \end{bmatrix}. \tag{64}$$

376 For these boundary conditions, the important displacements and stresses in the matrix, fiber and the interface  
 377 are given by

$$\begin{aligned}
 u_z^{(i)}(z) &= e^A z, \\
 u_r^{(i)}(r) &= e^T r U_r^{(i)}(r) \quad \text{with } U_r^{(i)}(r) = \left[ \Xi_1^{(i)} + \Xi_2^{(i)} \frac{1}{[r/r_1]^2} \right], \\
 \sigma_{rr}^{(i)}(r) &= e^T \Sigma_{rr}^{(i)}(r) + e^A l^{(i)} \quad \text{with } \Sigma_{rr}^{(i)}(r) = 2\kappa_{tr}^{(i)} \Xi_1^{(i)} - 2\mu_{tr}^{(i)} \Xi_2^{(i)} \frac{1}{[r/r_1]^2}, \\
 \sigma_{zz}^{(i)} &= e^T \Sigma_{zz}^{(i)} + e^A n^{(i)} \quad \text{with } \Sigma_{zz}^{(i)} = 2l^{(i)} \Xi_1^{(i)}, \\
 \bar{\sigma}_{\theta\theta} &= e^T \bar{\Sigma}_{\theta\theta} + e^A \bar{l} \quad \text{with } \bar{\Sigma}_{\theta\theta} = \frac{\bar{m}}{2} \left[ \Xi_1^{(1)} + \Xi_1^{(2)} + \Xi_2^{(1)} + \Xi_2^{(2)} \right], \\
 \bar{\sigma}_{zz} &= e^T \bar{\Sigma}_{zz} + e^A \bar{n} \quad \text{with } \bar{\Sigma}_{zz} = \frac{\bar{l}}{2} \left[ \Xi_1^{(1)} + \Xi_1^{(2)} + \Xi_2^{(1)} + \Xi_2^{(2)} \right],
 \end{aligned} \tag{65}$$

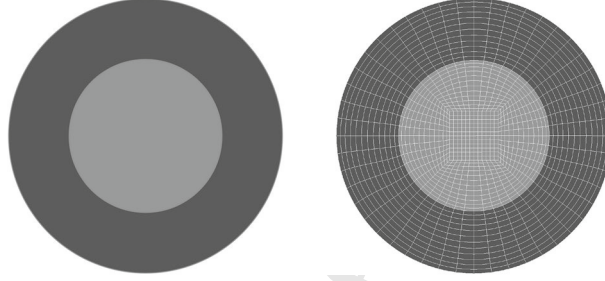
379 for  $i = 1, 2$  where  $i = 1$  corresponds to the fiber and  $i = 2$  corresponds to the matrix. The unknowns that  
 380 need to be defined are  $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_1^{(2)}$  and  $\Xi_2^{(2)}$ . The boundary and interface conditions necessitate

$$\begin{aligned}
 u_r^{(1)} \text{ finite at } r = 0 &\rightarrow \Xi_2^{(1)} = 0, \\
 \bar{t}_r = \bar{k}_r \llbracket u_r \rrbracket &\rightarrow \sigma_{rr}^{(2)}(r_1) + \sigma_{rr}^{(1)}(r_1) = 2\bar{k}_r \left[ u_r^{(2)}(r_1) - u_r^{(1)}(r_1) \right], \\
 \llbracket \text{div } \bar{\boldsymbol{\sigma}} \rrbracket_r + \llbracket t_r \rrbracket = 0 &\rightarrow -\frac{\bar{\sigma}_{\theta\theta}}{r_1} + \sigma_{rr}^{(2)}(r_1) - \sigma_{rr}^{(1)}(r_1) = 0, \\
 u_r^{(2)}(r \rightarrow \infty) = e^T r &\rightarrow \Xi_1^{(2)} = 1.
 \end{aligned} \tag{66}$$

382 Solving the above linear system, the average strain and stress in the fiber/interface system are

$$\begin{aligned}
 \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^- &= \begin{bmatrix} U_r^{(1)}(r_1) e^T & 0 & 0 \\ 0 & U_r^{(1)}(r_1) e^T & 0 \\ 0 & 0 & e^A \end{bmatrix}, & \langle \boldsymbol{\varepsilon} \rangle_{\Omega_1}^+ &= \begin{bmatrix} U_r^{(2)}(r_1) e^T & 0 & 0 \\ 0 & U_r^{(2)}(r_1) e^T & 0 \\ 0 & 0 & e^A \end{bmatrix}, \\
 \langle \boldsymbol{\sigma} \rangle_{\Omega_1}^+ &= \begin{bmatrix} \Sigma_{rr}^{(2)}(r_1) & 0 & 0 \\ 0 & \Sigma_{rr}^{(2)}(r_1) & 0 \\ 0 & 0 & \Sigma_{zz}^{(1)} + \frac{2\bar{\Sigma}_{zz}}{r_1} \end{bmatrix} e^T + \begin{bmatrix} l^{(2)} & 0 & 0 \\ 0 & l^{(2)} & 0 \\ 0 & 0 & n^{(1)} + \frac{2\bar{n}}{r_1} \end{bmatrix} e^A.
 \end{aligned} \tag{67}$$

384 At this stage, two cases are examined:



**Fig. 8** Mesh quality of the RVE for finite element analysis. The domain is discretized using biquadratic Lagrange elements

- 385 •  $e^A = 0$  and  $e^T = 1$ : The constants from the solution of the linear system are denoted as  $\Xi_{11}^{(1)}$  and  $\Xi_{21}^{(2)}$ . For  
386 this condition, the general forms of the dilute concentration tensors in Eq. (53) permit to write

$$387 \begin{aligned} \langle \varepsilon_{xx} \rangle_{\Omega_1}^- &= T_{11}^{(1)} + [T_{11}^{(1)} - T_{44}^{(1)}], & \langle \varepsilon_{xx} \rangle_{\Omega_1}^+ &= T_{11} + [T_{11} - T_{44}], \\ \langle \sigma_{xx} \rangle_{\Omega_1}^+ &= H_{11} + [H_{11} - 2H_{44}], & \langle \sigma_{zz} \rangle_{\Omega_1}^+ &= 2H_{31}. \end{aligned} \quad (68)$$

388 From (67), clearly we have

$$389 \begin{aligned} T_{11}^{(1)} &= \frac{1}{2} [\Xi_{11}^{(1)} + T_{44}^{(1)}], & T_{11} &= \frac{1}{2} [1 + \Xi_{21}^{(2)} + T_{44}], \\ H_{11} &= \kappa_{tr}^{(2)} - \mu_{tr}^{(2)} \Xi_{21}^{(2)} + H_{44}, & H_{31} &= l^{(1)} \Xi_{11}^{(1)} + \frac{\bar{l}}{2r_1} [1 + \Xi_{11}^{(1)} + \Xi_{21}^{(2)}]. \end{aligned} \quad (69)$$

- 390 •  $e^A = e^T = 1$ : The constants from the solution of the linear system are denoted as  $\Xi_{12}^{(1)}$  and  $\Xi_{22}^{(2)}$ . For this  
391 condition, the general forms of the dilute concentration tensors in Eq. (53) permit to write

$$392 \begin{aligned} \langle \varepsilon_{xx} \rangle_{\Omega_1}^- &= T_{11}^{(1)} + [T_{11}^{(1)} - T_{44}^{(1)}] + T_{13}^{(1)}, & \langle \varepsilon_{xx} \rangle_{\Omega_1}^+ &= T_{11} + [T_{11} - T_{44}] + T_{13}, \\ \langle \sigma_{xx} \rangle_{\Omega_1}^+ &= H_{11} + [H_{11} - 2H_{44}] + H_{13}, & \langle \sigma_{zz} \rangle_{\Omega_1}^+ &= 2H_{31} + H_{33}. \end{aligned} \quad (70)$$

