# Morphologically representative pattern-based bounding in elasticity

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# MORPHOLOGICALLY REPRESENTATIVE PATTERN-BASED BOUNDING IN ELASTICITY

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A general theory for the homogenization of heterogeneous linear elastic materials that relies on the concept of "morphologically representative pattern" is given. It allows the derivation of rigorous bounds for the effective behaviour of the Voigt–Reuss-type, which apply to any distribution of patterns, or of the Hashin–Shtrikman-type, which are restricted to materials whose pattern distributions are isotropic. Particular anisotropic distributions of patterns can also be considered: Hashin Shtrikman-type bounds for aniso-tropic media are then generated. The resolution of the homogenization problem leads to a complex composite inclusion problem with no analytical solution in the general case. Here it is solved by a numerical procedure based on the finite element method. As an example of possible application, this procedure is used to derive new bounds for matrix–inclusion composites with cubic symmetry as well as for transversely isotropic materials.

## 1. INTRODUCTION

Powerful variational methods have been developed in order to derive bounds for the overall moduli of heterogeneous linear elastic materials. The classical Voigt–Reuss and Hashin–Shtrikman bounds (Hashin and Shtrikman, 1963; Walpole, 1966) involve only the volume fractions of the constituent phases. The first ones are valid for any heterogeneous medium, whereas the second ones apply to macroscopically isotropic materials, but with no other specific assumption on the microstructural distribution of the phases. The latter have more recently been generalized to anisotropic behaviour (Walpole, 1969; Willis, 1977, 1978; Milton and Kohn, 1988; Ponte Castañeda and Willis, 1995). Recent trends in the analysis of inhomogeneous elastic random media are the derivation of bounds for their overall characteristics which could be closer and closer for an increasing knowledge of their structural morphology. The so-called "systematic theory" (Kröner and Koch, 1976; Kröner, 1977) is based on the use of point-correlation functions of the elastic moduli of the constituent phases. It allows the derivation of $n$th order bounds for the elastic properties of the effective medium, which involve the $i$th order correlation functions, for $i < n$. A particular case is obtained when these $n$-point phase correlation functions satisfy some particular conditions involving the non-local part of the modified Green's tensor of the infinite medium. The generated bounds can then be derived analytically thanks to the local part of the modified Green's tensor; the corresponding conditions describe the so-

called "graded disorder". When $n$ tends to infinity, the upper and lower bounds tend to a unique limit, which corresponds to the classical self-consistent estimate (Hershey, 1954; Kröner, 1958; Hill, 1965). Unfortunately the practical significance of these $n$th order conditions is not so clear, except for $n = 2$ which corresponds to the previously mentioned classical Hashin–Shtrikman bounds. The case $n = \infty$ describes the so-called "perfect disorder", and has proved its efficiency for the description of non-textured polycrystals, in which the orientations of the grains are randomly distributed and not correlated with the grain geometry. Other approaches are able to take into account the particular microgeometrical features of the considered materials, for instance through conditional probabilities (Willis, 1981) or through the determination of some particular parameters (Milton and Phan-Thien, 1982). The obtained bounds are closer and thus provide better estimates for the effective behaviour, since they involve more microstructural information; conversely the effect of particular microstructural features on the macroscopic behaviour may in principle also be investigated.

Nevertheless in practice it is very difficult to take benefit of such approaches in order to take into account some primary morphological characteristics such as the phase continuity or discontinuity, the presence of inclusions in a matrix, the shape and orientation of such inclusions, or local phase concentration fluctuations... As has been proposed recently (Stolz and Zaoui, 1991), such properties may be accounted for more conveniently by describing the considered materials as assemblages of adequate composite patterns. In this approach, the material is completely characterized by the description of these "morphologically representative patterns" and their spatial distribution. The concept of "phase" is then generalized to the one of "morphological phase": such a morphological phase is the domain occupied by all the realizations $D_i^r$ in the material of a given pattern $D_i$, which contains a specific and representative disposition of some of the constitutive "mechanical phases" $r$. Hashin's composite spheres assemblage (CSA) (Hashin, 1962) provides the prototype for microstructures that are advantageously described in such a way: in this case, the material is described as an assemblage of composite patterns, all made of a spherical inclusion of material 1 embedded in a concentric spherical shell of material 2, the ratio between the radii being constant and compatible with the phase concentration; some fractal construction is required to map the whole space with such spherical patterns of different sizes. The CSA provides a first model for materials with a clearly identified matrix–inclusion morphology; the composite cylinders assemblage (CCA) is a straightforward extension of this model to long fibre-reinforced materials (Hashin and Rosen, 1964).

This description has been combined with the powerful Hashin–Shtrikman variational principle (Hashin and Shtrikman, 1962) and the use of non-piecewise uniform polarization stress fields in order to derive rigorous bounds for the effective elastic moduli of heterogeneous materials with patterns isotropically distributed with respect to each other. In this paper the derivation of such bounds is thoroughly presented and generalized to anisotropic cases. In particular the concept of "ellipsoidal distribution", initially proposed by Willis (1977), which extends the concept of isotropic distribution of patterns, is redefined in a way similar to the one proposed by Ponte Castañeda and Willis (1995) for homogeneous inclusions. It is shown that the effective resolution of the variational problem leads to an inclusion problem, in which the inclusion is

heterogeneous and has an ellipsoidal outer shape. Such a problem has usually no known analytical solution and numerical techniques are required. Finite elements provide a convenient way to solve these mechanical auxiliary problems. Several examples are treated.

The first part of the paper (Section 2) is concerned with the adaptation of the classical and the Hashin–Shtrikman variational principles to a morphologically representative pattern (MRP in the following) -based description of a heterogeneous medium. The non-piecewise uniform polarization stress fields used in conjunction with the latter principle are precisely described. The second part (Section 3) deals with the effective computation of the bounds in case of an ellipsoidal distribution of patterns; the practical meaning of such a distribution and its consequences on the pattern definition are discussed. It is also shown how the derivation of the bounds leads to several composite inclusion problems. A possible application of this general method is the derivation of bounds for the effective properties of the matrix inclusion composites, in which the inclusions might be non-spherical and anisotropically distributed. In the last part (Section 4), we present some results for composites with aligned cubic inclusions, isotropically distributed in a matrix, which exhibit macroscopic cubic symmetry. Rigorous bounds for the shear moduli are compared to existing bounds. The case of transversely isotropic materials is chosen for a detailed comparison of the proposed method to the one recently developed by Ponte Castañeda and Willis (1995) for particulate microstructures. Only the results are presented and discussed; the numerical implementation of the method is described elsewhere (Bornert, 1996).

## 2. MRP-BASED BOUNDS

Consider a representative volume element $\Omega$ in a heterogeneous medium, with boundary $\partial\Omega$, in which the tensor of elastic moduli at point $x$ is $C(x)$, with inverse $S(x)$. Let $u$, $\varepsilon$ and $\sigma$ be the displacement, strain and stress fields. Hill's macrohomogeneity conditions are assumed: the potential energy $W$ in $\Omega$ depends only on the average strain $\langle\varepsilon\rangle$ over $\Omega$ and not on the particular applied boundary conditions. Thus, we consider only the case of homogeneous strain boundary conditions

$$u(x) = E \cdot x, \quad \forall x \in \partial\Omega. \tag{1}$$

The effective tensor of elastic moduli $C^{\text{eff}}$ is then defined as

$$\frac{2}{|\Omega|} W = \langle\varepsilon : C : \varepsilon\rangle = \langle\varepsilon\rangle : C^{\text{eff}} : \langle\varepsilon\rangle = E : C^{\text{eff}} : E, \tag{2}$$

where $|X|$ is the volume of domain $X$ and $\langle x\rangle$ is the average of $x$ over $\Omega$. The classical theorems of potential and complementary energy ensure that

$$2\langle\sigma^*\rangle : E - \langle\sigma^* : S : \sigma^*\rangle \leqslant \frac{2}{|\Omega|} W \leqslant \langle\varepsilon^* : C : \varepsilon^*\rangle, \tag{3}$$

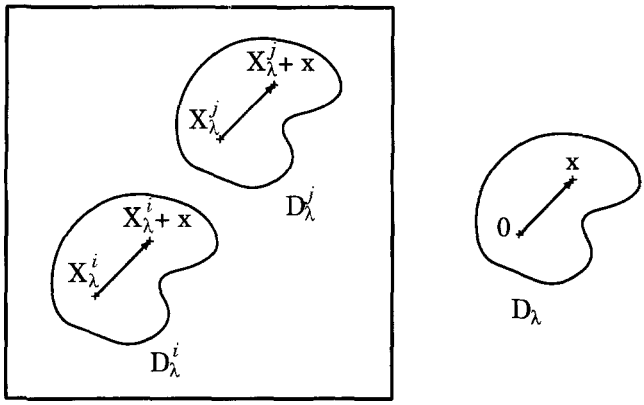



Fig. 1. A morphologically representative pattern.

where $\varepsilon^*$ is any strain field kinematically admissible with condition (1), and $\sigma^*$ any statically admissible stress field.

