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Designing isotropic composites reinforced by aligned transversely isotropic particles of spheroidal shape

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Abstract

The aim of this paper is to study the design of isotropic composites reinforced by aligned spheroidal particles made of a transversely isotropic material. The problem is investigated analytically using the framework of mean-field homogenization. Conditions of macroscopic isotropy of particle-reinforced composites are derived for the dilute and Mori-Tanaka’s schemes. This leads to a system of three nonlinear equations linking seven material constants and two geometrical constants. A design tool is finally proposed which permits to determine admissible particles achieving macroscopic isotropy for a given isotropic matrix behavior and a given particle aspect ratio. Correlations between transverse and longitudinal moduli of admissible particles are studied for various particle shapes. Finally, the design of particles is investigated for aluminum and steel matrix composites.

Keywords: Transverse isotropy; Spheroidal particles; Homogenization schemes; Composites

1 Introduction

Composite materials constitute one of the most advanced class of materials whose popularity in industrial applications keeps growing exponentially [1]. Their advent has been aided by the development of new processing methods, theoretical approaches of homogenization [2, 3] and numerical simulations of heterogeneous materials [4]. This class of materials is commonly divided into three categories [5]: (i) **fibrous composites** consisting of continuous fibers embedded in a matrix, (ii) **laminated composites** consisting of various stacked layers and (iii) **particle-reinforced composites** composed of particles in a matrix. We are interested in this work in particle-reinforced composites which cover a large range of existing materials, due to the various combinations of particles and matrices including notably concrete and polymer composites (nonmetallic particles in a nonmetallic matrix), solid-rocket propellants (metallic particles in nonmetallic matrix) and metal-matrix composites (nonmetallic particles in metallic matrix), and the various manufacturing processes including powder metallurgy and eutectic solidification, among others.

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The modeling of particle-reinforced composites can be tackled in a unified approach using homogenization techniques which are based on the distributions and the mechanical behaviors of the phases. Mean-field homogenization techniques are based on the concept of representative volume element together with appropriate averaging relations permitting to achieve a scale transition, known as the Hill-Mandel macrohomogeneity condition [6, 7]. The determination of the overall behavior of linear composites can then be performed using either (i) bounds, as the rigorous first-order bounds of Voigt and Reuss on the effective moduli and the second-order bounds of Hashin and Shtrikman based on variational principles [8], or (ii) estimates, as the dilute scheme [9, 10], Mori-Tanaka’s scheme [11] and the generalized self-consistent scheme [12, 13], which are all based on Eshelby’s ellipsoidal inclusion problem [14].

In practical applications, reinforcements commonly induce anisotropy due to their crystalline orientation (material anisotropy) and their shape (morphological anisotropy). In the case of a hexagonal crystallographic symmetry, which covers a large range of materials, the material anisotropy reduces to transverse isotropy. Thus, in the quite general situation of aligned spheroidal transversely isotropic particles embedded in an isotropic matrix, it is natural to expect a transversely isotropic overall behavior when these two sources of anisotropy are combined. Unfortunately, the induced anisotropy restricts the possibilities of engineering composites because, in most of industrial applications, anisotropy is often seen as a drawback while macroscopic isotropy is pursued to simplify materials processing. However one can wonder if the two sources of anisotropy (material and morphological) can cancel each other to lead to a macroscopic isotropic composite. This would permit to open new possibilities of engineering macroscopic composites made of anisotropic reinforcements. With the design of macroscopic isotropic enhanced composites in mind, it is thus of interest to understand the coupling between crystalline and particle-shape anisotropies and the conditions permitting to achieve macroscopic isotropy, in the framework of theoretical homogenization. The aim of this work is to provide a design tool for isotropic composites reinforced by aligned transversely isotropic particles particles. Section 2 presents the problem considered and notably the theoretical approach of mean-field homogenization. The condition of macroscopic isotropy is then derived in Section 3. Finally, a design tool is proposed in Section 4; correlations between transverse and longitudinal moduli of admissible particles are notably investigated.

2 Position of the problem

2.1 Preliminaries

We investigate the overall behavior of a two-phase composite made of an isotropic matrix reinforced by aligned transversely isotropic particles. The isotropic matrix is characterized by its shear and bulk moduli $G_0$ and $K_0$. The stiffness and compliance tensors of the matrix are denoted $C_0$ and $S_0$ respectively. The volume fraction of the matrix is denoted $f_0$. The particles are supposed to be transversely isotropic with stiffness and compliance tensors denoted $C_1$ and $S_1$ respectively. The shape of the particles is assumed to be spheroidal
with an aspect ratio $w$ ($w < 1$ corresponds to an oblate particle, $w = 1$ spherical and $w > 1$ prolate). Both material anisotropy and spheroidal axes are supposed to coincide with axis $e_3$, so it is expected that the overall behavior is transversely isotropic. Finally, the volume fraction of the particle is denoted $f_1 = 1 - f_0$.

In order to derive the overall behavior of the composite, it will be easy to express elasticity tensors with Walpole formalism [15], which provides a convenient framework to manipulate transversely isotropic tensors. Using this formalism, the transversely isotropic stiffness tensor $C_1$ is given by

$$C_1 = [2k_1, l_1, n_1, 2m_1, 2p_1],$$

and the compliance tensor $S_1$ reads

$$S_1 = \begin{bmatrix} n_1 / 2\Delta_1 & -l_1 / 2\Delta_1 & k_1 / \Delta_1 & 1 / 2m_1 & 1 / 2p_1 \end{bmatrix},$$

where $\Delta_1$ is given by

$$\Delta_1 = k_1 n_1 - l_1^2 / k_1.$$  

Positive definiteness of $C_1$ (and $S_1$) requires that all $k_1, m_1, p_1$ and $n_1 - l_1^2 / k_1$ are positive [15]. The moduli $k_1, l_1, n_1, m_1$ and $p_1$ can be expressed in terms of the components $C_{1,ijkl}$ through the following relations:

$$\begin{cases} k_1 = \frac{C_{1,1111} + C_{1,1122}}{2} = C_{1,1111} - C_{1,1212} \\ l_1 = C_{1,1133} = C_{1,2233} \\ n_1 = C_{1,3333} \\ m_1 = C_{1,1212} \\ p_1 = C_{1,2323} = C_{1,1313}. \end{cases}$$