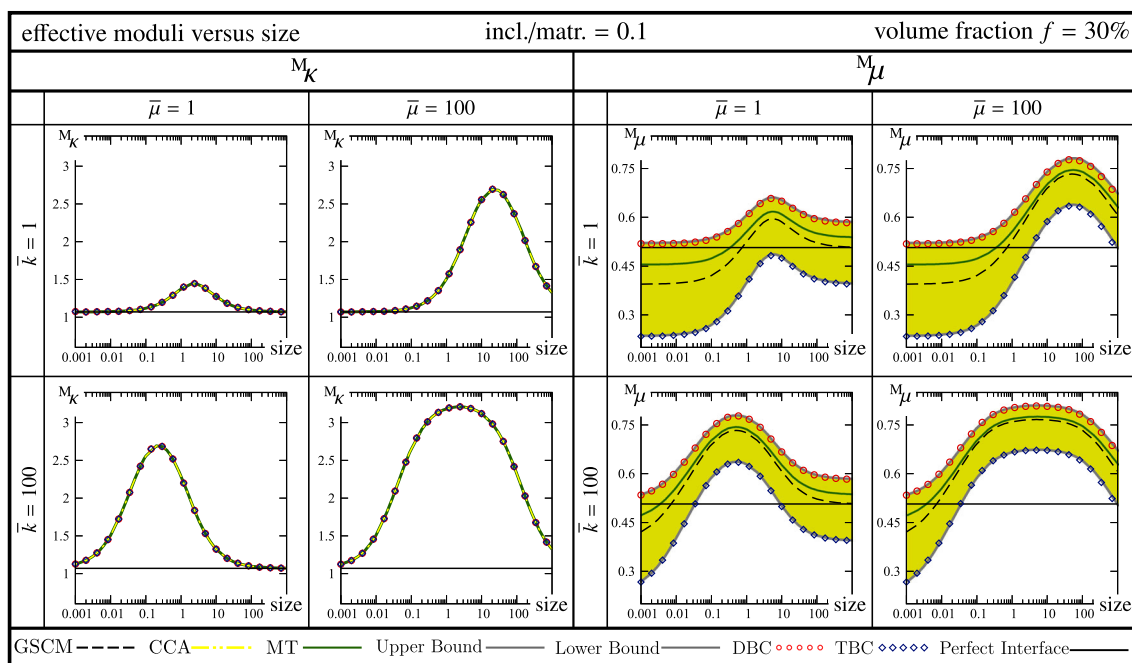
393 Combining the last expression with (67) and (69) yields

$$394 \begin{aligned} T_{13}^{(1)} &= \Xi_{12}^{(1)} + T_{44}^{(1)} - 2T_{11}^{(1)}, \\ T_{13} &= 1 + \Xi_{22}^{(2)} + T_{44} - 2T_{11}, \\ H_{13} &= 2\kappa_{tr}^{(2)} - 2\mu_{tr}^{(2)} \Xi_{22}^{(2)} + l^{(2)} + 2H_{44} - 2H_{11}, \\ H_{33} &= 2l^{(1)} \Xi_{12}^{(1)} + \frac{\bar{l}}{r_1} [1 + \Xi_{12}^{(1)} + \Xi_{22}^{(2)}] + n^{(1)} + \frac{2\bar{n}}{r_1} - 2H_{31}. \end{aligned} \quad (71)$$

395 Expressions (58), (63), (69) and (71) provide all the required coefficients for the interaction tensors, which  
396 in turn can be implemented in the Mori–Tanaka scheme to identify the macroscopic elasticity tensor of fiber  
397 composites. The components of  ${}^M\mathbf{L}$  are expressed as given in Eq. (10).

#### 398 4 Numerical results

399 The goal of this section is to evaluate the performance of the proposed analytical solutions through a series  
400 of numerical examples. In doing so, the influence of the general interfaces on the overall material response  
401 is investigated and compared against computational simulations using the finite element method elaborated  
402 in [91]. The computational analysis is carried out using our in-house finite element code applied to the RVE  
403 discretized by biquadratic Lagrange elements as shown in Fig. 8. For all examples, the solution procedures  
404 are robust and show asymptotically the quadratic rate of convergence associated with the Newton–Raphson  
405 scheme. For all the cases, the volume fraction  $f = 30\%$  is assumed. The RVE size varies from 0.001 to 1000,  
406 and three different stiffness ratios of 0.1, 1 and 10 are studied. The stiffness ratio denoted as  $\text{incl./matr.}$  is the

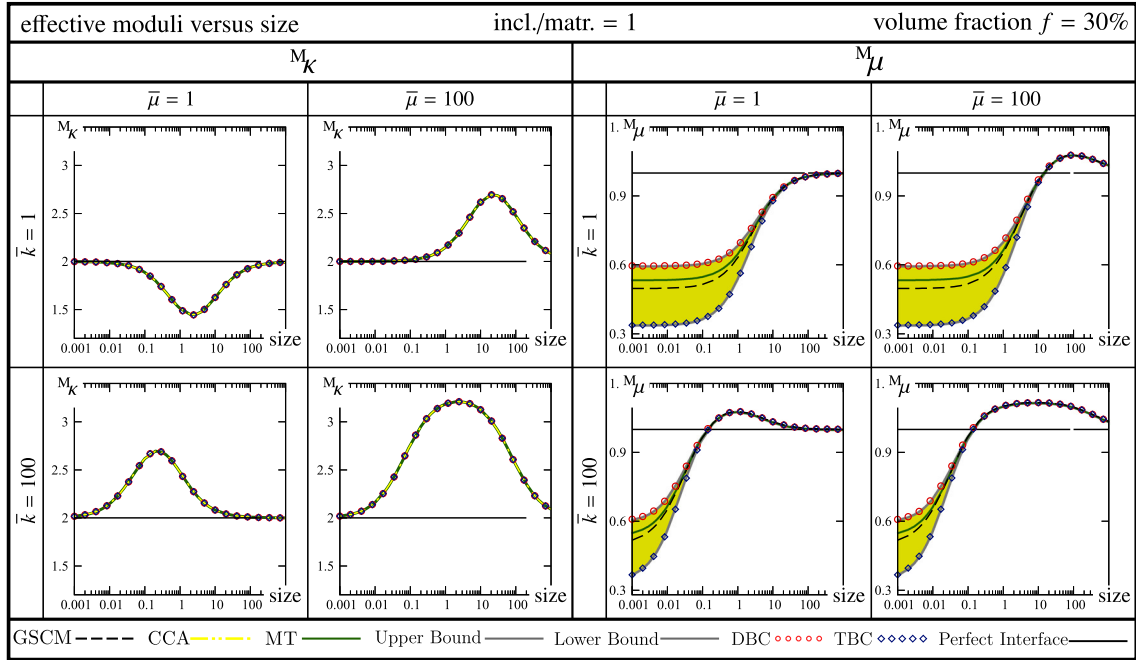


**Fig. 9** The effective bulk and shear moduli versus size for  $\text{incl./matr.} = 0.1$ . The lines correspond to the analytical solutions, and dots correspond to the numerical results using the finite element method. “CCA” and “GSCM” indicate the effective properties obtained via the solution proposed in Sects. 3.2.1 and 3.2.2. “Upper Bound” and “Lower Bound” refer to our proposed bounds in Sects. 3.2.3 and 3.2.4. “MT” corresponds to our proposed solution in Sect. 3.3

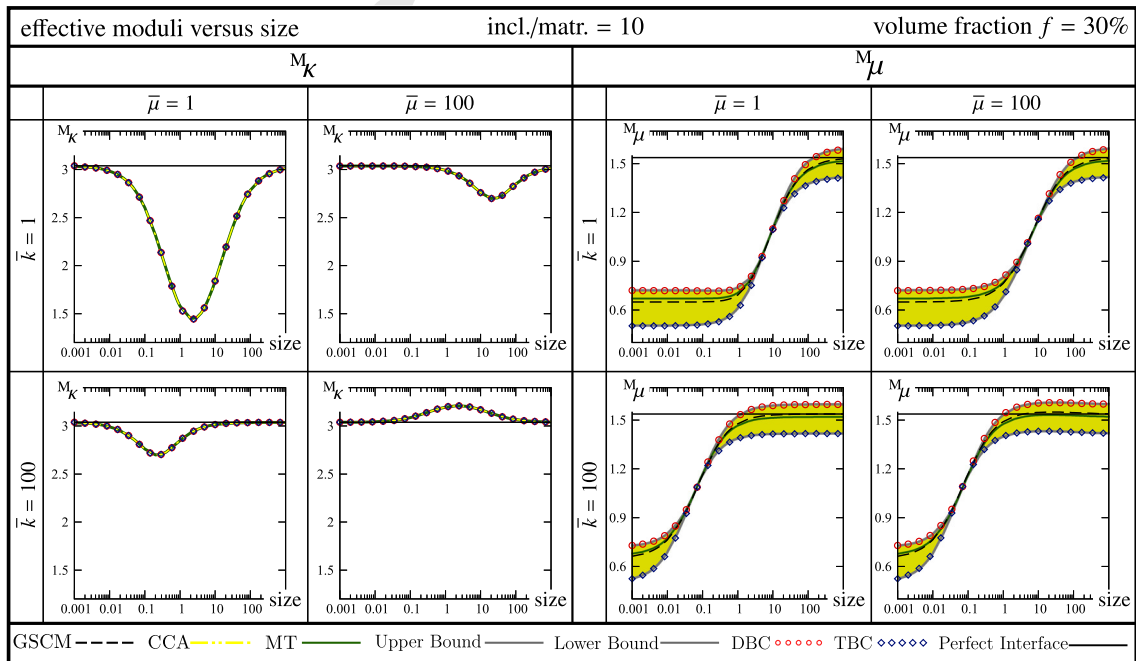
407 ratio of the inclusion to matrix Lamé parameters. The stiffness ratio 0.1 corresponds to a matrix 10 times stiffer  
 408 than the inclusion and in the limit of  $\text{incl./matr.} \rightarrow 0$ , the inclusion resembles a void. The stiffness ratio 10  
 409 corresponds to an inclusion 10 times stiffer than the matrix and in the limit of  $\text{incl./matr.} \rightarrow \infty$ , the inclusion  
 410 acts as being rigid. Clearly, the stiffness ratio 1 represents identical inclusion and matrix. Throughout the  
 411 numerical examples, the matrix Lamé parameters are  $\lambda_2 = \mu_2 = 1$  and the inclusion Lamé parameters vary in  
 412 accordance with the prescribed stiffness ratios. The interface in-plane resistance  $\bar{\mu}$  corresponds to the resistance  
 413 of the interface against stretch and is set to  $\bar{\mu} = 1$  indicating a low in-plane resistance and  $\bar{\mu} = 100$  indicating  
 414 a very high resistance. On the other hand, the two considered values for the orthogonal interface resistance  
 415 are  $\bar{k} = 1$  indicating a low opening resistance and  $\bar{k} = 100$  indicating a high opening resistance. In the limit  
 416  $\bar{k} \rightarrow \infty$ , the interface remains coherent and does not allow for opening. On the contrary,  $\bar{k} \rightarrow 0$  indicates  
 417 no orthogonal resistance and the fiber behaves entirely detached from the matrix. It shall be emphasized that  
 418 depending on the choice of the general interface parameters any of the perfect, elastic or cohesive interface  
 419 models could be recovered, as shown in Fig. 1. The conditions  $\bar{\mu} \neq 0$  and  $\bar{k} \rightarrow \infty$  recover the elastic interface  
 420 model. The cohesive interface is recovered when  $\bar{\mu} = 0$  and  $\bar{k} \rightarrow \infty$ . Finally, the perfect interface model is  
 421 recovered when  $\bar{\mu} = 0$  and  $\bar{k} \rightarrow \infty$ .