### 2.1. *Morphologically representative patterns*

The heterogeneous medium is now described as a set of disjoint subdomains that map the whole domain $\Omega$. It is assumed that these domains may be grouped into families with identical geometries and mechanical properties within the same family. These families are called "morphologically representative patterns". More precisely (see Fig. 1), if $D_\lambda^i$ and $D_\lambda^j$ are two members of the MRP $\lambda$, centred at points $X_\lambda^i$ and $X_\lambda^j$, then for any $x \in D_\lambda$ such that $(X_\lambda^i + x)$ belongs to $D_\lambda^i$, $(X_\lambda^j + x)$ belongs to $D_\lambda^j$ and $C(X_\lambda^i + x) = C(X_\lambda^j + x)$. A particular pattern is characterized by the domain $D_\lambda$ which describes its extension and by the material content defined by the known local distribution of elastic moduli $C_\lambda(x)$, $\forall x \in D_\lambda$. The heterogeneous medium is completely characterized by the description of all its patterns and the positions of the centres $X_\lambda^i$ of all the members of the patterns. No assumption is yet made either on the size of the domains, or on the geometrical distribution of the centres of the domains. Let $c_\lambda$ be the volume fraction of the domain occupied by the pattern $\lambda$. We define also a pattern-based average procedure, which transforms any field $f$ on $\Omega$ into local fields $f_\lambda^M$ on $D_\lambda$

$$f_\lambda^M(x) = \frac{1}{N_\lambda} \sum_{i=1}^{N_\lambda} f(X_\lambda^i + x), \quad \forall x \in D_\lambda, \quad \forall \lambda, \tag{4}$$

where the sum is taken over the $N_\lambda$ members of the pattern $\lambda$.

Note that any heterogeneous material can be described in such a way, at least with patterns reducing to single points and as many patterns as mechanical phases. The pattern-based averaging process leads in this latter case to the classical phase averaging and the $c_\lambda$ reduce to the classical phase volume fractions. In the following such a description will be referred to as the "punctual approach". Several different pattern-based descriptions of a given material are possible, but some of them lead to more accurate models than others, because they involve more microstructural information.

For instance, for the CSA, the punctual approach leads to bounds which are less efficient then those obtained when the composite spheres are used as patterns, as will be shown further.

### 2.2. *Voigt–Reuss-type bounds*

The classical Voigt–Reuss bounds (Voigt, 1889; Reuss, 1929; Hill, 1952; Paul, 1960) are obtained when uniform strain and stress fields are used in (3). On the one hand, $\varepsilon^* = E$ is a kinematically admissible field which leads to the Voigt bound

$$\langle C \rangle - C^{\text{eff}} \quad \text{positive.} \tag{5}$$

On the other hand, $\sigma^* = \Sigma^*$, with $\Sigma^*$ uniform, is a statically admissible field, which leads to a lower bound for $C^{\text{eff}}$. The optimal choice $\Sigma^* = \langle S \rangle^{-1} : E$ leads to the Reuss bound

$$\langle S \rangle^{-1} - C^{\text{eff}} \quad \text{negative.} \tag{6}$$

This classical approach may be generalized in a MRP-based approach. Voigt-type trial fields can be generated by computing the stress and strain fields in the patterns, when all of them are submitted to the same homogeneous strain boundary condition

$$u^*(x) = E \cdot x, \quad \forall x \in \partial D_\lambda^j, \quad \forall D_\lambda^j \subset \Omega. \tag{7}$$

The obtained strain field $\varepsilon^*$ is clearly kinematically admissible and leads to a "MRP-based Voigt bound" $C^{\text{V}}$ such that

$$C^{\text{V}} - C^{\text{eff}} \quad \text{positive,} \tag{8}$$

with

$$\forall E, \quad C^{\text{V}} : \langle \varepsilon^* \rangle = \langle C : \varepsilon^* \rangle = \sum_\lambda c_\lambda \langle C(x) : \varepsilon^*(x) \rangle_\lambda, \tag{9}$$

where $\langle x \rangle_\lambda$ is the average of $x$ in the pattern $D_\lambda$. A "MRP-based Reuss bound" is obtained in the same way, when a homogeneous stress condition is applied at the boundary of the patterns to generate statically admissible stress fields $\sigma^*(x)$

$$\sigma^*(x) \cdot n(x) = \Sigma^* \cdot n(x), \quad \forall x \in \partial D_\lambda^j, \quad \forall D_\lambda^j \subset \Omega, \tag{10}$$

$n$ being the outward unit normal vector to $\partial D_\lambda^j$, and $\Sigma^*$ a uniform stress field. The best choice for $\Sigma^*$ for a given $E$ leads to the bound

$$S^{\text{R}^{-1}} - C^{\text{eff}} \quad \text{negative,} \tag{11}$$

with $S^{\text{R}}$ such that

$$\forall \Sigma, \quad S^{\text{R}} : \langle \sigma^* \rangle = \langle S : \sigma^* \rangle = \sum_\lambda c_\lambda \langle S(x) : \sigma^*(x) \rangle_\lambda. \tag{12}$$

The tensors $[C^{\text{V}}]_{ijkl}$ and $[S^{\text{R}}]_{ijkl}$ are symmetric in $(i,j)$ and $(k,l)$ by definition. Their $(ij,kl)$ symmetry can be checked easily: it derives from the symmetry of the local tensors $C(x)$ and $S(x)$. Since they are upper bounds for $C^{\text{eff}}$ and $S^{\text{eff}}$, respectively, which are assumed to be positive definite, they are positive definite as well.

The computation of the average stress or strain tensors in the patterns requires the resolution of a mechanical problem for each pattern, which has to be performed with an appropriate method. In the most general case, the computation of all the 21 components of $C^{V}$ or $S^{R}$ requires the computation of these averages for six linearly independent applied strain $E$ or stress $\Sigma^*$ tensors. When particular symmetry properties are satisfied by $C^{eff}$, less computations may be sufficient. For instance, in the case of isotropy, one computation, with $E$ such that $\mathrm{tr}(E) \neq 0$ and $\mathrm{dev}(E) \neq 0$, allows derivation of the bounds for the shear and bulk moduli ($\mathrm{tr}(X)$ and $\mathrm{dev}(X)$ are the trace and the deviatoric part of tensor $X$, respectively). Other particular symmetries are addressed further (Section 4).

Note that the classical Voigt and Reuss bounds are no more than the MRP-based Voigt and Reuss bounds obtained when the punctual approach is used to describe the microstructure. Such MRP-based Voigt and Reuss bounds have already been proposed by Hashin for the CSA (Hashin, 1962) in the case of an isotropic behaviour of the constituents; these results are known as Hashin's bounds for matrix–inclusion composites. They improve the classical Voigt and Reuss bounds, because they take into account important morphological information on the microstructure, namely the fact that one phase is present as spherical inclusion embedded in a matrix. The improvement is such that these bounds lead to a unique estimate for the bulk modulus, whose upper and lower bounds coincide. But of course their validity is limited to this specific morphology of materials.