For practical reasons it is also convenient to introduce the so-called engineering notations defining the transverse and longitudinal Young’s moduli $E_t$ and $E_l$, the transverse and longitudinal shear moduli $G_t$ and $G_l$, and the longitudinal Poisson ratio $\nu_l$. These coefficients are related to the moduli $(k_1, l_1, n_1, m_1, p_1)$ through

$$\begin{cases} E_l = n_1 - l_1^2 / k_1 \\ E_t = \frac{1}{4k_1} + \frac{1}{4m_1} + \frac{1}{4} \left( n_1 \frac{k_1^2}{l_1^2} - k_1 \right) \\ G_t = m_1 \\ G_l = p_1 \\ \nu_l = \frac{l_1}{2k_1}. \end{cases}$$

---

1 Elements of Walpole formalism are recalled in Appendix A.
The isotropic stiffness tensor $C_0$ can also be expressed in Walpole formalism:

$$C_0 = [2k_0, l_0, n_0, 2m_0, 2p_0], \quad (6)$$

where

$$m_0 = p_0 = G_0, \quad k_0 = K_0 + \frac{1}{3}G_0, \quad l_0 = K_0 - \frac{2}{3}G_0, \quad n_0 = K_0 + \frac{4}{3}G_0.$$

We finally recall that the Young’s modulus $E_0$ and Poisson ratio $\nu_0$ of the matrix are related to the bulk and shear moduli $K_0$ and $G_0$ through

$$E_0 = \frac{9K_0G_0}{3K_0 + G_0}, \quad \nu_0 = \frac{3K_0 - 2G_0}{2(3K_0 + G_0)}. \quad (7)$$

2.2 Macroscopic behavior of a particle-reinforced composite

The effective behavior of the composite material is investigated by the mean-field approach of homogenization. Since classical homogenization schemes make intensive use of Eshelby’s tensors, we recall that Eshelby’s polarization tensor $P$ (also known as Hill’s tensor) obtained from the Eshelby (classical) tensor $S^{\text{esh}}$ [14] is given by

$$P = S^{\text{esh}}.$$

(8)

Tensor $P$ depends on the moduli $G_0$ and $K_0$ of the matrix and on the aspect ratio $w$ of the particle. It possesses the symmetry of a transversely isotropic tensor and thus can be written under the form

$$P = [2k_p, l_p, n_p, 2m_p, 2p_p], \quad (9)$$

where the expressions of coefficients $k_p, l_p, n_p, m_p$ and $p_p$ are given in Appendix B and have the physical dimension of a compliance.

First, we consider the dilute scheme [9, 10] which applies for aligned ellipsoidal particles with a very small volume fraction. In its “primal” form, the macroscopic stiffness tensor, denoted $C^D$, is given by

$$C^D = C_0 + f_1 \left( P + (C_1 - C_0)^{-1} \right)^{-1}. \quad (10)$$

In its “dual” form, the macroscopic compliance tensor, denoted $S^D$, is given by

$$S^D = S_0 - f_1S_0 : \left( P + (C_1 - C_0)^{-1} \right)^{-1} : S_0. \quad (11)$$

It should be noted that $S^D \neq (C^D)^{-1}$, which means that the dilute scheme exhibits a “duality gap".  

4
Then, we consider Mori-Tanaka’s scheme [11] which applies for aligned ellipsoidal particles with a moderate volume fraction. For this model, the macroscopic stiffness tensor, denoted $\mathcal{C}^{MT}$, is given by

$$
\mathcal{C}^{MT} = \mathcal{C}_0 + f_1 \left(f_0 \mathcal{P} + (\mathcal{C}_1 - \mathcal{C}_0)^{-1}\right)^{-1}.
$$

(12)

Since Mori-Tanaka’s scheme does not exhibit a “duality gap”, the macroscopic compliance tensor $\mathcal{S}^{MT}$ simply reads $\mathcal{S}^{MT} = (\mathcal{C}^{MT})^{-1}$.

In order to simplify the notations, the effective behavior of the composite, denoted $\bar{\mathcal{C}}$, can thus be written under the generic form

$$
\bar{\mathcal{C}} = \mathcal{C}_0 + f_1 \left(f_c \mathcal{P} + (\mathcal{C}_1 - \mathcal{C}_0)^{-1}\right)^{-1},
$$

(13)

where $f_c = 1$ corresponds to the dilute scheme and $f_c = f_0$ corresponds to the model of Mori-Tanaka.

### 3 Condition of macroscopic isotropy

#### 3.1 Generalities

The aim of this Section is to derive the conditions that the particle and the matrix must fulfill so that the macroscopic behavior given by equation (13) becomes isotropic. Obviously, from equations (10), (11) and (12), a sufficient and necessary condition to ensure macroscopic isotropy is that the tensor

$$
A = f_c \mathcal{P} + (\mathcal{C}_1 - \mathcal{C}_0)^{-1}
$$

(14)

is isotropic (since $\mathcal{C}_0$ and $\mathcal{S}_0$ are isotropic). It is interesting to note that the tensor $A$ depends on (i) the coefficients of the isotropic matrix through $\mathcal{P}$ and $\mathcal{C}_0$, (ii) the anisotropy of the particles through $\mathcal{C}_1$ and (iii) the shape and volume fraction of the particle. Thus the condition of macroscopic isotropy will result in a subtle coupling between material anisotropy and shape of the particle.