422 Figures 9, 10 and 11 illustrate the effective bulk modulus  $M_K$  and shear modulus  $M_\mu$  versus size for different  
 423 stiffness ratios. Each column corresponds to a specific in-plane resistance  $\bar{\mu}$ , and each row corresponds to a  
 424 specific orthogonal resistance  $\bar{k}$ . The solid straight black line shows the effective response due to the perfect  
 425 interface. Lines indicate the analytical solutions corresponding to the analytical approaches developed in  
 426 Sects. 3.2.1 and 3.3. Red circular points and blue rectangular points correspond to computational results using  
 427 the finite element method obtained via prescribing DBC and TBC, respectively.

428 A remarkable agreement between the analytical solutions and the computational results are consistently  
 429 observed for all the examples. For all the cases, a size-dependent response is observed due to the presence of  
 430 the general interface. For the bulk modulus, all the solutions render a consistent behavior with respect to the  
 431 perfect interface solution. The results coincide with the perfect interface solution at small sizes. Increasing  
 432 the size results in deviation from the perfect interface solution until a critical size at which an extremum is  
 433 reached. Further increase in size yields asymptotic convergence of the results to the perfect interface solution  
 434 which is due to the diminished interface effects at large sizes. For  $\text{incl./matr.} = 0.1$ , the results corresponding



**Fig. 10** The effective bulk and shear moduli versus size for  $\text{incl./matr.} = 1$ . The lines correspond to the analytical solutions, and dots correspond to the numerical results using the finite element method. “CCA” and “GSCM” indicate the effective properties obtained via the solution proposed in Sects. 3.2.1 and 3.2.2. “Upper Bound” and “Lower Bound” refer to our proposed bounds in Sects. 3.2.3 and 3.2.4. “MT” corresponds to our proposed solution in Sect. 3.3.



**Fig. 11** The effective bulk and shear moduli versus size for  $\text{incl./matr.} = 10$ . The lines correspond to the analytical solutions, and dots correspond to the numerical results using the finite element method. “CCA” and “GSCM” indicate the effective properties obtained via the solution proposed in Sects. 3.2.1 and 3.2.2. “Upper Bound” and “Lower Bound” refer to our proposed bounds in Sects. 3.2.3 and 3.2.4. “MT” corresponds to our proposed solution in Sect. 3.3.

Author Proof

435 to general interface always overestimate to those obtained from the perfect interface model. However, for the  
 436 other stiffness ratios, depending on the interface parameters, the results render either a weaker or a stronger  
 437 response compared to the perfect interface solution. Evidently, if the interface parameters are taken enough  
 438 large, the response due to the general interface is stiffer than those of the perfect interface. Overall, an important  
 439 observation and especially useful for computational material design is that in the presence of interfaces, even  
 440 if the inclusion is identical to the matrix, various combinations of parameters could result in substantially  
 441 different but also size-dependent overall material behavior. For the shear modulus, there is perfect agreement  
 442 between the upper bound and DBC and the lower bound and TBC. When  $\text{incl./matr.} = 0.1$ , the bounds  
 443 never coincide. When  $\text{incl./matr.} = 1$  in Fig. 10, the upper and the lower bounds *converge* at larger sizes since  
 444  $\text{incl./matr.} = 1$  implies identical matrix and inclusion and hence, identical responses are seen when the interface  
 445 effects become negligible enough at large sizes. For  $\text{incl./matr.} = 10$ , the bounds tend to approach to each  
 446 other until they coincide at a specific sizes and then they distant from each other as size increases. A particular  
 447 significant observation is that the generalized self-consistent method and the modified Mori–Tanaka method  
 448 do not provide similar estimates for the effective shear modulus. For  $\text{incl./matr.} = 0.1$  and  $\text{incl./matr.} = 1$ , the  
 449 response obtained from GSCM underestimates that of MT method. However, when  $\text{incl./matr.} = 10$ , the results  
 450 corresponding to GSCM underestimate the ones obtained from MT before the bounds coincide, whereas the  
 451 opposite story holds after the bounds coincidence.

452 *Remark* In view of the behavior of the effective bulk modulus  $M_K$ , it is observed that the general interface  
 453 model at both limits of small and large sizes converges to the perfect interface model. The interface effect is  
 454 decreasing when increasing the size, and thus, its behavior at large sizes is fairly obvious. At small scales,  
 455 however, further discussion is required to justify the influence of the interface on the overall material response.  
 456 The effective behavior of the general interface model can be explained by the fact that it combines the two  
 457 opposing cohesive and elastic interface models, schematically illustrated in Fig. 1. The elastic interface model  
 458 results in a *smaller-stronger* effect in contrast to the *smaller-weaker* effect of the cohesive interface model.  
 459 At large sizes, neither of the interface effects is present. But at small sizes, both of the interface effects are  
 460 present and eventually cancel each other. Furthermore, we can elaborate on this observation from an analytical  
 461 perspective. To do so, we re-express the effective bulk modulus (25) as

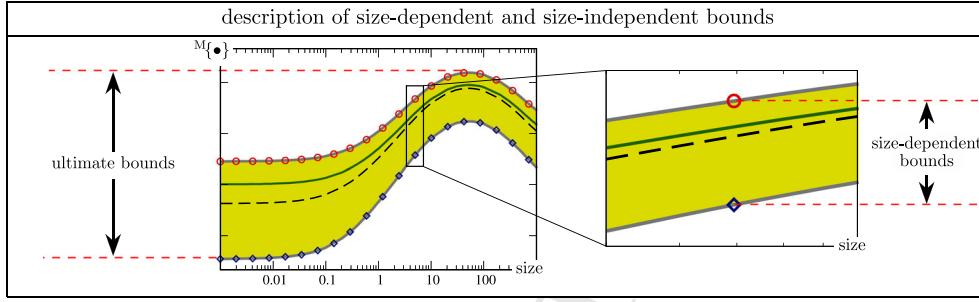
$$462 \quad M_K = \lambda_2 + \mu_2 + \frac{f}{\frac{1}{\frac{[\lambda_1 + \mu_1][4\bar{k}r_1^3 + 2\bar{\mu}r_1] + 4\bar{k}\bar{\mu}r_1^2}{4r_1^2[2\lambda_1 + 2\mu_1 + \bar{k}r_1] + 2\bar{\mu}r_1} - [\lambda_2 + \mu_2]} + \frac{1-f}{\lambda_2 + 2\mu_2}},$$

463 thereby gaining a better insight on  $M_K$  in terms of  $r_1$ . This relation in both limits simplifies to