### 2.3. *Hashin–Shtrikman-type bounds*

2.3.1. *Hashin–Shtrikman formulation.* According to Hashin–Shtrikman's approach, trial fields are generated by means of an auxiliary mechanical problem with the same geometry and boundary conditions but defined on a homogeneous reference medium with tensor of elastic moduli $C^0$, and an arbitrary polarization stress field of symmetric second order tensors $p^*$, such that

$$\begin{cases} u^* = E \cdot x, \quad \forall x \in \partial\Omega, \\ e^* = \frac{1}{2}(\nabla u^* + \nabla^T u^*), \\ \mathrm{div}\,\sigma^* = 0, \\ \sigma^* = C^0 : \varepsilon^* + p^*. \end{cases} \tag{13}$$

The solutions $\varepsilon^*$ and $\sigma^*$ of this problem can be used in inequalities (3), which after a few manipulations read classically

$$\int_\Omega \delta^* : S : G : S : \delta^* \, \mathrm{d}\omega + \mathrm{HS}(p^*, E) \leqslant W \leqslant \mathrm{HS}(p^*, E) + \int_\Omega \delta^* : H : \delta^* \, \mathrm{d}\omega, \tag{14}$$

where

$$\mathrm{HS}(p^*, E) = \frac{|\Omega|}{2}[E : C^0 : E + E : \langle p^* \rangle + \langle \varepsilon^*(p^*) : p^* \rangle - \langle p^* : H : p^* \rangle] \tag{15}$$

is the Hashin–Shtrikman functional and with

$$H=(C-C^0)^{-1},\quad G=(S^0-S)^{-1},\quad \delta^*=\sigma^*-C:\varepsilon^*. \tag{16}$$

Note that if $p^*$ is such that $\varepsilon^*(p^*)=H:p^*$, then the fields $u^*$, $\varepsilon^*$ and $\sigma^*$ are the solutions of the initial problem on the heterogeneous medium, and $\delta^*=0$, so that $W=\mathrm{HS}(p^*,E)$.

Since $C(x)$ is not completely known in the general case, one has to test trial fields varying in a subspace of the space of symmetric second order tensor fields over $\Omega$ in order to generate bounds for $W$. To ensure that the functional HS generates bounds, one has to choose $C^\bullet$ such that the sign of $W-\mathrm{HS}(p^*,E)$ is known:

- If $H$ or $G$ is negative definite at any $x\in\Omega$, then $\mathrm{HS}(p^*,E)$ is an upper bound for $W$.
- If $H$ or $G$ is positive definite at any $x\in\Omega$, then $\mathrm{HS}(p^*,E)$ is a lower bound for $W$.

For a given choice of $C^\bullet$, the best bounds are obtained for values of the polarization field that ensure the stationarity of the functional HS. Let $p_0^*$ be such a field

$$\frac{\partial \mathrm{HS}}{\partial p}(p_0^*,E)=0. \tag{17}$$

This optimality condition for $p_0^*$ can be rewritten as

$$\langle(\varepsilon^*(p_0^*)-H:p_0^*):\mathrm{d}p\rangle=0,\quad \forall\,\mathrm{d}p, \tag{18}$$

which in turn leads to the well-known relation

$$\mathrm{HS}(p_0^*,E)=\frac{|\Omega|}{2}[E:C^0:E+E:\langle p_0^*\rangle]. \tag{19}$$

With $\sigma_0^*=C^\bullet:\varepsilon_0^*(p_0^*)+p_0^*$ and using the condition $\langle\varepsilon_0^*(p_0^*)\rangle=E$, this can be written as

$$\mathrm{HS}(p_0^*,E)=\frac{|\Omega|}{2}E:\langle\sigma_0^*\rangle=\frac{|\Omega|}{2}E:C^{\mathrm{HS}}:E, \tag{20}$$

with $C^{\mathrm{HS}}$ symmetric (see Appendix) and such that

$$\langle\sigma_0^*\rangle=C^{\mathrm{HS}}:E. \tag{21}$$

The tensor $C^{\mathrm{HS}}$ is a bound for $C^{\mathrm{eff}}$ when $C^0$ is chosen in an appropriate way, but its value depends on the space over which $p^*$ is optimized, and the possibility to compute it effectively depends on the available microstructural information. Optimal bounds are obtained when the choice of the subspace for $p^*$ is fully adapted to this information.

2.3.2. *Particular choices of polarization fields.* In the *classical (or punctual) approach*, $p^*$ is chosen uniform over each mechanical phase $s$

$$p^*(x)=p_s^*,\quad \forall x\in\Omega_s,\quad \forall s, \tag{22}$$

where $\Omega_s$ is the domain of mechanical phase $s$. Optimal bounds are obtained for optimal values of the tensors $p_s^*$.

In the *pattern-based approach*, one chooses $p^*$ so that it takes the same value at all homologous points of the subdomains $D'_\lambda$ of each pattern $D_\lambda$. Such a polarization field is characterized by as many *local fields* $p^*_\lambda(x)$ as morphologically representative patterns

$$p^*(X^i_\lambda + x) = p^*_\lambda(x), \quad \forall x \in D_\lambda, \quad \forall i, \quad \forall \lambda. \tag{23}$$

Optimal bounds are obtained when these local fields satisfy the condition (18) which reads now

$$\varepsilon^{*M}_\lambda(x) - [C_\lambda(x) - C^0]^{-1} : p^*_\lambda(x) = 0, \quad \forall x \in D_\lambda, \quad \forall \lambda. \tag{24}$$

This condition involves the pattern-based average strain fields $\varepsilon^{*M}_\lambda(x)$ over each "morphological phase" $\lambda$, which can be computed by means of the modified Green operator $\Gamma^0$ associated with the medium $C^0$, the geometry of $\Omega$ and the adopted homogeneous displacement boundary conditions. Classically (Kröner and Koch, 1976), one has

$$\varepsilon^*(p^*)(x) = E - \int_\Omega \Gamma^0(x, y) : p^*(y)\, \mathrm{d}y \tag{25}$$

$$= E - \sum_\lambda \sum_{i=1}^{N_\lambda} \int_{D'_\lambda} \Gamma^0(x, y) : p^*_\lambda(y)\, \mathrm{d}y. \tag{26}$$

The local optimal polarization fields $p^*_{\lambda 0}(x)$ are then determined by the following system of equations

$$E - \sum_\mu [\tilde{\Gamma}^0_{\lambda\mu} * p^*_\mu](x) = [C_\lambda(x) - C^0]^{-1} : p^*_\lambda(x), \quad \forall x \in D_\lambda, \tag{27}$$

where $\tilde{\Gamma}^0_{\lambda\mu}$ is a convolution operator that transforms any tensor field $p$ on $D_\mu$ on a tensor field on $D_\lambda$ according to

$$[\tilde{\Gamma}^0_{\lambda\mu} * p](x) = N_\mu \int_{D_\mu} \Gamma^{0MM}_{\lambda\mu}(x, y) : p(y)\, \mathrm{d}y, \quad \forall x \in D_\lambda \tag{28}$$

$$= \frac{1}{N_\lambda} \int_{D_\mu} \sum_{i=1}^{N_\lambda} \sum_{j=1}^{N_\mu} \Gamma^0(X^i_\lambda + x, X^j_\mu + y) : p(y)\, \mathrm{d}y, \quad \forall x \in D_\lambda. \tag{29}$$

The system (27) cannot be solved in the general case, since the operators $\tilde{\Gamma}^0_{\lambda\mu}$ are not known. But some particular properties and a few additional assumptions allow drastic simplification, as shown in the next section; $C^{\mathrm{HS}}$ can then be determined.

Note that in case of punctual patterns, the above convolution operators reduce to the tensors used in the classical approach. The optimal polarization fields are then piecewise uniform and identical to those obtained classically.