#### 3.2 Derivation of the isotropy condition

Using Walpole formalism, the tensor $A$ reads

$$
A = \begin{bmatrix}
2f_c k_p + \frac{n_1 - n_0}{2\Delta_A}, f_c l_p - \frac{l_1 - l_0}{2\Delta_A}, f_c n_p + \frac{k_1 - k_0}{\Delta_A}, \\
2f_c m_p + \frac{1}{2(m_1 - m_0)}, 2f_c p_p + \frac{1}{2(p_1 - p_0)}
\end{bmatrix},
$$

(15)
where $\Delta_A$ is given by

$$\Delta_A = (k_1 - k_0)(n_1 - n_0) - (l_1 - l_0)^2.$$  \hspace{1cm} (16)

The isotropy condition implies that the tensor $A$ must be written under the form

$$A = [2(a + b), a, a + 2b, 2b, 2b],$$  \hspace{1cm} (17)

where $a$ and $b$ are arbitrary constants (see Appendix A). It should be noted that the parameters $a$ and $b$ are not related to a bulk and shear moduli since the tensor $A$ is not a stiffness tensor, but have the physical dimension of a compliance. Thus, the isotropy condition leads to the following system

$$\begin{cases} 
2f_cm_p + \frac{1}{2(m_1 - m_0)} = 2f_cl_p + \frac{1}{2(p_1 - p_0)} \\
2f_kp + \frac{n_1 - n_0}{2\Delta_A} = 2fkl_p - \frac{l_1 - l_0}{\Delta_A} + 2fcl_p + \frac{1}{2(p_1 - p_0)} \\
f_cm_p + \frac{k_1 - k_0}{\Delta_A} = f_cl_p - \frac{l_1 - l_0}{2\Delta_A} + 2fcl_p + \frac{1}{2(p_1 - p_0)}.
\end{cases}$$  \hspace{1cm} (18)

The isotropy condition consists in a system of three equations linking nine parameters, seven material constants ($K_0$, $G_0$, $k_1$, $l_1$, $n_1$, $m_1$, $p_1$), one morphological constant ($w$) and a constant related to the volume fraction of particles ($f_c$).

It should be noted that in the case of the dilute scheme, corresponding to $f_c = 1$, the isotropy condition is independent of the volume fraction of reinforcements.

3.3 Macroscopic behavior

When the isotropy condition (18) is verified, it is possible to express the macroscopic stiffness tensor of the isotropic composite from equation (13), denoted $\mathcal{C}^{iso}$, in a very compact way:

$$\mathcal{C}^{iso} = \left[2\left(\frac{1}{3}\overline{K} + \frac{1}{3}\overline{G}\right), \frac{2}{3}\overline{G}, \frac{4}{3}\overline{G}, 2\overline{G}, 2\overline{G}\right],$$  \hspace{1cm} (19)

where

$$3\overline{K} = 3K_0 + f_1\frac{1}{3c + 2d}, \quad 2\overline{G} = 2G_0 + f_1\frac{1}{2d},$$

$$c = f_cl_p - \frac{l_1 - l_0}{2\Delta_A}, \quad d = f_cm_p + \frac{1}{4m_1 - m_0}.$$
4 Design of transversely isotropic spheroidal particles achieving macroscopic isotropy

4.1 Generalities

The aim of this Section is to provide a design tool of transversely isotropic particles permitting to obtain macroscopic isotropic composites. Our objectives are twofold:

(1) We aim at providing analytic expressions of the components of the tensor $C_1$ for a given matrix $C_0$, a given shape $w$ and a given volume fraction $f_c$ of particles.

(2) We are interested in studying the correlation between material anisotropy through the coefficients of $C_1$ and morphological anisotropy through the coefficients $f_c$ and $w$.

The parameters $K_0$, $G_0$, $f_c$ and $w$ are thus assumed to be known and the problem reduces in finding the moduli $k_1$, $l_1$, $m_1$, $p_1$ which verify system (18). First, it is interesting to note that system (18) can be written under a dimensionless form by multiplying every terms by $G_0$; this leads to

$$
\begin{align*}
2f_cG_0m_p + \frac{1}{2 \left( \frac{m_1}{G_0} - 1 \right)} &= 2f_cG_0p_p + \frac{1}{2 \left( \frac{p_1}{G_0} - 1 \right)} \\
2f_cG_0k_p + \frac{n_1}{G_0} - \frac{K_0}{G_0} - \frac{4}{3} \frac{\Delta_A}{2} &= 2f_cG_0l_p - \frac{m_1}{G_0} - \frac{K_0}{G_0} + \frac{2}{3} \frac{\Delta_A}{2} + 2f_cG_0p_p + \frac{1}{2 \left( \frac{p_1}{G_0} - 1 \right)} \\
f_cG_0n_p + \frac{k_1}{G_0} - \frac{K_0}{G_0} - \frac{1}{3} \frac{\Delta_A}{3} &= f_cG_0l_p - \frac{l_1}{G_0} - \frac{K_0}{G_0} + \frac{2}{3} \frac{\Delta_A}{2} + 2f_cG_0p_p + \frac{1}{2 \left( \frac{p_1}{G_0} - 1 \right)}
\end{align*}
$$

(20)

where

$$
\tilde{\Delta}_A = \left( \frac{k_1}{G_0} - \frac{K_0}{G_0} - \frac{1}{3} \right) \times \left( \frac{n_1}{G_0} - \frac{K_0}{G_0} - \frac{4}{3} \right) - \left( \frac{l_1}{G_0} - \frac{K_0}{G_0} + \frac{2}{3} \right)^2.
$$

(21)
Here, the coefficients $G_0 k_p$, $G_0 l_p$, $G_0 n_p$, $G_0 m_p$ and $G_0 p_p$ are given by

\[
\begin{align*}
G_0 k_p &= \frac{7h(w) - 2w^2 - 4w^2 h(w) + (h(w) - 2w^2 + 2w^2 h(w))3K_0/G_0}{8(1-w^2)(4+3K_0/G_0)} \\
G_0 l_p &= \frac{(2w^2 - h(w) - 2w^2 h(w)) \times (1 + 3K_0/G_0)}{4(1-w^2)(4+3K_0/G_0)} \\
G_0 n_p &= \frac{6 - 5h(w) - 8w^2 h(w) + (h(w) - 2w^2 + 2w^2 h(w))3K_0/G_0}{2(1-w^2)(4+3K_0/G_0)} \\
G_0 m_p &= \frac{15h(w) - 2w^2 - 12w^2 h(w) + (3h(w) - 2w^2)3K_0/G_0}{16(1-w^2)(4+3K_0/G_0)} \\
G_0 p_p &= \frac{8 - 6h(w) - 4w^2 + (2 - 3h(w) + 2w^2 - 3w^2 h(w))3K_0/G_0}{8(1-w^2)(4+3K_0/G_0)},
\end{align*}
\]

where $h(w)$ is given in Appendix A.