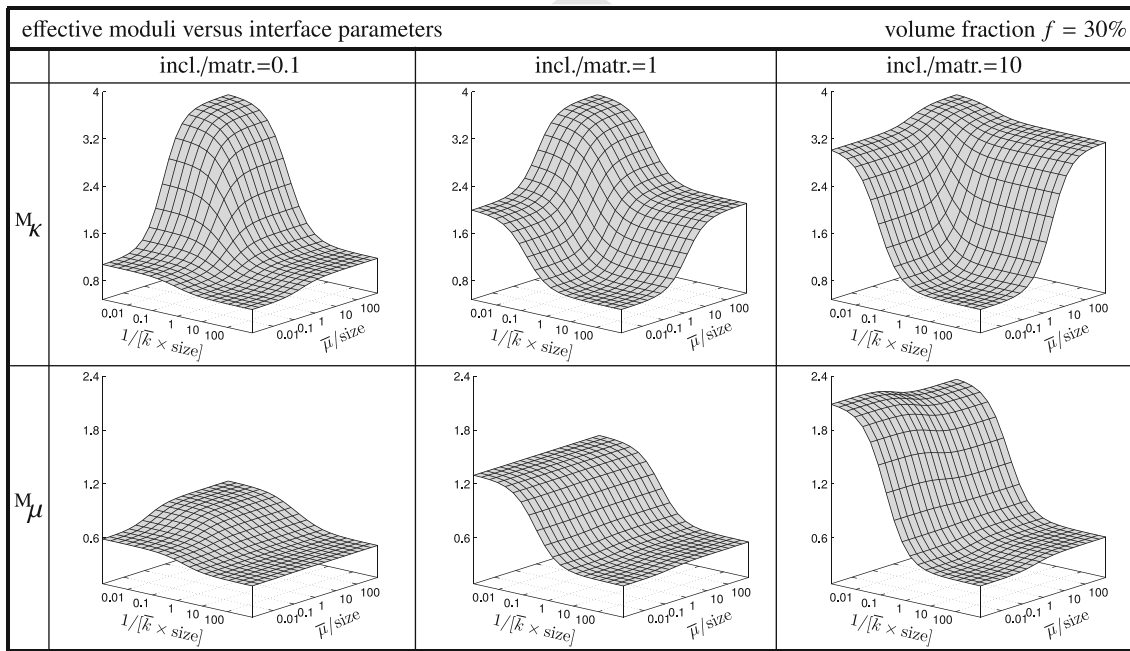
$$464 \quad r \rightarrow 0 \quad \text{or} \quad r \rightarrow \infty \quad \Rightarrow \quad M_K = \lambda_2 + \mu_2 + \frac{f}{\frac{1}{[\lambda_1 + \mu_1] - [\lambda_2 + \mu_2]} + \frac{1-f}{\lambda_2 + 2\mu_2}}, \quad (72)$$

465 which corresponds exactly to the solution associated with the perfect interface model.

466 Inspired by the observations made throughout the numerical examples, it is possible to distinguish between  
 467 two dissimilar bounds on the overall behavior of the microstructure, namely *size-dependent bounds* and *ultimate*  
 468 *bounds*. Size-dependent bounds are the bounds on the effective behavior of the microstructure at any given  
 469 size. The upper and lower size-dependent bounds correspond to the solution of the boundary value problem  
 470 associated with DBC and TBC, respectively. On the other hand, we also observe that the macroscopic response  
 471 is always bounded between two specific values regardless of the size of the microstructure and thus, we refer to  
 472 them as ultimate bounds. In the case of a stiff inclusion within a more compliant matrix such as  $\text{incl./matr.} = 10$   
 473 shown in Fig. 11, the ultimate bounds are reached at extreme sizes. However, the ultimate bounds may be  
 474 reached at critical sizes and not necessarily at the limits, see, for instance, Fig. 9. In fact, Fig. 12 elucidates the  
 475 notions of ultimate and size-dependent bounds schematically. Size-dependent bounds are local in the sense  
 476 that for a specific interface and material parameters, they vary with respect to size. In contrast, the ultimate  
 477 bounds are independent of size and they entirely depend on the interface and bulk material properties. As  
 478 pointed out earlier, the size-dependent bounds coincide in the case of the effective bulk modulus  $M_K$  and are  
 479 only distinct in the case of the effective shear modulus  $M_\mu$ . One can mention that this conclusion for general  
 480 interface is in agreement with that derived by Hashin and Rosen for the case of a perfect interface [107].



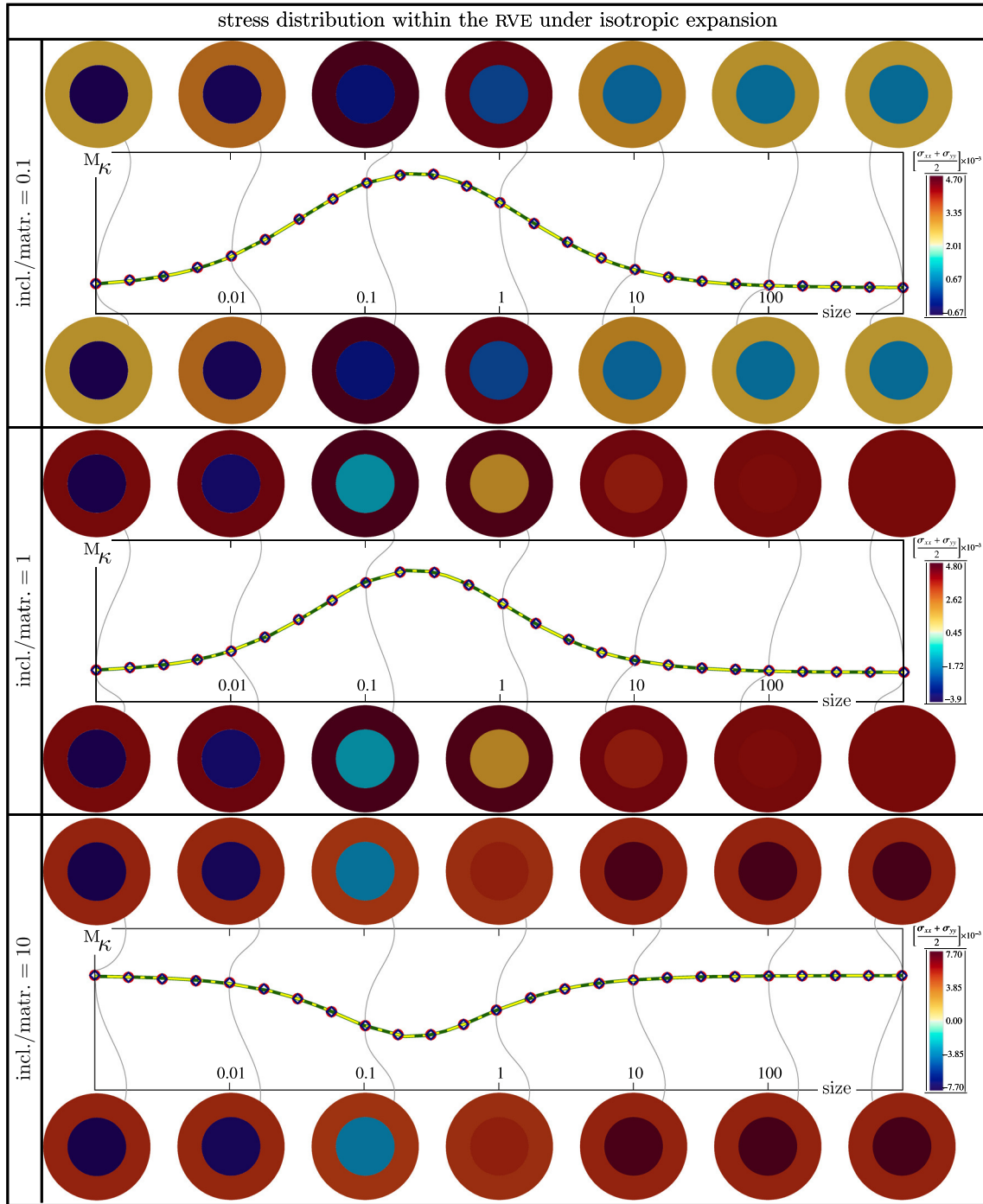
**Fig. 12** Schematic illustration of size-dependent and ultimate bounds. The size-dependent bounds are the bounds on the effective behavior of the microstructure at any given size. The ultimate bounds are independent of size, and they entirely depend on the interface and bulk material properties