## 3. EXPLICIT DERIVATION: ELLIPSOIDAL PHASE OR PATTERN DISTRIBUTIONS

We now assume that $\Omega$ is large enough to be identified to the whole three-dimensional space, and the boundary condition (1) is replaced by the weaker condition: $u(x)-E\cdot x$ tends to zero when $\|x\|$ tends to infinity. The polarization trial fields are now also defined over the whole three-dimensional space. The associated convergence problem can be solved by making the Green operator act on $p^*(y)-\langle p^*(y)\rangle$. Alternatively, following Kröner and Koch (1976), relation (25) may be rewritten as

$$\varepsilon^*(p^*)(x) = E^0 - \int \Gamma^0_\infty(x-y) : p^*(y)\,\mathrm{d}y, \tag{30}$$

where $\Gamma^0_\infty$ is the modified Green operator associated to the infinite medium with the elastic moduli $C^0$ and $E^0$ is a uniform tensor which might be different from $E$. In this expression the convergence of the integral is ensured only for polarization exhibiting some particular properties. But in the following the pattern distributions that will be considered will guarantee that the previously described derivations are compatible with such requirements.

The pattern-based averages are now to be understood as the limits of the averages previously defined on finite domains, when the extension of these domains tends to infinity. We assume that these averages can be computed on domains with finite extension: there exists a domain $\tilde{\Omega}$ with finite but large enough extension to allow the definition of domains $\tilde{\Omega}_x$ with the property $y\in\tilde{\Omega}_x \Leftrightarrow (y-x)\in\tilde{\Omega}$ and such that $f_\lambda^{M_{\tilde{\Omega}_x}}$ does not depend on $x$ and is equal to the pattern-based averages of $f$ over $\Omega$, for any field $f$ on $\Omega$. The superscript $M_{\tilde{\Omega}_x}$ denotes that the average $\cdot_\lambda^{M}$ is taken over the patterns in finite number $\tilde{N}_\lambda$ that belong to $\tilde{\Omega}_x$.

The system of equations for the optimal polarization fields $p^*_\lambda(x)$ reads now

$$E^0 - \sum_\mu [\tilde{\Gamma}^0_{\infty\lambda\mu} * p^*_\mu](x) = [C_\lambda(x)-C^0]^{-1} : p^*_\lambda(x), \quad \forall x\in D_\lambda, \quad \forall\lambda, \tag{31}$$

with

$$[\tilde{\Gamma}^0_{\infty\lambda\mu} * p](x) = \frac{1}{\tilde{N}_\lambda}\sum_{i=1}^{\tilde{N}_\lambda}\sum_{j=1}^{\infty}\int_{D_\mu}\Gamma^0_\infty(X^i_\mu - X^j_\mu + x - y) : p(y)\,\mathrm{d}y, \quad \forall x\in D_\lambda, \tag{32}$$

where $\tilde{N}_\lambda$ is the number of members of the pattern $\lambda$ in $\tilde{\Omega}$.

From now on, we assume some particular properties on pattern distributions such that, taking benefit of some general property of $\Gamma^0_\infty$, all non-diagonal terms in the above systems of equations vanish

$$\tilde{\Gamma}^0_{\infty\lambda\mu} = 0, \quad \text{for} \quad \lambda\neq\mu. \tag{33}$$

Furthermore the remaining diagonal terms are formally identical to those obtained in the case of the computation of the effective polarization in an inclusion embedded in an infinite medium with moduli $C^0$, subjected to homogeneous boundary conditions at infinity.

We first assume that the number of patterns in the volume $\tilde{\Omega}$ is sufficiently large so

that one can define the function $\Psi_{\lambda\mu}$ such that $\Psi_{\lambda\mu}(u)\,du$ is the number of couples $(i,j)$ ensuring that $(X_\lambda^i - X_\mu^j)$ belongs to the volume $du$ around $u$. The operator $\tilde{\Gamma}^0_{\lambda\mu}$ can then be rewritten as

$$[\tilde{\Gamma}^0_{\lambda\mu} * p](x) = \frac{1}{\tilde{N}_\lambda} \int du \int_{D_\mu} dy\, \Psi_{\lambda\mu}(u)\Gamma^0_\lambda(u+x-y) : p(y), \quad \forall x \in D_\lambda. \tag{34}$$

The basic assumption is now that the centres of the patterns are distributed according to an ellipsoidal symmetry, i.e. that $\Psi_{\lambda\mu}$ can be written as

$$\Psi_{\lambda\mu}(u) = \psi_{\lambda\mu}(\| B \cdot u \|), \tag{35}$$

$\psi_{\lambda\mu}$ being any positive real function and $B$ any positive definite symmetric second order matrix normalized according to an appropriate norm. This definition for the ellipsoidal distribution of patterns derives from the definition of the ellipsoidal distribution of phases initially proposed by Willis (1977) in a way similar to the one proposed by Ponte Castañeda and Willis (1995) for an ellipsoidal distribution of *homogeneous inclusions*.

This assumption induces some restrictions on the outer shape of the patterns. In fact any pattern $\lambda$ is necessarily ellipsoidal and characterized by the equations $\| B \cdot u \| \leqslant r_\lambda$, where the scalars $r_\lambda$ determine the patterns' extensions. To establish this property, consider for instance, in the case of an isotropic distribution in which $B$ reduces to identity, two patterns $\lambda$ and $\mu$, which contain at least two members $D_\lambda^i$ and $D_\mu^j$ that touch one another. Such patterns do exist since the pattern members have to map the whole three-dimensional space. If one of the patterns has a finite extension, then $\psi_{\lambda\mu}$ vanishes in a neighbourhood of 0 (excluding 0 for the case $\lambda = \mu$), since two different subdomains cannot lie at the same location. The lowest value for $x$ for which $\psi_{\lambda\mu}(x)$ does not vanish corresponds to the minimal distance between the centres of subdomains $\lambda$ and $\mu$, that is the distance between them when they touch one another. To satisfy the assumption on the distribution of centres this indicates that the distance at which these patterns become in contact does not depend on their relative orientation. This can only be satisfied when their outer shapes are spheres. The complete mathematical demonstration of the latter assertion can be established by some simple algebra.

The case of an anisotropic ellipsoidal distribution can be treated in the same way, by considering it as the result of an isotropic distribution that has been stretched along the principal directions of the matrix $B^T \cdot B$. So this proves that isotropic distributions can only be obtained with spherical patterns, and ellipsoidal distributions with ellipsoidal patterns having all the same outer shape characterized by tensor $B^T \cdot B$. Figure 2 gives an example of an isotropic distribution. If all the patterns are composite spheres with the same volume fraction this corresponds to Hashin's CSA (b), for which one has to define as many patterns as composite inclusion sizes; it is possible to generate other microstructures based on the same pattern distribution but with other "internal" pattern structures (c). Figure 3 shows an ellipsoidal distribution that has been obtained by stretching the previous isotropic one along the vertical direction. The content of each pattern may vary as well, generating several different