The isotropy condition consists in a system of three equations that links the dimensionless moduli $k_1/G_0$, $l_1/G_0$, $n_1/G_0$, $m_1/G_0$, $p_1/G_0$ to $w$, $f_c$ and the ratio $K_0/G_0$. It is thus remarkable that these dimensionless ratios only depend on the matrix behavior through its Poisson ratio since the quantity $K_0/G_0$ reads, using equation (7):

\[
\frac{3K_0}{G_0} = \frac{2(1 + \nu_0)}{1 - 2\nu_0}.
\]

(23)

The resolution consists in finding five unknowns verifying three equations for which there is \textit{a priori} an infinity of solutions. In order to determine a set of admissible material constants, it is however possible to fix arbitrarily two coefficients, $n_1/G_0$ and $l_1/G_0$ for instance, and to deduce the remaining three coefficients which are given by

\[
\begin{align*}
k_1 &= \frac{K_0}{G_0} + \frac{1}{3} + \frac{\frac{l_1}{G_0} + \frac{n_1}{G_0} - 2 \frac{K_0}{G_0} - \frac{2}{3} - 2f_c(2G_0 k_p - G_0 l_p - G_0 n_p) \left( \frac{l_1}{G_0} - \frac{K_0}{G_0} + \frac{2}{3} \right)^2}{2 \left( 1 - f_c(2G_0 k_p - G_0 l_p - G_0 n_p) \left( \frac{n_1}{G_0} - \frac{K_0}{G_0} - \frac{4}{3} \right)^2 \right)} \\
p_1 &= 1 + \frac{\Delta_A}{\frac{p_1}{G_0} - 1} \\
m_1 &= 1 + \frac{\Delta_A}{1 + 4f_c \left( \frac{p_1}{G_0} - 1 \right) (G_0 p_p - G_0 m_p)},
\end{align*}
\]

(24)

where $\Delta_A$ is given in terms of $n_1/G_0$ and $l_1/G_0$ using equations (21) and (24). Thus, if one explores accurately the space of $n_1/G_0$ and $l_1/G_0$, it is possible to obtain a large
set of admissible values for the material constants and thus deduce the set of admissible particles for a given matrix behavior, shape and volume fraction of particles.

4.2 Correlation between transverse and longitudinal shear moduli

First, we study the relation between transverse and longitudinal dimensionless shear moduli $G_t/G_0$ and $G_l/G_0$ which are given by

$$\begin{align*}
\frac{G_t}{G_0} &= \frac{m_1}{G_0}, \\
\frac{G_l}{G_0} &= \frac{p_1}{G_0},
\end{align*}$$

(25)

where $m_1/G_0$ and $p_1/G_0$ are related to each other by equation (24). Thus, the transverse shear modulus $G_t/G_0$ can be expressed in terms of the longitudinal shear modulus $G_l/G_0$ by the equation

$$\frac{G_t}{G_0} = 1 + \frac{G_l}{G_0} - 1 \times g\left(f_c, w, \frac{K_0}{G_0}\right),$$

(26)

where the function $g\left(f_c, w, \frac{K_0}{G_0}\right)$ is given by

$$g\left(f_c, w, \frac{K_0}{G_0}\right) = f_c \frac{16 - 27h(w) - 6w^2 + 12h(w)w^2 + (4 - 9h(w) + 6w^2 - 6w^2h(w))3K_0}{4(1 - w^2)\left(4 + 3\frac{K_0}{G_0}\right)}.$$  

(27)

It is remarkable that the shear moduli $G_t/G_0$ and $G_l/G_0$ of a particle achieving macroscopic isotropy are related to each other through a formula that only depends on the particle shape $w$, the ratio $K_0/G_0$ related to the Poisson ratio of the matrix, and the parameter $f_c$ which is related to the volume fraction $f_0$. For illustrative purpose, the transverse shear modulus $G_t/G_0$ versus the longitudinal shear modulus $G_l/G_0$ is represented in Figure 1 for the value $f_c = 1$ (which corresponds to the dilute scheme), various values of the particle shape $w$ and various values of $K_0/G_0$ corresponding to different families matrix materials: $K_0/G_0 = 1/6$ or $\nu_0 = -1/2$ (auxetic matrix), $K_0/G_0 = 4/3$ or $\nu_0 = 2/5$ (concrete), $K_0/G_0 = 8/3$ or $\nu_0 = 1/3$ (metallic alloys), $K_0/G_0 = 100$ or $\nu_0 = 0.495$ (rubber).
Fig. 1. Dimensionless transverse shear modulus $G_t/G_0$ versus longitudinal shear modulus $G_l/G_0$ in the case $f_c = 1$ (high dilution). (a) $K_0/G_0 = 1/6$ or $\nu_0 = -1/2$ (auxetic matrix), (b) $K_0/G_0 = 4/3$ or $\nu_0 = 2/5$ (concrete), (c) $K_0/G_0 = 8/3$ or $\nu_0 = 1/3$ (metallic alloys) and (d) $K_0/G_0 = 100$ or $\nu_0 = 0.495$ (rubber)
Some comments are in order:

- For prolate particles \((w > 1)\), the transverse shear modulus of a particle achieving macroscopic isotropy is greater than the longitudinal shear modulus. Thus, the morphological anisotropy induced by the particle shape is balanced by an increase of the transverse shear modulus. In the asymptotic geometrical case \(w \to +\infty\) corresponding to fibers, equation (26) reduces to

\[
\frac{G_t}{G_0} = 1 + \frac{G_l - 1}{1 - \frac{3f_c}{2(4 + 3K_0/G_0)} \times \left(\frac{G_l}{G_0} - 1\right)}.
\]

(28)

It is thus possible to achieve macroscopic isotropy with parallel anisotropic cylindrical fibers but their shear modulus is limited by the value

\[
\left(\frac{G_t}{G_0}\right)_{\text{max}} = 1 + \frac{2}{3f_c} \left(4 + 3K_0/G_0\right).
\]

(29)

- For spherical particles \((w = 1)\), one gets \(g = 0\) and thus \(G_t = G_l\). This is of course expected since in this case, the only way to achieve macroscopic isotropy is to consider isotropic particles.