**Fig. 13** Effective moduli versus dimensionless interface parameters

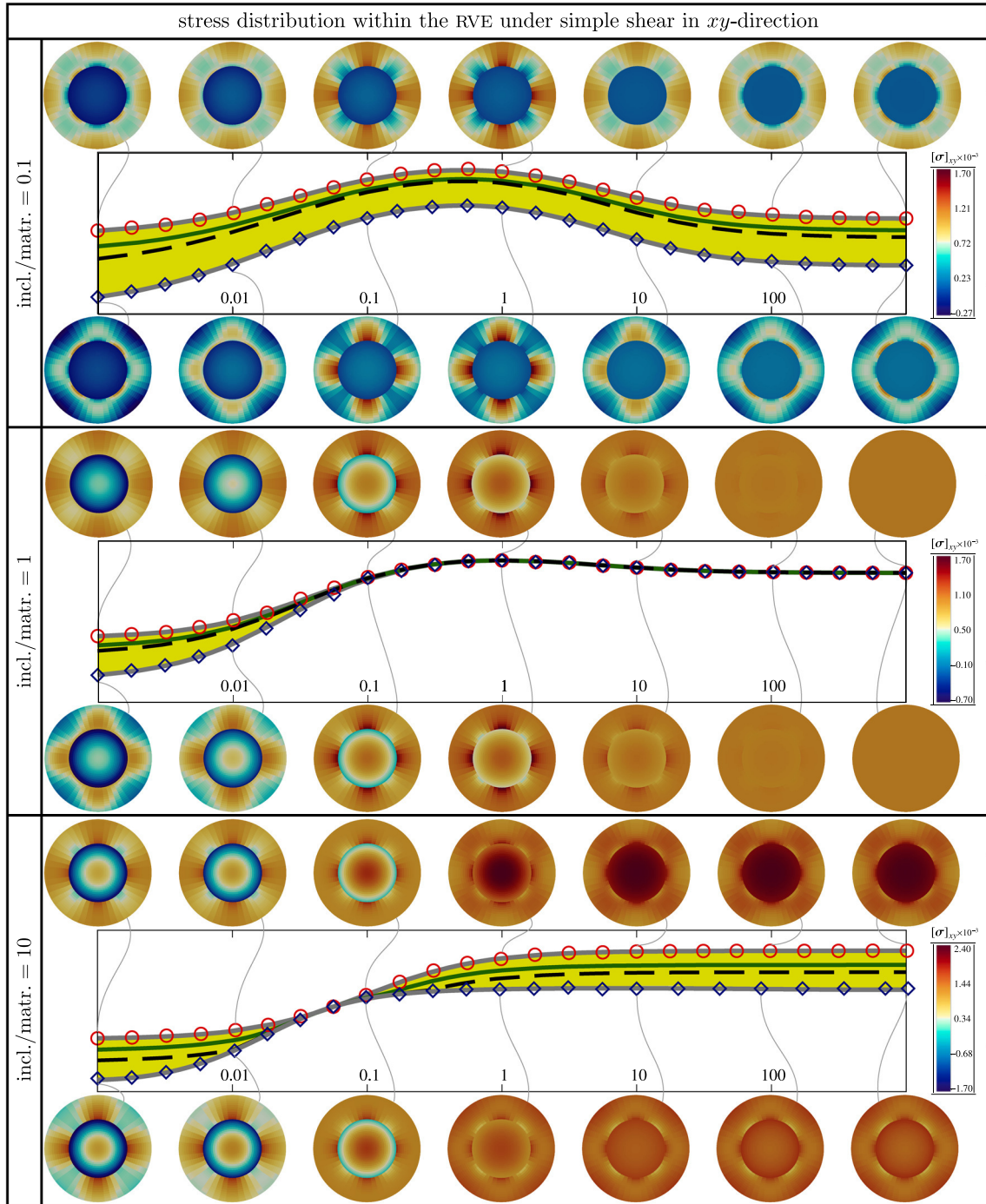
481 To pinpoint the effects of the interface parameters on the overall material response of composites with  
 482 general interfaces, Fig. 13 illustrates the variation of the effective moduli versus interface parameters. Each  
 483 column corresponds to a specific stiffness ratio. The top row corresponds to effective bulk modulus  $M_K$ , and the  
 484 bottom row corresponds to the effective shear modulus  $M_\mu$ . Note that the interface orthogonal resistance  $\bar{k}$  has  
 485 the inverse length dimension and thus multiplied to the size to become dimensionless. On the other hand, the  
 486 interface elastic parameter  $\bar{\mu}$  has the length dimension and thus divided by the size to become dimensionless.  
 487 For the effective bulk modulus, increasing any of the interface parameters results in stiffer material response.  
 488 For two extreme cases of very strong and very weak interfaces, the associated overall response is similar for  
 489 all stiffness ratios. On the other hand, for the shear modulus, when  $\text{incl./matr.} = 0.1$ , increasing the interface  
 490 parameters stiffens the response. For  $\text{incl./matr.} = 1$ , the overall response shows no sensitivity to  $\bar{\mu}$ , whereas  
 491 increasing  $\bar{k}$  yields stronger response. An interesting observation arises for  $\text{incl./matr.} = 10$  where increasing  
 492  $\bar{k}$  results in stiffer response but increasing  $\bar{\mu}$  might lead to either softer or stiffer response depending on the  
 493 size.

494 Figures 14 and 15 illustrate the stress distribution within the microstructure at different sizes and for  
 495 different stiffness ratios. More precisely, the color patterns display  $[\sigma_{xx} + \sigma_{yy}]/2$  in Fig. 14 and  $[\sigma]_{xy}$  in  
 496 Fig. 15. This choice is made to provide meaningful stress distributions for each case. In the case of Fig. 14,  
 497 volumetric expansion is prescribed on the RVE to compute the effective bulk modulus  $M_K$  and thus, a pressure-



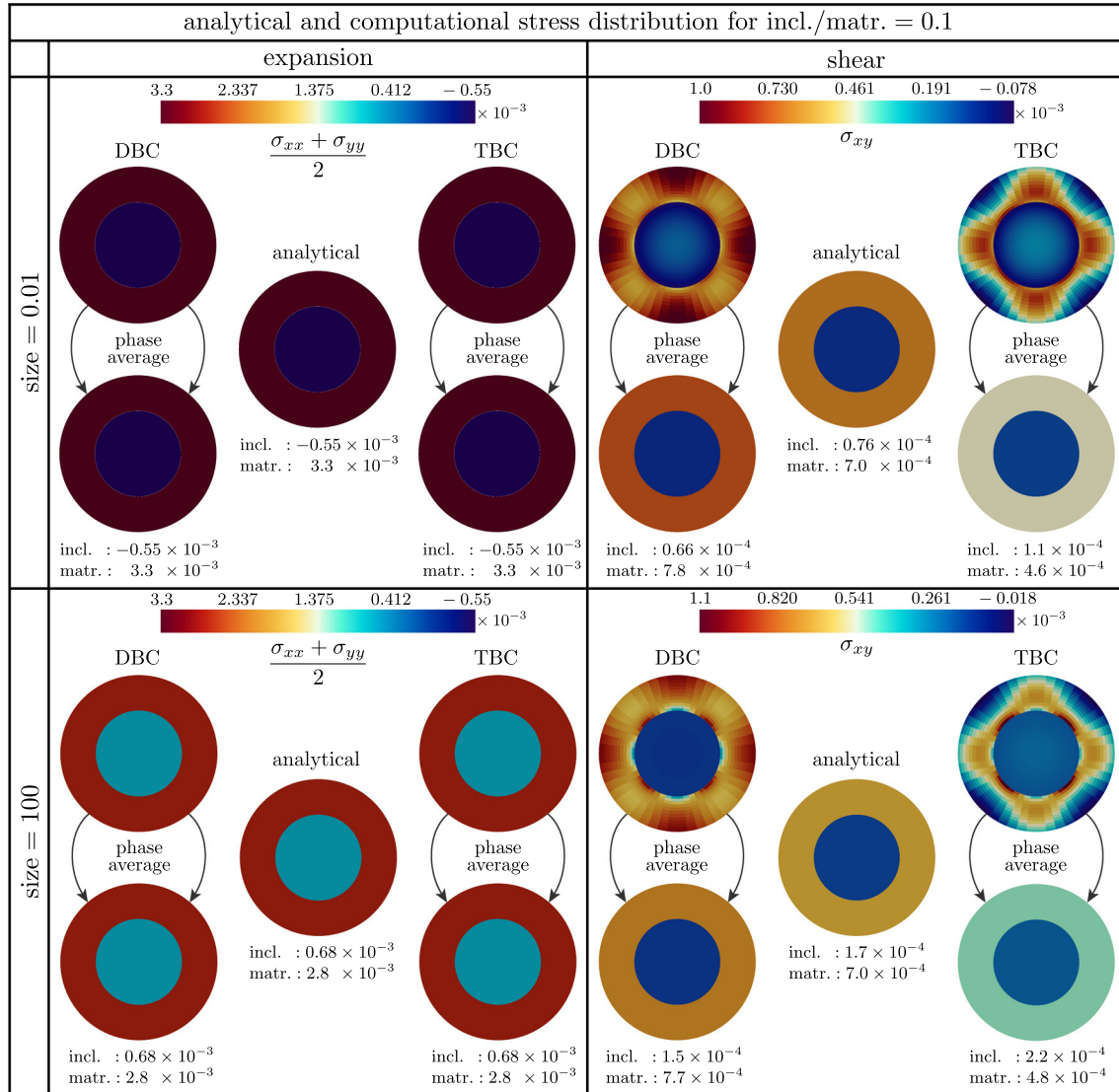
**Fig. 14** Illustration of the stress distribution within the microstructure due to isotropic expansion at different sizes and for different stiffness ratios. The upper row of stress distributions on each graph correspond to DBC and the lower row to TBC

498 like quantity  $[\sigma_{xx} + \sigma_{yy}]/2$  is more relevant and informative. On the other hand, in the case of Fig. 15, a simple  
 499 shear is prescribed on the RVE to compute the effective shear modulus  $M\mu$  in which case the shear component  
 500 of the stress  $[\sigma]_{xy}$  is a more appropriate quantity to look at. Obviously, for the sake of a better presentation, all  
 501 the RVEs are scaled to the same size. On each graph, the upper row and lower row show the stress distributions  
 502 corresponding to DBC and TBC, respectively. Both figures compare the cases with the interface parameters  
 503  $\bar{k} = 100$  and  $\bar{\mu} = 1$  from Figs. 9, 10 and 11. For the expansion case in Fig. 14, the stress patterns due to DBC



**Fig. 15** Illustration of the stress distribution within the microstructure due to simple shear at different sizes and for different stiffness ratios. The upper row of stress distributions on each graph corresponds to DBC, and the lower row to TBC