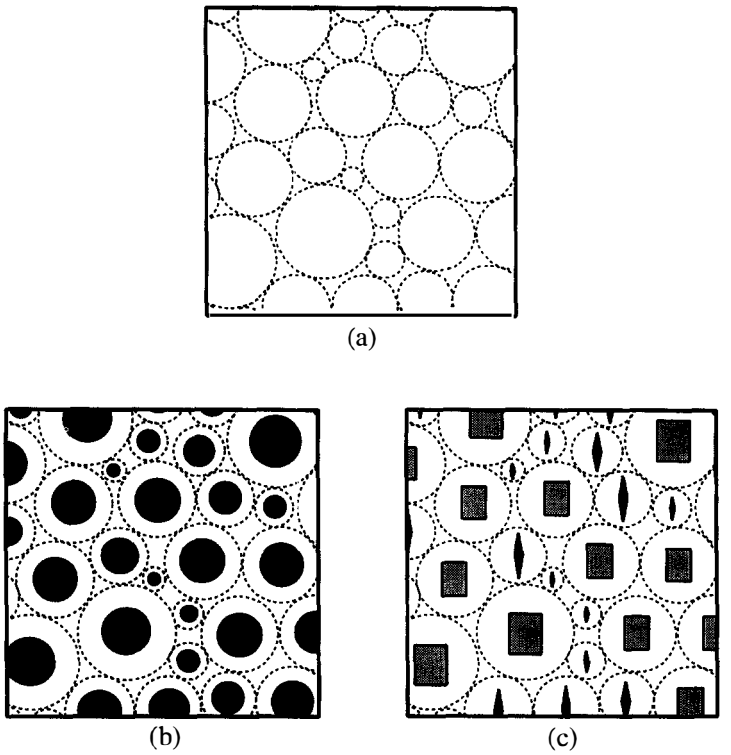


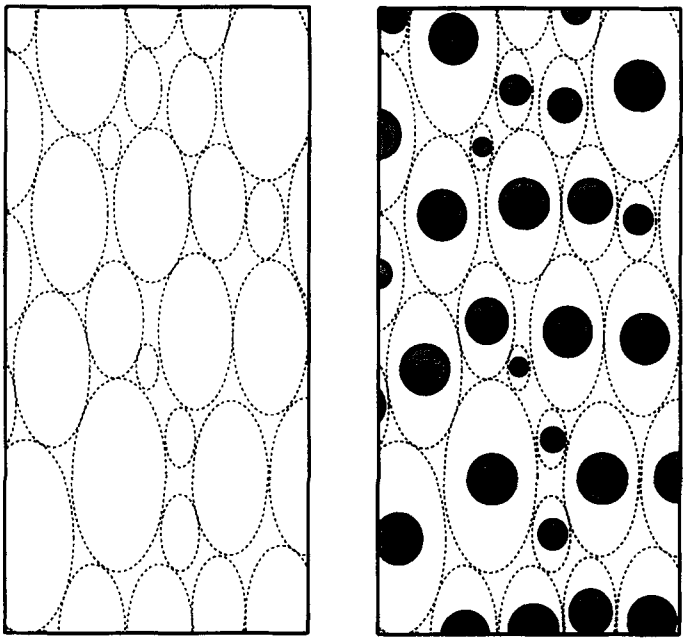

Fig. 2. Isotropic distribution of patterns: (a) isotropic distribution; (b) the corresponding composite spheres assemblage; and (c) another microstructure with the same distribution.

microstructures. Note that in all cases some fractal construction is required to map the whole space, as for Hashin's CSA.

Let $E_r$ be the ellipsoid with equation $\| B \cdot u \| \leqslant r$. In (34) $x$ and $y$ belong, respectively, to the ellipsoids $E_{r_\lambda}$ and $E_{r_\mu}$ so that, since these ellipsoids have the same principal directions and aspect ratios, $x-y$ belongs to the ellipsoid $E_{r_\lambda+r_\mu}$. After application of Fubini's relation, the integration domain for $u$ can be decomposed into ellipsoidal domains $E_{r+\mathrm{d}r} \backslash E_r$, over which $\psi_{\lambda\mu}(u)$ is constant. These terms vanish for $r \geqslant r_\lambda + r_\mu$ by application of the following property of the modified Green's tensor, which is basically a consequence of the absence of characteristic length in Eshelby's inclusion problem (Eshelby, 1957)

$$\int_{E_r} \Gamma^0_\infty(x-y)\,\mathrm{d}y = \int_{E_1} \Gamma^0_\infty(x-y)\,\mathrm{d}y, \quad \forall r \geqslant 1, \quad \forall x \in \boldsymbol{E}_1. \tag{36}$$

The integration over $u$ reduces then to the integration over the domain $E_{r_\lambda+r_\mu}$. But since $\Psi_{\lambda\mu}$ vanishes on this domain for $\lambda \neq \mu$ the integral finally equals zero in this case. For $\lambda = \mu$, $\Psi_{\lambda\lambda}(x)$ vanishes also inside this ellipsoid except at the origin since one has $\Psi_{\lambda\lambda}(0) = \tilde{N}_\lambda$ so that only this punctual contribution of the modified Green's operator subsists and one has



(a) (b)

Fig. 3. Ellipsoidal distribution of patterns: (a) ellipsoidal distribution; and (b) possible microstructure based on it.

$$[\tilde{\Gamma}^0_{\lambda\mu} * p](x) = \delta_{\lambda\mu} \int_{D_\mu} \Gamma^0_\lambda(x-y) : p(y)\, dy, \quad \forall x \in D_\lambda. \tag{37}$$

Thus, the optimal local polarization fields in the patterns are characterized by the relations

$$E^0 - \int_{D\lambda} \Gamma^0_\lambda (x-y) : p^*_\lambda(y)\, dy = [C_\lambda(x) - C^0]^{-1} : p^*_\lambda(x), \quad \forall x \in D_\lambda, \quad \forall \lambda. \tag{38}$$

They are formally identical to those one obtains for the computation of the effective polarization in ellipsoidal inclusions, with the same heterogeneous content than the patterns $\lambda$, embedded in an infinite medium with moduli $C^0$ and subjected to homogeneous strain condition $E^0$ at infinity. Moreover, the pattern-based averages of the optimal trial stress $\sigma_0^*$ or strain $\varepsilon_0^*$ fields are the fields one computes in such composite inclusions.

In previous relations, the tensor $E^0$ is not known as a function of $E$. It is only determined by the condition that $E$ equals the average trial strain field $\langle \varepsilon_0^* \rangle$. But in fact one does not need to know its exact value. The purpose is to determine the bounds $C^{HS}$ for the effective elastic moduli, which are characterized by relations $\langle \sigma_0^* \rangle = C^{HS} : \langle \varepsilon_0^* \rangle$. So instead of computing $E^0$ for each chosen $E$, one should preferably compute $E = \langle \varepsilon_0^* \rangle$ for enough choices of $E_0$ so as to be able to compute $C^{HS}$ completely, with an adequate choice of $C^0$.

In the case of the punctual approach, the assumption of ellipsoidal distribution of patterns is equivalent to the assumption of ellipsoidal distribution of phases used by Willis (1977). It can be checked that the resulting Hashin–Shtrikman-type bounds are then identical to those proposed by this author.

Note finally that all these derivations have been presented in case of homogeneous strain conditions at the boundary of $\Omega$. The simplification brought by the recourse to the modified Green's operator of the infinite medium makes in fact that identical results would have been obtained in case of a homogeneous stress approach, since homogeneous stress or strain conditions at infinity are equivalent for inclusion problems.

## 4. NEW BOUNDS FOR ANISOTROPIC MATRIX–INCLUSION COMPOSITES

### 4.1. *General procedure*

The general procedure to compute such generalized Hashin–Shtrikman bounds requires first the computation of the average stress and strain fields in a composite inclusion with ellipsoidal outer shape but arbitrary content, embedded in a homogeneous medium and subjected to homogeneous conditions $E^0$ at infinity. A known analytical solution to such a problem is the one related to spherical $n$-layered spheres (Hervé and Zaoui, 1993). The case of $n$-layered cylinders can also be addressed analytically (Hervé and Zaoui, 1995) but since the boundary conditions at infinity along the direction of the fibre that are to be adopted are somewhat particular, its rigorous treatment cannot be considered immediately in the present approach, even if, in a sense, this problem can be considered as the limit case of prolate ellipsoids with very large aspect ratios embedded in a matrix.

Other cases have to be addressed by numerical methods. In the present study, we have resorted to finite element techniques, since they provide an easy way to compute local fields and their averages and since many softwares are available, but any other appropriate method could be used. The composite inclusion as well as the medium in which it is embedded are meshed. Since anisotropy is considered, 3D models are generally required in order to be able to compute all the components of the tensor $C^{HS}$. The numerical aspects of this method are more thoroughly addressed by Bornert (1996). The approximations owing to the discretization and to the fact that the infinite reference medium in which the patterns are embedded has in practice to be truncated at a finite extent where the homogeneous boundary conditions are applied, are discussed. It is shown that, since only average quantities are required for the computation of the bounds, the meshes do not need to be too fine. The extension of the reference medium can be limited to three or four times the characteristic size of the ellipsoidal patterns. The average trial stress or strain fields within each pattern can thus be computed within reasonable computation times.