- For oblate particles \((w < 1)\), the transverse shear modulus of a particle achieving macroscopic isotropy is lower than the longitudinal shear modulus. Again, the morphological anisotropy induced by the particle shape is balanced by an increase of material anisotropy. In the asymptotic case \(w \to 0\) corresponding to penny shape particles, equation (26) reduces to

\[
\frac{G_t}{G_0} = 1 + \frac{G_l - 1}{1 + f_c \left(\frac{G_l}{G_0} - 1\right)}.
\]

(30)

Thus, it is also possible to achieve macroscopic isotropy with parallel penny shape particles, but their transverse shear modulus is limited by the value

\[
\left(\frac{G_t}{G_0}\right)_{\text{max}} = 1 + \frac{1}{f_c}.
\]

(31)
4.3 Correlation between transverse and longitudinal Young’s moduli

We study now the correlation between transverse and longitudinal Young’s moduli. From equation (5), the dimensionless transverse and longitudinal Young’s moduli \( E_t/E_0 \) and \( E_l/E_0 \) are given by

\[
\begin{align*}
E_t/E_0 &= \left( \frac{9K_0}{3K_0/G_0 + 1} \right) \left( \frac{n_1}{G_0} - \left( \frac{l_1}{G_0} \right)^2 \frac{G_0}{k_1} \right), \\
E_l/E_0 &= \frac{36K_0/G_0}{3K_0/G_0 + 1} \times \frac{G_0}{k_1 + \frac{G_0}{m_1} + \frac{n_1}{G_0} \left( \frac{k_1}{G_0} \right)^2 \left( \frac{G_0}{l_1} \right)^2 - \frac{k_1}{G_0}},
\end{align*}
\]

where the coefficients \( k_1/G_0 \) and \( m_1/G_0 \) are given in terms of \( n_1/G_0 \) and \( l_1/G_0 \) by equation (24). It appears that the transverse and longitudinal Young’s moduli are both expressed only in terms of \( n_1/G_0 \) and \( l_1/G_0 \) in a very nonlinear way. In contrast to the case of the shear moduli studied in Section 4.2, it is impossible to obtain an analytic relation between \( E_t/E_0 \) and \( E_l/E_0 \) involving only \( f_c, w \) and \( K_0/G_0 \). However, it is still possible to determine a set of admissible values \( E_l/E_0 \) and \( E_t/E_0 \) by exploring the space of \( n_1/G_0 \) and \( l_1/G_0 \) as explained in Section 4.1. A large number of values is considered which permits to plot in Figure 2 the ratio \( E_t/E_0 \) versus \( E_l/E_0 \) for the same \( K_0/G_0 \) values as in Figure 1. Again, the value \( f_c = 1 \) is considered in all cases.

Overall, the results are similar to those obtained for the shear moduli in particular for \( K_0/G_0 = 4/3 \) and \( K_0/G_0 = 8/3 \). It is worth noting that the relation between the transverse and longitudinal moduli is no longer a bijection: for a given value \( E_l/E_0 \) there are multiple admissible values \( E_t/E_0 \) that are bounded, the size of the domain depending on the values of \( w \) and \( K_0/G_0 \). For prolate particles achieving macroscopic isotropy, the transverse Young’s modulus is in general greater than the longitudinal one. Conversely, for oblate particles achieving macroscopic isotropy, the transverse Young’s modulus is in general lower than the longitudinal one. It should be noted that peculiar behaviors are observed mainly for a rubber matrix (\( K_0/G_0 = 100 \) or \( \nu_0 = 0.495 \)), where the transverse Young’s modulus can be lower than the longitudinal one for prolate particles and the transverse Young’s modulus greater than the longitudinal one for oblate particles. These peculiar behaviors are notably due to admissible materials which possess a negative transverse Poisson ratio given by \( \nu_t = E_t/(2G_t) - 1 \).
Fig. 2. Dimensionless transverse Young’s modulus $E_t/E_0$ versus longitudinal Young’s modulus $E_l/E_0$ in the case $f_c = 1$ (high dilution). (a) $K_0/G_0 = 1/6$ or $\nu_0 = -1/2$ (auxetic matrix), (b) $K_0/G_0 = 4/3$ or $\nu_0 = 2/5$ (concrete), (c) $K_0/G_0 = 8/3$ or $\nu_0 = 1/3$ (metallic alloys) and (d) $K_0/G_0 = 100$ or $\nu_0 = 0.495$ (rubber).
4.4 Application to metal-matrix composites

We investigate finally the design of particles for aluminum and steel matrix composites, and notably their possible relation with popular particles such as silicon carbide (SiC) and titanium diboride (TiB₂).

If it is unlikely that a 9-tuplets \((K_0, G_0, k_1, l_1, n_1, m_1, p_1, w, f_c)\) could lead to macroscopic isotropy in the exact case of Al-SiC and Fe-TiB₂ composites, it is however possible to determine admissible materials constituting the particles achieving macroscopic isotropy, called ideal materials, that are close to the desired materials (SiC or TiB₂), called real materials. The closeness between real and ideal materials is characterized by the distance between their stiffness tensors, denoted \(C_{\text{real}}\) and \(C_{\text{ideal}}\) respectively. The Log-Euclidean distance \([16, 17]\) is used in order to provide a relative error between tensors denoted \(\text{dist}(C_{\text{real}}, C_{\text{ideal}})\) and given by:

\[
\text{dist}(C_{\text{real}}, C_{\text{ideal}}) = \frac{||\log(C_{\text{real}}) - \log(C_{\text{ideal}})||}{\sqrt{6}}. \tag{33}
\]

The procedure to obtain the logarithm of a matrix can be found in \([16]\). The choice of the Log-Euclidean distance over the classical Euclidean distance is motivated by the fact that it preserves the invariance under the operation of inversion and thus the duality between stiffness and compliance \([16, 17]\). It should be noted that the coefficient \(\sqrt{6}\) in equation (33) has been added to the classical Log-Euclidean distance so that the distance between two tensors \(C_1\) and \(\alpha C_1\), with \(\alpha\) a non-negative scalar, reduces to \(\text{dist}(C_1, \alpha C_1) = \log(\alpha)\); this permits to extend the notion of “relative error” to the tensorial case.