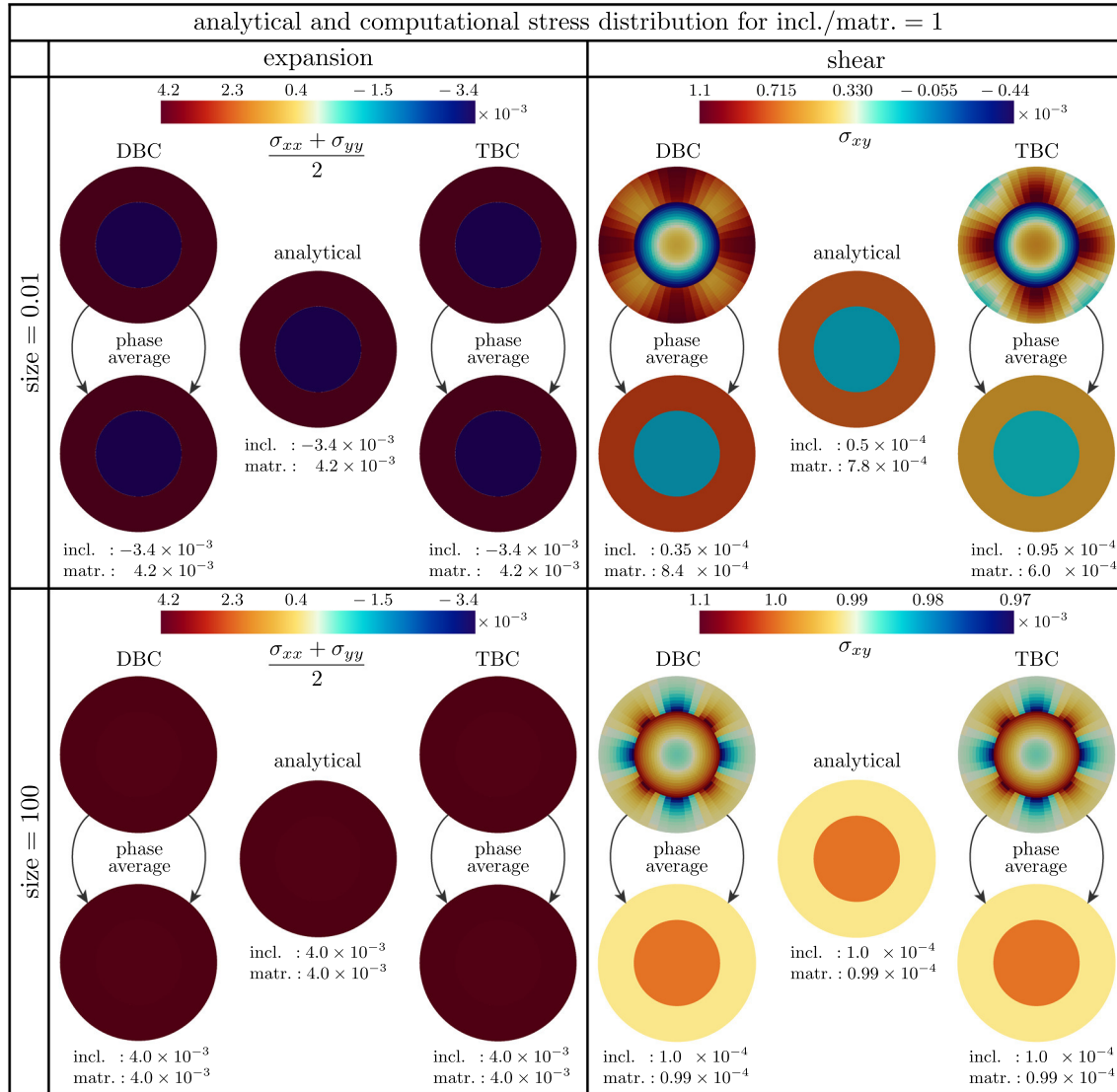
504 and TBC are identical, and thus, the effective bulk modulus  $M_k$  is same, at any given size. But that is not the  
 505 case for the effective shear modulus. For the non-coinciding cases, the stress due to DBC always overestimates  
 506 the stress due to TBC and hence stiffer overall response. For the coinciding cases, the stresses due to DBC  
 507 and TBC are identical which justifies the same overall response. Moreover, for  $\text{incl./matr.} = 0.1$ , the stress in  
 508 the fiber is less than the matrix at any size. For  $\text{incl./matr.} = 1$ , the same story holds at small sizes, whereas  
 509 at large size, the stresses become similar since interface effects become negligible and the bulk materials are



**Fig. 16** Comparison of the analytical and numerical stress distributions within the RVE at different sizes for incl./matr. = 0.1. On each block, the top microstructures corresponds to the local stress distribution due to DBC and TBC. The analytical stress distribution is shown at the center. The bottom microstructures render the average of the computational stresses due to DBC and TBC

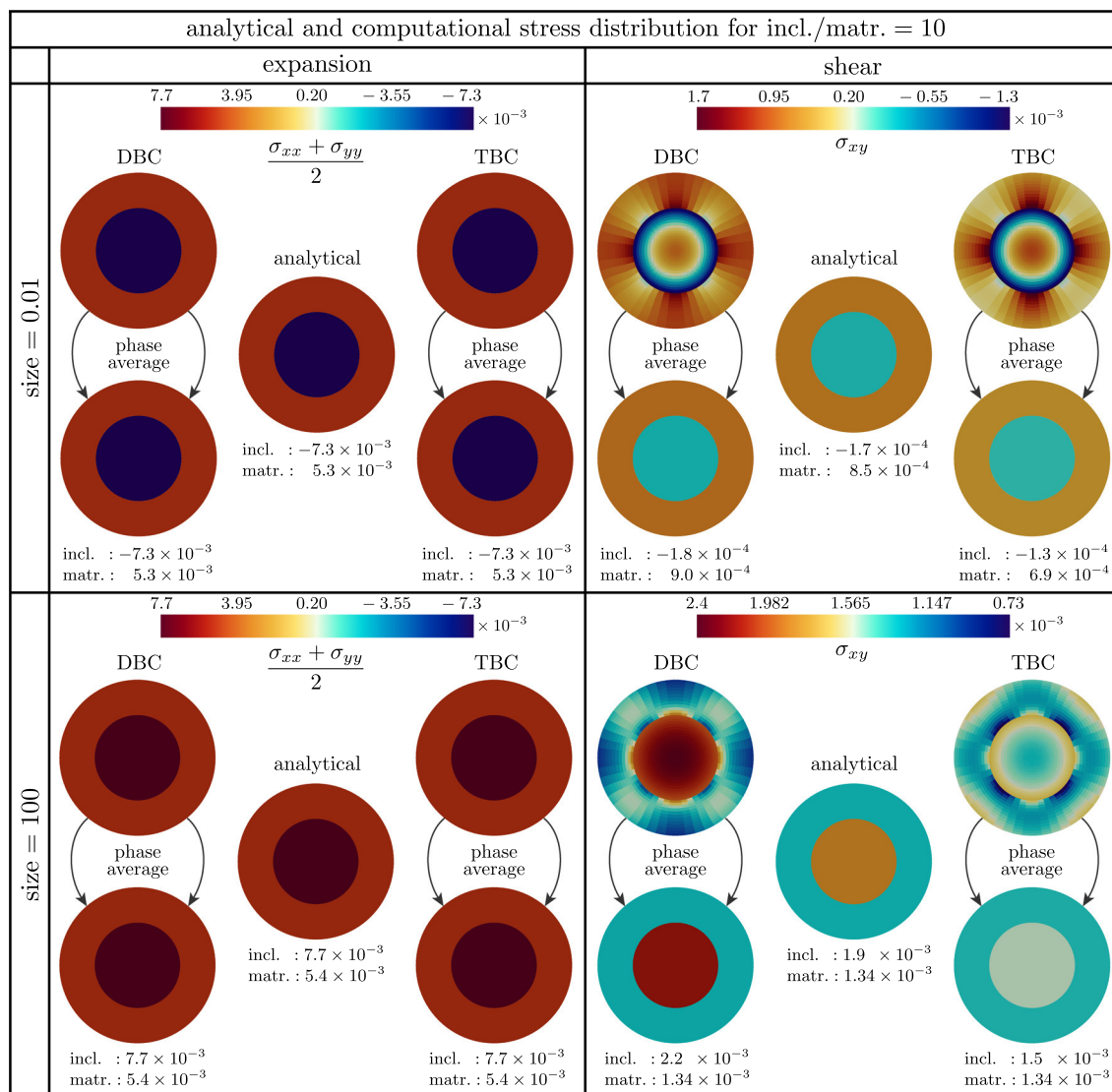
510 identical. Finally, when incl./matr. = 10, fiber undergoes less stress than the matrix at small sizes, whereas the  
 511 opposite story holds at large sizes.