Once the inclusion problems with an adequate choice of $C^0$ are solved, one has to compute the average of these averages weighted by the volume fraction of the patterns. Finally the components of $C^{HS}$ are obtained by the relation $\langle\sigma\rangle = C^{HS} : \langle\varepsilon\rangle$ which

has to be explicited for as many values of $E^0$ as needed. In case of isotropy, one load is generally enough. Shear $\mu$ and bulk $K$ moduli are determined by relations

$$\mathrm{tr}(\langle\sigma\rangle) = 3K\,\mathrm{tr}(\langle\varepsilon\rangle) \quad \text{and} \quad \mathrm{dev}(\langle\sigma\rangle) = 2\mu\,\mathrm{dev}(\langle\varepsilon\rangle). \tag{39}$$

One has just to choose $E^0$ such that both $\mathrm{tr}(\langle\varepsilon\rangle)$ and $\mathrm{dev}(\langle\varepsilon\rangle)$ are non-zero. In the most general anisotropic case, the computation of all the 21 components of $C^{\mathrm{HS}}$ requires the computation of these averages for six applied strain tensors $E^0$ which generate six linearly independent average strains $\langle\varepsilon\rangle$. The components of $C^{\mathrm{HS}}$ are then determined by a linear system of equations. In intermediate situations for which the symmetries of the material ensure particular properties of the effective medium, this number of required applied strain tensors may be less than six.

Voigt and Reuss generalized pattern-based bounds can be obtained within the same framework. The only difference is that homogeneous stress or strain boundary conditions are applied at the boundary of the patterns, which are not required to have an ellipsoidal outer shape. The procedure to compute the components of the tensor of elastic moduli is then identical. Another way to compute these bounds is to use exactly the same procedure than for the Hashin–Shtrikman bounds, but with moduli of the reference medium, in which the composite patterns are embedded, much harder or much weaker than the moduli of the constitutive phases. The homogeneous boundary condition applied at the boundaries of the reference medium then result in homogeneous strain and stress conditions at the boundary of the patterns, respectively.

### 4.2. *Material with cubic symmetry*

Materials with cubic symmetry are characterized by their symmetry axes and three elastic constants which are all eigenvalues of the tensor of elastic moduli. Let $(e_x, e_y, e_z)$ be the unit vectors along the directions $x$, $y$ and $z$ of the cubic symmetry. The eigenvector that corresponds to the bulk modulus $K$ is $e_x \otimes e_x + e_y \otimes e_y + e_z \otimes e_z$. The first shear modulus $\mu_a$ has multiplicity 2 and admits $e_x \otimes e_x - e_y \otimes e_y$ and $e_x \otimes e_x - e_z \otimes e_z$ as eigenvectors. The second shear modulus $\mu_d$ has multiplicity three and eigenvectors $e_x \otimes e_y + e_y \otimes e_x$, $e_y \otimes e_z + e_z \otimes e_y$ and $e_z \otimes e_x + e_x \otimes e_z$. These constants can be determined within one computation as soon as $E^0$ is chosen such that $\langle\varepsilon\rangle$ has non-vanishing components along one eigenvector of each eigenvalue. Then, one has for instance

$$3K = \frac{\mathrm{tr}(\langle\sigma\rangle)}{\mathrm{tr}(\langle\varepsilon\rangle)}, \tag{40}$$

$$2\mu_a = \frac{\langle\sigma\rangle_{xx} - \langle\sigma\rangle_{yy}}{\langle\varepsilon\rangle_{xx} - \langle\varepsilon\rangle_{yy}} = \frac{\langle\sigma\rangle_{xx} - \langle\sigma\rangle_{zz}}{\langle\varepsilon\rangle_{xx} - \langle\varepsilon\rangle_{zz}} = \frac{\langle\sigma\rangle_{yy} - \langle\sigma\rangle_{zz}}{\langle\varepsilon\rangle_{yy} - \langle\varepsilon\rangle_{zz}}, \tag{41}$$

$$2\mu_d = \frac{\langle\sigma\rangle_{xy}}{\langle\varepsilon\rangle_{xy}} = \frac{\langle\sigma\rangle_{xz}}{\langle\varepsilon\rangle_{xz}} = \frac{\langle\sigma\rangle_{yz}}{\langle\varepsilon\rangle_{yz}}. \tag{42}$$

The shear moduli are overdetermined; the results of different definitions might give slightly different results because the mesh might not respect exactly the cubic symmetry and because of possible numerical errors. The discrepancies give a measure of the accuracy of the numerical model.

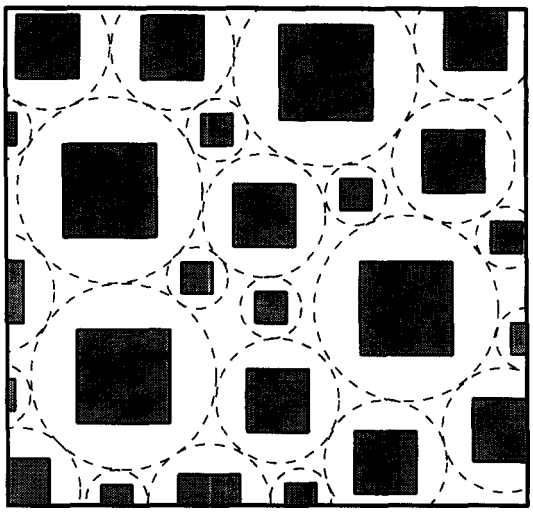


Fig. 4. A composite with cubic inclusions distributed isotropically.

As an illustration, we give here some results for materials with cubic inclusions isotropically distributed in a matrix. Inclusions and matrix are assumed to exhibit local isotropic behaviour, so that the global behaviour exhibits cubic symmetry. The patterns used to describe such microstructures are made of cubic inclusions of material 1, with moduli $K_1$ and $\mu_1$, embedded in a spherical shell of material 2, with moduli $K_2$ and $\mu_2$. Several pattern sizes can be used, but thanks to the absence of characteristic length, there is only one composite inclusion problem to be solved, as for the CSA. Figure 4 gives a representation of the kind of materials that are modelled by such patterns and Fig. 5 gives an example of the meshes used to compute Hashin–Shtrikman bounds. The reference media used to derive lower and upper Hashin–Shtrikman bounds are isotropic with moduli $(K_2, \mu_2)$ and $(K_1, \mu_1)$, respectively.

The bounds for the shear moduli $\mu_a$ and $\mu_d$ of the composite can be compared to the corresponding bounds for the classical CSA. The discrepancy reflects the effect of the inclusion shape. Figure 6 compares the new Voigt–Reuss-type bounds to classical Hashin's bounds, in Hill's diagram for an inclusion volume fraction varying from 0–35%. (The maximal volume fraction, obtained when the inclusion touches the boundary of the spherical shell, is $2/\pi\sqrt{3} \approx 37\%$.) Figure 7 gives the same result for Hashin–Shtrikman-type bounds; the new bounds for the anisotropic composite are here compared to the bounds recently proposed by Hervé *et al.* (1991), which improve Hashin's bounds for the CSA, in the case of an isotropic distribution of patterns. One can see that the possible range for both shear moduli of the anisotropic composite lie above the corresponding domain for the isotropic composite: it seems that, for this particular configuration, the effect of the non-sphericity of the inclusions is to harden the composite for any mechanical solicitation. This hardening effect is more important for $\mu_a$ than for $\mu_d$. One can also note that the domains for $\mu_a$ and $\mu_d$ determined by the Voigt–Reuss-type bounds intersect, whereas those obtained with Hashin–Shtrikman-type bounds are almost disjoined.