**Case of Al-SiC.** First, we consider the case of an aluminum matrix \((E_0 = 68.8 \text{ GPa}, \; G_0 = 26 \text{ GPa}, \; v_0 = 0.32)\) reinforced by silicon carbide particles (Al-SiC), which constitutes one of the most popular metal-matrix composites due to an increase of tensile strength, hardness and wear resistance \([18]\). Silicon carbides can be found under various polytypes (cubic, hexagonal or rhombohedral) inducing various elastic behaviors, according to the Landolt-Bornstein database. We consider here the 6H-SiC which is the most commonly used SiC polytype \([19]\), for which there are several existing sets of elastic constants in the literature. We consider two sets of elastic constants, obtained from (i) a bond charge model calculation \([20]\) (case 1) and (ii) Brillouin scattering experiments \([21]\) (case 2). The stiffness tensors obtained from these two approaches are slightly different (see Tables 1 and 2) and the relative error between these two tensors takes the value

\[
\text{dist}(C_{\text{case1}}^{\text{real}}, C_{\text{case2}}^{\text{real}}) = 0.231. \tag{34}
\]

This value permits to express the degree of uncertainty that is made on the knowledge of the material behavior. The elastic constants of the closest ideal particles achieving macroscopic isotropy, together with the associated relative errors, are given for various particles shapes in Tables 1 and 2, for the cases 1 and 2 respectively. For the case 1, it is possible to achieve isotropy with a material reasonably close to the real 6H-SiC \([20]\) for \(f_1 = 0.1\) and \(w = 0.96\), with a distance that takes the value 0.091. For the case 2,
it is possible to achieve isotropy with a material also reasonably close to the second real 6H-SiC [21] for \( f_1 = 0.1 \) and \( w = 0.97 \), with a distance that takes this time the value 0.145. Thus, in both cases, it is possible to achieve macroscopic isotropy with slightly oblate particles made of materials that are close to real SiC, with a relative error that is of the order of the uncertainty made on the SiC constants.

| Material | \( C_{1111} \) | \( C_{1122} \) | \( C_{1133} \) | \( C_{3333} \) | \( C_{2323} \) | \( E_l \) | \( E_t \) | \( G_l \) | \( G_t \) | \( \nu_l \) | dist \\
|----------|----------------|----------------|----------------|----------------|----------------|-------------|-------------|-------------|-------------|--------------|----------|
| 6H-SiC Case 1 [20] | 498 | 186 | 176 | 567 | 141 | 476 | 404 | 141 | 156 | 0.257 | - \\
| Ideal particle | \( f_1 = 0.1 \), \( w = 0.5 \) | 333 | 140 | 186 | 685 | 168 | 538 | 254 | 168 | 96 | 0.39 | 0.354 \\
| \( f_1 = 0.1 \), \( w = 0.8 \) | 447 | 178 | 192 | 595 | 164 | 477 | 350 | 164 | 134 | 0.31 | 0.136 \\
| \( f_1 = 0.1 \), \( w = 0.9 \) | 478 | 186 | 191 | 546 | 160 | 435 | 376 | 160 | 146 | 0.29 | 0.096 \\
| \( f_1 = 0.1 \), \( w = 0.96 \) | 492 | 189 | 191 | 517 | 157 | 410 | 388 | 157 | 151 | 0.28 | 0.091 \\
| \( f_1 = 0.1 \), \( w = 2 \) | 544 | 177 | 188 | 331 | 125 | 233 | 426 | 125 | 184 | 0.26 | 0.311 \\

Table 1  
Closest materials to a real 6H-SiC [20] achieving macroscopic isotropy for various aspect ratios \( w \). The elastic moduli \( C_{ijkl} \), \( E_l \), \( E_t \), \( G_l \) and \( G_t \) are expressed in GPa.

| Material | \( C_{1111} \) | \( C_{1122} \) | \( C_{1133} \) | \( C_{3333} \) | \( C_{2323} \) | \( E_l \) | \( E_t \) | \( G_l \) | \( G_t \) | \( \nu_l \) | dist \\
|----------|----------------|----------------|----------------|----------------|----------------|-------------|-------------|-------------|-------------|--------------|----------|
| 6H-SiC Case 2 [21] | 501 | 111 | 52 | 553 | 163 | 544 | 473 | 163 | 195 | 0.085 | - \\
| Ideal particle | \( f_1 = 0.1 \), \( w = 0.5 \) | 298 | 87 | 82 | 625 | 212 | 590 | 267 | 212 | 106 | 0.21 | 0.441 \\
| \( f_1 = 0.1 \), \( w = 0.8 \) | 416 | 101 | 86 | 573 | 204 | 544 | 384 | 204 | 158 | 0.17 | 0.203 \\
| \( f_1 = 0.1 \), \( w = 0.9 \) | 449 | 98 | 89 | 522 | 198 | 493 | 418 | 198 | 175 | 0.16 | 0.157 \\
| \( f_1 = 0.1 \), \( w = 0.97 \) | 471 | 97 | 94 | 492 | 194 | 461 | 439 | 194 | 187 | 0.17 | 0.145 \\
| \( f_1 = 0.1 \), \( w = 2 \) | 526 | 43 | 118 | 295 | 146 | 246 | 479 | 146 | 241 | 0.21 | 0.375 \\

Table 2  
Closest materials to a real 6H-SiC [21] achieving macroscopic isotropy for various aspect ratios \( w \). The elastic moduli \( C_{ijkl} \), \( E_l \), \( E_t \), \( G_l \) and \( G_t \) are expressed in GPa.

**Case of Fe-TiB\(_2\).** Then, we consider the case of a steel (\( E_0 = 208 \) GPa, \( G_0 = 80 \) GPa, \( \nu_0 = 0.3 \)) reinforced by titanium diboride (Fe-TiB\(_2\)), which is a promising material with improved specific properties [22]. As in the case of SiC, there are several sets of elastic constants available in the literature. We consider two sets obtained from (i) the pulse-echo method [23] (case 3) (ii) the rectangular parallelepiped resonance method [24] (case 4). The associated stiffness tensors are again quite different (see Tables 3 and 4) and their distance takes the value

\[
\text{dist}(\mathbf{c}^{\text{case3}}_{\text{real}}, \mathbf{c}^{\text{case4}}_{\text{real}}) = 0.556. \tag{35}
\]

The elastic constants of the closest ideal particles achieving macroscopic isotropy, together with the associated relative errors, are given for various particles shapes in Tables 3 and 4, for the cases 3 and 4 respectively. For the case 3, it is possible to achieve isotropy with
a material reasonably close to the real TiB$_2$ [23] for $f_1 = 0.1$ and $w = \infty$, with a distance that takes the value 0.312. For the case 2, it is possible to achieve isotropy with a material very close close to the second real TiB$_2$ [24] for $f_1 = 0.1$ and $w = 4$, with a distance that takes this time the value 0.066. Thus, in both cases, it is possible to achieve macroscopic isotropy with elongated particles made of materials that are close to TiB$_2$ with a relative error that is smaller than the uncertainty made on TiB$_2$ elastic constants.