512 A significant feature of this contribution is that our novel formalism through the modified Mori–Tanaka  
 513 approach does not only determine the overall response of composites, but also it provides information about the  
 514 local fields for each phase of the medium. The purpose of the next set of examples is to evaluate the analytical  
 515 stress fields and compare them against the associated numerical solutions. Figures 16, 17 and 18 provide a  
 516 thorough comparison between the numerical and analytical stress distributions for different stiffness ratios at  
 517 different sizes. In each figure, the rows correspond to specific sizes, whereas the columns correspond to the  
 518 deformation type. Similar to Figs. 14 and 15, the stress component of the interest for the expansion and shear  
 519 deformations are  $[\sigma_{xx} + \sigma_{yy}]/2$  and  $[\sigma_{xy}]$ , respectively. On each block, the top microstructures render the  
 520 computational stress distribution due to DBC and TBC obtained from the finite element method. The analytical  
 521 stress distribution is shown at the center of each block. Since our proposed analytical approach determines the  
 522 average stress in the constituents, the bottom microstructures render the computational average stresses due to  
 523 DBC and TBC suitable for comparison with analytical stresses. For the sake of clarity, the value of the average



**Fig. 17** Comparison of the analytical and numerical stress distributions within the RVE at different sizes for incl./matr. = 1. On each block, the top microstructures correspond to the local stress distribution due to DBC and TBC. The analytical stress distribution is shown at the center. The bottom microstructures render the average of the computational stresses due to DBC and TBC

524 stresses in the inclusion and the matrix is shown at the bottom of each microstructure. For the expansion case,  
 525 the analytical stress is outstandingly precise and the stresses in the inclusion and matrix are exactly similar to  
 526 the computational stresses. However, this is not the case for the shear deformation where various conclusions  
 527 can be drawn. When incl./matr. = 0.1, the average stress due to DBC overestimates the analytical stress in the  
 528 matrix. On the other hand, the average stress due to TBC underestimates the analytical stress in the matrix.  
 529 For the stress in the inclusion, TBC results in the highest average stress and DBC renders the lowest average  
 530 stress with the analytical stress being in between. The same story holds for incl./matr. = 1 when size is small.  
 531 When size is large, both the analytical and computational stresses resemble which conforms to the coinciding  
 532 bounds at large sizes in Fig. 15. For incl./matr. = 10, when size = 0.01, the stress due to DBC is the highest in  
 533 the matrix and the lowest in the inclusion. TBC renders the highest inclusion average stress and lowest matrix  
 534 average stress. The analytical stress in both the inclusion and the matrix are between those obtained by DBC  
 535 and TBC. Finally, for incl./matr. = 10 and size = 100, both analytical and computational average stresses are  
 536 similar in the matrix. However, the average stress in the inclusion is highest for DBC and the lowest for TBC  
 537 with the analytical stress being in between.



**Fig. 18** Comparison of the analytical and numerical stress distributions within the RVE at different sizes for incl./matr. = 10. On each block, the top microstructures correspond to the local stress distribution due to DBC and TBC. The analytical stress distribution is shown at the center. The bottom microstructures render the average of the computational stresses due to DBC and TBC

## 538 5 Conclusion and outlook

539 This contribution establishes novel bounds and estimates to determine the overall behavior of composites  
 540 through homogenization enhanced by general interfaces and hence the size effects. The bounds are obtained  
 541 via extension of the CCA approach to account for interfaces and by prescribing displacement-type and traction-  
 542 type boundary conditions on the microstructure, respectively. Our proposed strategy to compute an estimate  
 543 for the effective material response, on the other hand, extends the Mori–Tanaka approach. Not only does our  
 544 methodology furnish accurate results for the effective properties, but also it provides additional information  
 545 about the local fields in the constituents including the interface. The proposed framework here is generic  
 546 and versatile, and thus, it can readily recover perfect, cohesive and elastic interface models. Throughout a  
 547 series of numerical examples, we have shown that our proposed analytical solutions are in excellent agreement  
 548 with the computational results obtained from the finite element method. Furthermore, the notions of *size-*  
 549 *dependent bounds* and *ultimate bounds* were introduced which give a crucial insight into the problem from a  
 550 computational material design perspective. We believe this contribution provides a deeper understanding of the

551 interface effects and size-dependent behavior of continua with a variety of applications in nano-composites.  
 552 Our next immediate plan is to extend the current work to 3D and study the size effects in particulate composites  
 553 due to interfaces.

554

## 555 Appendix A: System of equations for the estimate and bounds on the shear modulus

556 In this section, we elaborate on the system of equations used to obtain the estimate and the bounds on the  
 557 macroscopic shear modulus explained in Sect. 3.

### 558 Appendix A.1: Effective shear modulus

559 For this problem, the displacement fields in the matrix, fiber and the effective medium are given in Eq. (27)  
 560 resulting in ten unknowns  $\Xi_1^{(1)}, \Xi_2^{(1)}, \Xi_3^{(1)}, \Xi_4^{(1)}, \Xi_1^{(2)}, \Xi_2^{(2)}, \Xi_3^{(2)}, \Xi_4^{(2)}, \Xi_3^{(\text{eff})}$  and  $\Xi_4^{(\text{eff})}$ . We concluded that  
 561 since the displacement at the center of the RVE must be finite,  $\Xi_3^{(1)}$  and  $\Xi_4^{(1)}$  must vanish. Applying the energetic  
 562 criterion expressed in Eq. (30) yields  $\Xi_4^{(\text{eff})}$ . The remaining seven unknowns are determined using the below  
 563 system which is deduced from Eq. (29)

$$564 \quad \mathbf{Q} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -\frac{3}{2} \\ \frac{3}{2} \end{bmatrix} \Xi_3^{(\text{eff})}, \quad (\text{A.1})$$

565 with

$$566 \quad \mathbf{Q} = \begin{bmatrix} \frac{3\bar{\mu}\zeta_2 r_1}{\zeta_3} & \frac{\bar{\mu}}{r_1} - 2\mu_1 & \frac{3\bar{\mu}\zeta_5 r_1}{\zeta_6} & \frac{\bar{\mu}}{r_1} + 2\mu_2 & \frac{3\bar{\mu}}{r_1^5} + \frac{6\mu_2}{r_1^4} & -\frac{4\zeta_4}{r_1^2} - \frac{\lambda_2 \bar{\mu}}{\mu_2 r_1^3} \\ \frac{6[\bar{\mu}\zeta_2 + \mu_1 \zeta_1 r_1] r_1}{\zeta_3} & \frac{2\bar{\mu}}{r_1} - 2\mu_1 & \frac{6[\bar{\mu}\zeta_5 - \mu_2 \zeta_4 r_1] r_1}{\zeta_6} & \frac{2\bar{\mu}}{r_1} + 2\mu_2 & -\frac{6\bar{\mu}}{r_1^5} - \frac{6\mu_2}{r_1^4} & \frac{2\zeta_4}{r_1^2} + \frac{2\bar{\mu}\lambda_2}{\mu_2 r_1^3} \\ \frac{\lambda_1 r_1^3}{\zeta_3} & \frac{\mu_1}{k} + r_1 & -\frac{\lambda_2 r_1^3}{\zeta_6} & \frac{\mu_2}{k} - r_1 & \frac{3\mu_2}{k r_1^4} + \frac{1}{r_1^3} & -\frac{2\zeta_4}{k r_1^2} - \frac{\zeta_5}{\mu_2 r_1} \\ \frac{3\mu_1 \zeta_1 r_1^2}{k \zeta_3} + r_1^3 & \frac{\mu_1}{k} + r_1 & \frac{3\mu_2 \zeta_4 r_1^2}{k \zeta_6} - r_1^3 & \frac{\mu_2}{k} - r_1 & -\frac{3\mu_2}{k r_1^4} - \frac{1}{r_1^3} & \frac{\zeta_4}{k r_1^2} - \frac{1}{r_1} \\ 0 & 0 & 0 & 2\mu_2 & \frac{6\mu_2}{r_2^4} & -\frac{4\zeta_4}{r_2^2} \\ 0 & 0 & \frac{6\mu_2 \zeta_4 r_2^2}{\zeta_6} & 2\mu_2 & -\frac{6\mu_2}{r_2^4} & \frac{2\zeta_4}{r_2^2} \end{bmatrix}, \quad (\text{A.2})$$

567 where

$$\zeta_1 = \lambda_1 + \mu_1, \quad \zeta_2 = \lambda_1 + 2\mu_1, \quad \zeta_3 = 2\lambda_1 + 3\mu_1, \quad \zeta_4 = \lambda_2 + \mu_2, \quad \zeta_5 = \lambda_2 + 2\mu_2, \quad \zeta_6 = 2\lambda_2 + 3\mu_2.$$

Note the above system of equations is nonlinear, and thus, special treatments must be applied. We express the solution of the above system in the form

$$\begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} + \begin{bmatrix} h_1 \\ h_2 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} \Xi_3^{(\text{eff})}. \quad (\text{A.3})$$