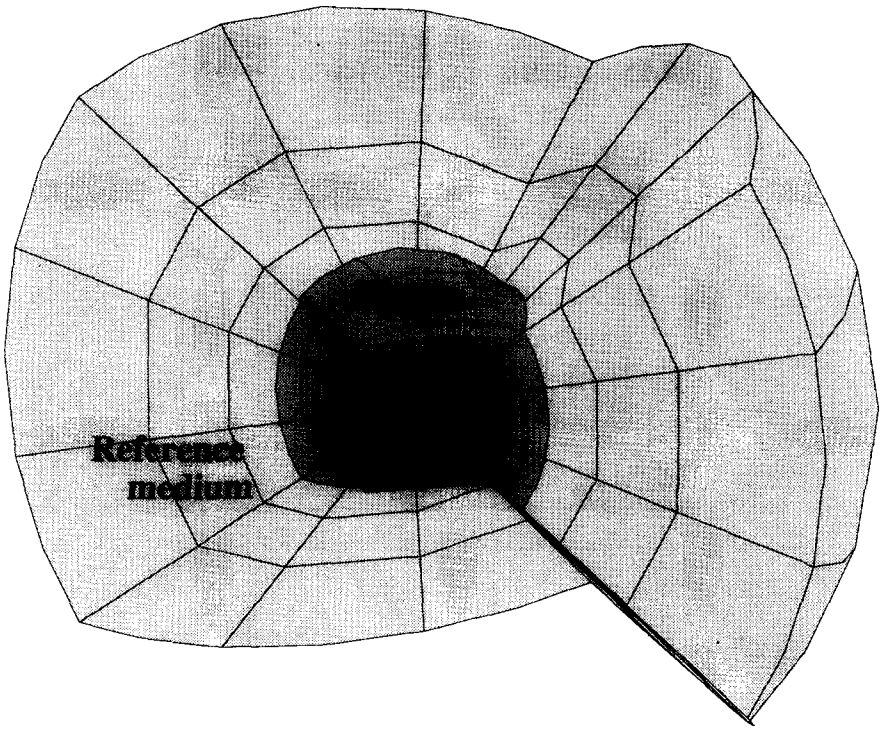



Fig. 5. Partial view of 3D mesh for the auxiliary problem for material of Fig. 4 (351 20-noded quadratic elements and 1528 nodes).

The anisotropic MRP-based Hashin–Shtrikman-type bounds can be compared to the bounds derived by Milton and Kohn (1988). In case of cubic symmetry, the latter lead to the following inequalities satisfied by $\mu_a$ and $\mu_d$, when $K_1 > K_2$ and $\mu_1 > \mu_2$

$$c_2\left[\frac{1}{\mu_1-\mu_a}+\frac{3}{2(\mu_1-\mu_d)}\right]\leqslant\frac{5}{2(\mu_1-\mu_2)}-\frac{3c_1(K_1+2\mu_1)}{\mu_1(3K_1+4\mu_1)}, \tag{43}$$

$$c_1\left[\frac{1}{\mu_a-\mu_2}+\frac{3}{2(\mu_d-\mu_2)}\right]\leqslant\frac{5}{2(\mu_1-\mu_2)}-\frac{3c_2(K_2+2\mu_2)}{\mu_2(3K_2+4\mu_2)}. \tag{44}$$

Figure 8 gives the possible domain for $\mu_a$ and $\mu_d$ for a fixed inclusion volume fraction of 25%. Several bounds have been reported. The classical Voigt and Reuss bounds are valid for any composite. The classical Hashin–Shtrikman bounds are valid for any composite that exhibits an isotropic macroscopic behaviour, in particular for the isotropic CSA. The above Milton and Kohn bounds apply to composite with macroscopic cubic symmetry, in particular to the considered composites with cubic inclusions isotropically distributed, but also to the isotropic CSA. The pattern-based Voigt–Reuss and Hashin–Shtrikman bounds for the CSA and for the composite with cubic inclusions are also plotted.

This diagram suggests several remarks. First the here proposed new bounds are

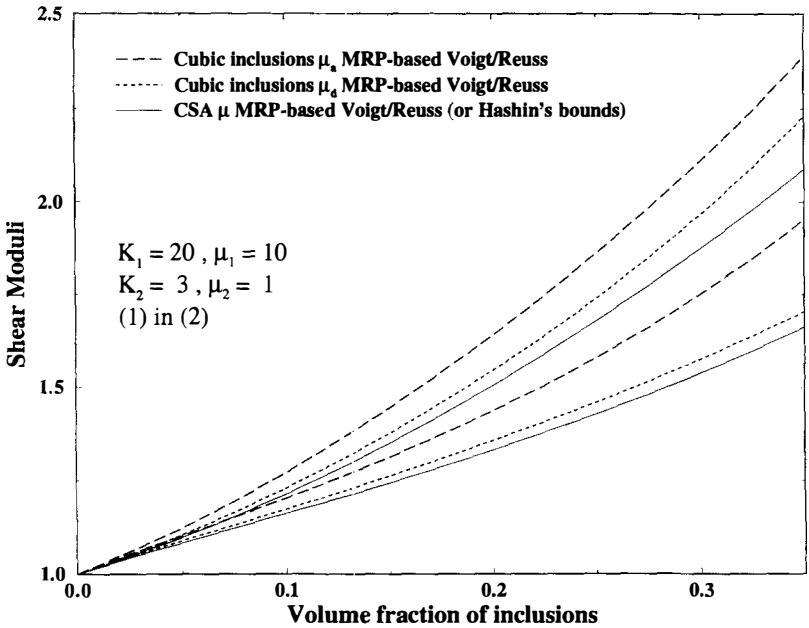



Fig. 6. MRP-based Voigt–Reuss bounds in Hill's diagram---composite with aligned cubic inclusions.

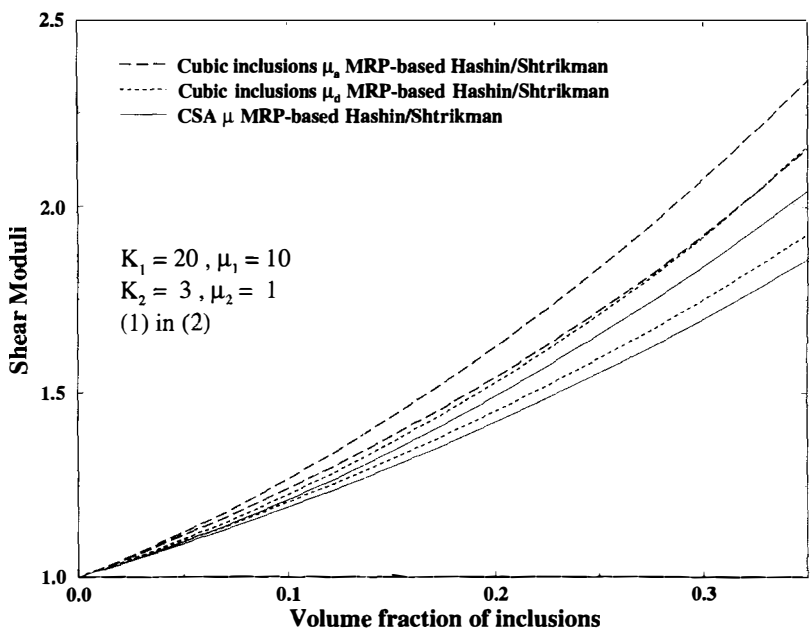



Fig. 7. MRP-based Hashin–Shtrikman bounds in Hill's diagram---composite with aligned cubic inclusions.