Table 3

Closest materials to a real TiB$_2$ [23] achieving macroscopic isotropy for various aspect ratios $w$. The elastic moduli $C_{ijkl}$, $E_l$, $E_t$, $G_l$ and $G_t$ are expressed in GPa.

<table>
<thead>
<tr>
<th>Material</th>
<th>$C_{1111}$</th>
<th>$C_{1122}$</th>
<th>$C_{1133}$</th>
<th>$C_{3333}$</th>
<th>$C_{2323}$</th>
<th>$E_l$</th>
<th>$E_t$</th>
<th>$G_l$</th>
<th>$G_t$</th>
<th>$\nu_l$</th>
<th>dist.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TiB$_2$ Case 3 [23]</td>
<td>690</td>
<td>410</td>
<td>320</td>
<td>440</td>
<td>250</td>
<td>254</td>
<td>389</td>
<td>250</td>
<td>140</td>
<td>0.29</td>
<td>-</td>
</tr>
<tr>
<td>Ideal particle</td>
<td>$f_1 = 0.1$, $w = 0.5$</td>
<td>593</td>
<td>276</td>
<td>298</td>
<td>692</td>
<td>176</td>
<td>487</td>
<td>417</td>
<td>176</td>
<td>158</td>
<td>0.34</td>
</tr>
<tr>
<td></td>
<td>$f_1 = 0.1$, $w = 1.5$</td>
<td>682</td>
<td>338</td>
<td>327</td>
<td>630</td>
<td>165</td>
<td>420</td>
<td>457</td>
<td>165</td>
<td>172</td>
<td>0.32</td>
</tr>
<tr>
<td></td>
<td>$f_1 = 0.1$, $w = 2$</td>
<td>682</td>
<td>333</td>
<td>319</td>
<td>604</td>
<td>165</td>
<td>404</td>
<td>461</td>
<td>165</td>
<td>175</td>
<td>0.31</td>
</tr>
<tr>
<td></td>
<td>$f_1 = 0.1$, $w = 5$</td>
<td>703</td>
<td>343</td>
<td>324</td>
<td>577</td>
<td>166</td>
<td>376</td>
<td>471</td>
<td>166</td>
<td>180</td>
<td>0.31</td>
</tr>
<tr>
<td></td>
<td>$f_1 = 0.1$, $w = \infty$</td>
<td>714</td>
<td>342</td>
<td>325</td>
<td>565</td>
<td>171</td>
<td>366</td>
<td>482</td>
<td>171</td>
<td>186</td>
<td>0.31</td>
</tr>
</tbody>
</table>

Table 4

Closest materials to a real TiB$_2$ [24] achieving macroscopic isotropy for various aspect ratios $w$. The elastic moduli $C_{ijkl}$, $E_l$, $E_t$, $G_l$ and $G_t$ are expressed in GPa.

<table>
<thead>
<tr>
<th>Material</th>
<th>$C_{1111}$</th>
<th>$C_{1122}$</th>
<th>$C_{1133}$</th>
<th>$C_{3333}$</th>
<th>$C_{2323}$</th>
<th>$E_l$</th>
<th>$E_t$</th>
<th>$G_l$</th>
<th>$G_t$</th>
<th>$\nu_l$</th>
<th>dist.</th>
</tr>
</thead>
<tbody>
<tr>
<td>TiB$_2$ Case 4 [24]</td>
<td>660</td>
<td>48</td>
<td>93</td>
<td>432</td>
<td>260</td>
<td>408</td>
<td>639</td>
<td>260</td>
<td>306</td>
<td>0.13</td>
<td>-</td>
</tr>
<tr>
<td>Ideal particle</td>
<td>$f_1 = 0.1$, $w = 0.5$</td>
<td>519</td>
<td>90</td>
<td>51</td>
<td>614</td>
<td>278</td>
<td>605</td>
<td>501</td>
<td>278</td>
<td>215</td>
<td>0.08</td>
</tr>
<tr>
<td></td>
<td>$f_1 = 0.1$, $w = 1.5$</td>
<td>627</td>
<td>54</td>
<td>89</td>
<td>556</td>
<td>255</td>
<td>532</td>
<td>610</td>
<td>255</td>
<td>287</td>
<td>0.13</td>
</tr>
<tr>
<td></td>
<td>$f_1 = 0.1$, $w = 2$</td>
<td>637</td>
<td>37</td>
<td>96</td>
<td>527</td>
<td>252</td>
<td>499</td>
<td>619</td>
<td>252</td>
<td>300</td>
<td>0.14</td>
</tr>
<tr>
<td></td>
<td>$f_1 = 0.1$, $w = 4$</td>
<td>643</td>
<td>22</td>
<td>113</td>
<td>485</td>
<td>247</td>
<td>446</td>
<td>617</td>
<td>247</td>
<td>310</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td>$f_1 = 0.1$, $w = \infty$</td>
<td>645</td>
<td>9</td>
<td>124</td>
<td>458</td>
<td>252</td>
<td>411</td>
<td>611</td>
<td>252</td>
<td>318</td>
<td>0.19</td>
</tr>
</tbody>
</table>

5 Conclusion

The aim of this paper was to study the design of isotropic composites made of an isotropic matrix reinforced by aligned transversely isotropic particles of spheroidal shape.