The last two equations in Eq. (29) can be written as

$$a_5 + b_5 \Xi_3^{(\text{eff})} = \frac{c_5 + c_6 \Xi_3^{(\text{eff})}}{M\mu}, \quad a_6 + b_6 \Xi_3^{(\text{eff})} = \frac{c_5 - c_6 \Xi_3^{(\text{eff})}}{M\mu}. \quad (\text{A.4})$$

with

$$\begin{aligned} a_5 &= \frac{\lambda_2 r_2^3}{2\lambda_2 + 3\mu_2} a_1 + r_2 a_2 - \frac{1}{r_2^3} a_3 + \frac{\lambda_2 + 2\mu_2}{\mu_2 r_2} a_4, \\ a_6 &= r_2^3 a_1 + r_2 a_2 + \frac{1}{r_2^3} a_3 + \frac{1}{r_2} a_4, \\ b_5 &= \frac{\lambda_2 r_2^3}{2\lambda_2 + 3\mu_2} b_1 + r_2 b_2 - \frac{1}{r_2^3} b_3 + \frac{\lambda_2 + 2\mu_2}{\mu_2 r_2} b_4, \\ b_6 &= r_2^3 b_1 + r_2 b_2 + \frac{1}{r_2^3} b_3 + \frac{1}{r_2} b_4, \\ c_5 &= \frac{r_2}{2}, \\ c_6 &= \frac{r_2}{4}. \end{aligned} \quad (\text{A.5})$$

Subtracting (A.4)<sub>1</sub> from (A.4)<sub>2</sub> gives

$$\Xi_3^{(\text{eff})} = \frac{[a_5 - a_6]M\mu}{2c_6 + [b_6 - b_5]M\mu}.$$

Substituting the final result in (A.4)<sub>1</sub>, after some algebra we obtain the below quadratic equation

$$[a_6 b_5 - a_5 b_6]M\mu^2 - [b_5 c_5 - b_6 c_5 + a_5 c_6 + a_6 c_6]M\mu + 2c_5 c_6 = 0.$$

From the two possible solutions, the positive value is the macroscopic shear modulus.

## Appendix A.2: Strain bound on the shear modulus

For this problem, the displacement fields in the matrix, fiber and the effective medium are given in Eq. (32) resulting in ten unknowns  $\Xi_1^{(1)}$ ,  $\Xi_2^{(1)}$ ,  $\Xi_3^{(1)}$ ,  $\Xi_4^{(1)}$ ,  $\Xi_1^{(2)}$ ,  $\Xi_2^{(2)}$ ,  $\Xi_3^{(2)}$  and  $\Xi_4^{(2)}$ . We concluded that since the

583 displacement at the center of the RVE must be finite,  $\Xi_3^{(1)}$  and  $\Xi_4^{(1)}$  must vanish. The remaining six unknowns  
584 are determined using the below system which is deduced from Eq. (33)

$$585 \begin{bmatrix} \frac{3\bar{\mu}\zeta_2 r_1}{\zeta_3} & \frac{\bar{\mu}}{r_1} - 2\mu_1 & \frac{3\bar{\mu}\zeta_5 r_1}{\zeta_6} & \frac{\bar{\mu}}{r_1} + 2\mu_2 & \frac{3\bar{\mu}}{r_1^5} + \frac{6\mu_2}{r_1^4} & -\frac{4\zeta_4}{r_1^2} - \frac{\lambda_2\bar{\mu}}{\mu_2 r_1^3} \\ -\frac{6[\bar{\mu}\zeta_2 + \mu_1\zeta_1 r_1]r_1}{\zeta_3} & -\frac{2\bar{\mu}}{r_1} - 2\mu_1 & -\frac{6[\bar{\mu}\zeta_5 - \mu_2\zeta_4 r_1]r_1}{\zeta_6} & -\frac{2\bar{\mu}}{r_1} + 2\mu_2 & -\frac{6\bar{\mu}}{r_1^5} - \frac{6\mu_2}{r_1^4} & \frac{2\zeta_4}{r_1^2} + \frac{2\bar{\mu}\lambda_2}{\mu_2 r_1^3} \\ \frac{\lambda_1 r_1^3}{\zeta_3} & \frac{\mu_1}{k} + r_1 & -\frac{\lambda_2 r_1^3}{\zeta_6} & \frac{\mu_2}{k} - r_1 & \frac{3\mu_2}{kr_1^4} + \frac{1}{r_1^3} & -\frac{2\zeta_4}{kr_1^2} - \frac{\zeta_5}{\mu_2 r_1} \\ \frac{3\mu_1\zeta_1 r_1^2}{k\zeta_3} + r_1^3 & \frac{\mu_1}{k} + r_1 & \frac{3\mu_2\zeta_4 r_1^2}{k\zeta_6} - r_1^3 & \frac{\mu_2}{k} - r_1 & -\frac{3\mu_2}{kr_1^4} - \frac{1}{r_1^3} & \frac{\zeta_4}{kr_1^2} - \frac{1}{r_1} \\ 0 & 0 & \frac{\lambda_2 r_2^3}{\zeta_6} & r_2 & -\frac{1}{r_2^3} & \frac{\zeta_5}{\mu_2 r_2} \\ 0 & 0 & r_2^3 & r_2 & \frac{1}{r_2^3} & \frac{1}{r_2} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ r_2 \\ r_2 \end{bmatrix}, \quad (A.6)$$

587 where

$$588 \zeta_1 = \lambda_1 + \mu_1, \quad \zeta_2 = \lambda_1 + 2\mu_1, \quad \zeta_3 = 2\lambda_1 + 3\mu_1, \quad \zeta_4 = \lambda_2 + \mu_2, \quad \zeta_5 = \lambda_2 + 2\mu_2, \quad \zeta_6 = 2\lambda_2 + 3\mu_2.$$

### 589 Appendix A.3: Stress bound on the shear modulus

590 For this problem, the displacement fields in the matrix, fiber and the effective medium are given in Eq. (32)  
591 resulting in ten unknowns  $\Xi_1^{(1)}$ ,  $\Xi_2^{(1)}$ ,  $\Xi_3^{(1)}$ ,  $\Xi_4^{(1)}$ ,  $\Xi_1^{(2)}$ ,  $\Xi_2^{(2)}$ ,  $\Xi_3^{(2)}$  and  $\Xi_4^{(2)}$ . We concluded that since the  
592 displacement at the center of the RVE must be finite,  $\Xi_3^{(1)}$  and  $\Xi_4^{(1)}$  must vanish. The remaining six unknowns  
593 are determined using the below system which is deduced from Eq. (37)

$$594 \begin{bmatrix} \frac{3\bar{\mu}\zeta_2 r_1}{\zeta_3} & \frac{\bar{\mu}}{r_1} - 2\mu_1 & \frac{3\bar{\mu}\zeta_5 r_1}{\zeta_6} & \frac{\bar{\mu}}{r_1} + 2\mu_2 & \frac{3\bar{\mu}}{r_1^5} + \frac{6\mu_2}{r_1^4} & -\frac{4\zeta_4}{r_1^2} - \frac{\lambda_2\bar{\mu}}{\mu_2 r_1^3} \\ -\frac{6[\bar{\mu}\zeta_2 + \mu_1\zeta_1 r_1]r_1}{\zeta_3} & -\frac{2\bar{\mu}}{r_1} - 2\mu_1 & -\frac{6[\bar{\mu}\zeta_5 - \mu_2\zeta_4 r_1]r_1}{\zeta_6} & -\frac{2\bar{\mu}}{r_1} + 2\mu_2 & -\frac{6\bar{\mu}}{r_1^5} - \frac{6\mu_2}{r_1^4} & \frac{2\zeta_4}{r_1^2} + \frac{2\bar{\mu}\lambda_2}{\mu_2 r_1^3} \\ \frac{\lambda_1 r_1^3}{\zeta_3} & \frac{\mu_1}{k} + r_1 & -\frac{\lambda_2 r_1^3}{\zeta_6} & \frac{\mu_2}{k} - r_1 & \frac{3\mu_2}{kr_1^4} + \frac{1}{r_1^3} & -\frac{2\zeta_4}{kr_1^2} - \frac{\zeta_5}{\mu_2 r_1} \\ \frac{3\mu_1\zeta_1 r_1^2}{k\zeta_3} + r_1^3 & \frac{\mu_1}{k} + r_1 & \frac{3\mu_2\zeta_4 r_1^2}{k\zeta_6} - r_1^3 & \frac{\mu_2}{k} - r_1 & -\frac{3\mu_2}{kr_1^4} - \frac{1}{r_1^3} & \frac{\zeta_4}{kr_1^2} - \frac{1}{r_1} \\ 0 & 0 & 0 & 2\mu_2 & \frac{6\mu_2}{r_2^4} & -\frac{4\zeta_4}{r_2^2} \\ 0 & 0 & \frac{6\mu_2\zeta_4 r_2^2}{\zeta_6} & 2\mu_2 & -\frac{6\mu_2}{r_2^4} & \frac{2\zeta_4}{r_2^2} \end{bmatrix} \begin{bmatrix} \Xi_1^{(1)} \\ \Xi_2^{(1)} \\ \Xi_1^{(2)} \\ \Xi_2^{(2)} \\ \Xi_3^{(2)} \\ \Xi_4^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}, \quad (A.7)$$

596 where

$$597 \zeta_1 = \lambda_1 + \mu_1, \quad \zeta_2 = \lambda_1 + 2\mu_1, \quad \zeta_3 = 2\lambda_1 + 3\mu_1, \quad \zeta_4 = \lambda_2 + \mu_2, \quad \zeta_5 = \lambda_2 + 2\mu_2, \quad \zeta_6 = 2\lambda_2 + 3\mu_2.$$

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