First, we derived analytical conditions for macroscopic isotropy of composites reinforced by aligned transversely isotropic particles of spheroidal shape in the framework of mean-field homogenization using the dilute and Mori-Tanaka’s schemes. This has permitted to
express the isotropy condition as a system of three nonlinear equations liking nine parameters. Sets of admissible anisotropic particles were then provided for a given matrix behavior and shape of the particles. Correlations between transverse and shear moduli have permitted to investigate the coupling between material and morphological anisotropies. In general, the transverse modulus is greater than the longitudinal modulus for prolate particles. Conversely, the transverse modulus is in general lower than the longitudinal modulus for oblate particles. Finally, the design of metal-matrix composite was investigated. In the case of an aluminum matrix, admissible oblate particles close to SiC have been found to achieve macroscopic isotropy, permitting the design of isotropic Al-SiC composites. In the case of a steel matrix, admissible elongated particles close to TiB$_2$ have been found to achieve macroscopic isotropy, permitting the design of isotropic Fe-TiB$_2$ composites.

The obtained design may be directly used in industrial applications to provide new isotropic composites made of standard, anisotropic reinforcements such as SiC or TiB$_2$ for instance. Interestingly, it could be also employed in more complicated situations where the mechanical properties are designed to be isotropic but other physical properties such as electrical or acoustic properties, may stay anisotropic due to the particle shape.

Finally, it should be noted that the design tool proposed in this paper only applies to some ideal situations. In order to extend this design to more realistic situations, several directions can be explored:

- The spatial distribution of the particles’ centers, which was supposed to be random, could be introduced in order to account for a more realistic microstructure. The effect of spatial distribution was investigated, in the theoretical homogenization framework, by Ponte Castañeda and Willis [25] through a distribution tensor that modifies Mori-Tanaka’s estimate. Thus, it would be possible to derive a condition of macroscopic isotropy including this effect (at the cost of additional parameters).
- Particles were supposed to be perfectly aligned and material anisotropy axes of the particles were supposed to coincide with the geometric anisotropy axes; these assumptions permitted to obtain a first estimate of the parameters achieving macroscopic isotropy. It could be interesting to complement the proposed approximate design by full-field simulations performed on real microstructures in order to investigate the effect of these assumptions on macroscopic isotropy.

Acknowledgments

Fruitful discussions with Z. Hamouche are gratefully acknowledged.
A  Walpole formalism

Walpole formalism [15] is a convenient framework to manipulate transversely isotropic fourth-order tensors. Let us consider two transversely isotropic tensors given by

\[
L_1 = [2k_1, l_1, n_1, 2m_1, 2p_1], \quad L_2 = [2k_2, l_2, n_2, 2m_2, 2p_2].
\]  

(A.1)

The product between \( L_1 \) and \( L_2 \) is given by

\[
L_1 : L_2 = [4k_1k_2 + 2l_1l_2, 2k_1l_2 + n_2l_1, 2l_1l_2 + n_1n_2, 4m_1m_2, 4p_1p_2],
\]  

(A.2)

and the inverse of \( L_1 \) is given by

\[
L_1^{-1} = \left[ \frac{n_1}{2\Delta_1}, -\frac{l_1}{2\Delta_1}, \frac{k_1}{\Delta_1}, \frac{1}{2m_1}, \frac{1}{2p_1} \right], \quad \Delta_1 = k_1n_1 - l_1^2.
\]  

(A.3)

An isotropic stiffness tensor \( C_{iso} \), with bulk and shear moduli denoted \( K_{iso} \) and \( G_{iso} \) respectively, can be written under the form

\[
C_{iso} = [2(\alpha + \beta), \alpha, \alpha + 2\beta, 2\beta, 2\beta],
\]  

(A.4)

where

\[
\beta = G_{iso}, \quad \alpha = K_{iso} - \frac{2}{3}G_{iso}.
\]  

(A.5)

The corresponding isotropic compliance tensor \( S_{iso} = C_{iso}^{-1} \) can also be written under the form

\[
S_{iso} = [2(\gamma + \delta), \gamma, \gamma + 2\delta, 2\delta, 2\delta],
\]  

(A.6)

where

\[
\delta = \frac{1}{4\beta} = \frac{1}{4G_{iso}}, \quad \gamma = \frac{1}{9\alpha + 6\beta} - \frac{1}{6\beta} = \frac{1}{9K_{iso}} - \frac{1}{6G_{iso}}.
\]  

(A.7)

B  Eshelby polarization tensor

The components of the Eshelby polarization tensor \( P \) for a spheroidal inclusion with aspect ratio \( w \) and axis of symmetry \( e_3 \) embedded in an isotropic matrix with shear and bulk
moduli $G_0$ and $K_0$ are given, in Walpole formalism, by [25]

\[
\begin{align*}
    k_p &= \frac{(7h(w) - 2w^2 - 4h^2(w))G_0 + 3(h(w) - 2w^2 + 2h^2(w))K_0}{8(1 - w^2)G_0(4G_0 + 3K_0)} \\
    l_p &= \frac{(2w^2 - h(w) - 2w^2h(w))(G_0 + 3K_0)}{8(1 - w^2)G_0(4G_0 + 3K_0)} \\
    n_p &= \frac{(6 - 5h(w) - 8w^2h(w))G_0 + 3(h(w) - 2w^2 + 2w^2h(w))K_0}{2(1 - w^2)G_0(4G_0 + 3K_0)} \\
    m_p &= \frac{(15h(w) - 2w^2 - 12w^2h(w))G_0 + 3(3h(w) - 2w^2)K_0}{16(1 - w^2)G_0(4G_0 + 3K_0)} \\
    p_p &= \frac{2(4 - 3h(w) - 2w^2)G_0 + 3(2 - 3h(w) + 2w^2 - 3w^2h(w))K_0}{8(1 - w^2)G_0(4K_0 + 3K_0)}.
\end{align*}
\] (B.1)

For oblate spheroids ($w < 1$), the function $h$ is given by

\[
h(w) = \frac{w \left( \arccos(w) - w\sqrt{w^2 - 1} \right)}{(1 - w^2)^{\frac{3}{2}}} \tag{B.2}
\]

and for prolate spheroids ($w > 1$), it reads

\[
h(w) = \frac{w \left( \sqrt{w^2 - 1} - \text{argcosh}(w) \right)}{(w^2 - 1)^{\frac{3}{2}}} \tag{B.3}
\]

The limit $w \to 1$ gives $h(1) = 2/3$ for a sphere.

References