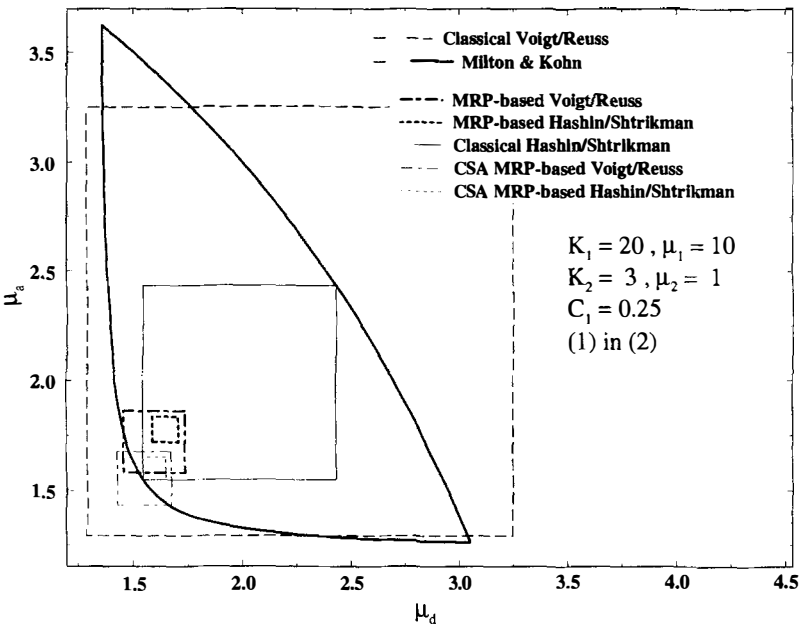



Fig. 8. Comparison between bounds—"hard cubic inclusions in weak matrix" configuration.

consistent with the existing ones: in particular the pattern-based Hashin–Shtrikman-type bounds lie within the domain determined by Milton and Kohn bounds. The explicit use of some microstructural information, namely the fact that the composite is particulate and that the inclusions are cubic, aligned and isotropically distributed, allows drastic reduction of the domain of possible values of the shear moduli. The domain determined by the MRP-based Voigt–Reuss bounds does not completely lie within Milton and Kohn's domain. The points that are outside correspond to composites that do not exhibit a cubic symmetry at the macroscopic level, because of their particular anisotropic pattern distribution. In case of the CSA, the lower pattern-based Hashin–Shtrikman-type bounds coincide with the classical Hashin–Shtrikman bounds: this is due to the spherical geometry of the pattern that represents the CSA and to the fact that the bulk and shear moduli of the constitutive phases are similarly ordered, so that the auxiliary composite problems are identical in the punctual and the pattern-based approach. But nothing similar stands in the case of cubic inclusions. Note that we used the analytical relation to plot the classical Hashin–Shtrikman bounds, whereas numerical results have been plotted for the MRP-based Hashin–Shtrikman-type bounds of the CSA (even if analytical relations also exist); the small discrepancy gives the order of magnitude of the numerical errors, which can be neglected from a practical point of view.

Figure 9 gives the same kind of results for the inverse morphology: this diagram corresponds to weak inclusions embedded in a hard matrix, with 75% hard material. The above comments stand also for this case, except that, in this configuration, even though $\mu_u$ still increases when the inclusions become cubic, $\mu_d$ now decreases. It can also be noted that in this configuration the MRP-based bounds are close to the upper

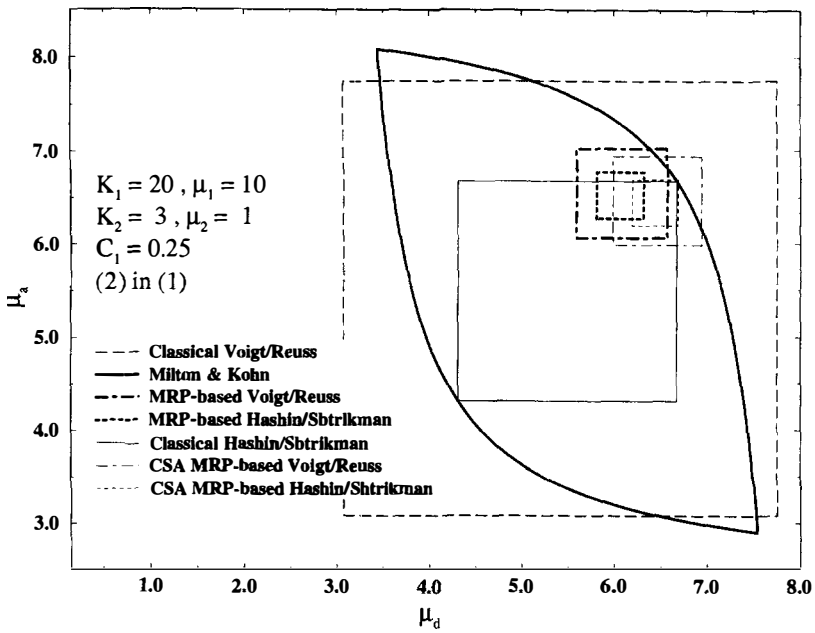



Fig. 9. Comparison between bounds—"weak cubic inclusions in hard matrix" configuration.

Hashin–Shtrikman or Milton and Kohn bounds, whereas they were close to the lower ones in the reverse configuration.

### 4.3. *Transversely isotropic materials*

In the case of transverse isotropy with symmetry axis $z$, two computations are sufficient to determine the five constants that characterize such a material: the transverse $\mu_{xy}$ and longitudinal $\mu_{xz}$ shear moduli, which are eigenvalues with multiplicity two of the tensor of elastic moduli, the longitudinal Young's modulus $E_{zz}$, the in-plane bulk modulus $K_{xy}$ and the longitudinal Poisson's ratio $v_{xz}$ (Bornert, 1996). Here we give some results that correspond to composites with identically shaped and oriented hard isotropic ellipsoidal inclusions distributed in a weak isotropic matrix according to an ellipsoidal symmetry. This case has recently been considered by Ponte Castañeda and Willis (1995), who derived explicit analytical Hashin–Shtrikman-type bounds, using *piecewise constant* polarization fields in the matrix and the inclusions, and assuming that the centres of the inclusions are distributed according to an ellipsoidal symmetry, but without the assumption of a "generalized Hashin's assemblage" microstructure.

As previously, let subscript 2 denote the matrix and 1 the inclusions; the tensors of moduli are $C_i$ and the volume fractions $c_i$, $i \in [1, 2]$. The shape of the inclusions is characterized by the ellipsoid $\Omega_{\text{inc}}$ and the distribution of the centres of the inclusions by the ellipsoid $\Omega_{\text{dis}}$. Following Ponte Castañeda and Willis (1995), we note $P^i_{\text{dis}}$ and $P^i_{\text{inc}}$ the following uniform tensors

$$P^i_{\text{inc}} = \int_{\Omega_{\text{inc}}} \Gamma^i_\infty(x-y)\,\mathrm{d}y, \quad \forall x \in \Omega_{\text{inc}}, \tag{45}\delta\gamma$$

$$P^i_{\text{dis}} = \int_{\Omega_{\text{dis}}} \Gamma^i_\infty(x-y)\,\mathrm{d}y, \quad \forall x \in \Omega_{\text{dis}}, \tag{46}$$

where the superscript $i$ refers to the reference medium $C_i$ to which the modified Green's operator $\Gamma^i_\infty$ is related. The lower Hashin–Shtrikman-type bound given in Ponte Castañeda and Willis (1995) is

$$C^{\text{HS}-}_{\text{PW}} = C_2 + c_1[(C_1 - C_2)^{-1} + P^2_{\text{inc}} - c_1 P^2_{\text{dis}}]^{-1}. \tag{47}$$

A similar upper bound can be inferred from the general relations given by these authors

$$C^{\text{HS}+}_{\text{PW}} = C_1 - c_2\left[(C_1 - C_2)^{-1} - \frac{c_1}{c_2} P^1_{\text{inc}} + \frac{(c_1)^2}{c_2} P^1_{\text{dis}}\right]^{-1}. \tag{48}$$

These bounds generalize the classical Hashin–Shtrikman bounds (Hashin and Shtrikman, 1963) to composites with non-isotropic distributions of ellipsoidal inclusions: it can be checked that in the case of spherical inclusions isotropically distributed in a matrix they coincide with these classical bounds, which indicates that, at least in this case, the particulate microstructure of the composite has not been fully utilized.

Several numerical results for transversely isotropic composites with spherical or ellipsoidal aligned inclusions, isotropically or "ellipsoidally" distributed in a matrix are given in Bornert (1996). For sake of conciseness, we restrict ourselves here to the case of spheroidal inclusions and spheroidal distributions, aligned with directions $z$ and with identical aspect ratios $w = b/a$, $a$ being the diameter of the spheroids in the transverse $xy$ plane and $b$ their length along the $z$ axis. In this case the tensors $P^i_{\text{inc}}$ and $P^i_{\text{dis}}$ are identical. In the numerical applications we have considered the same properties of the constitutive phases than in the previous section. The volume fraction of inclusions is 30%. Figures 10 and 11 give the transverse and longitudinal shear moduli as a function of the aspect ratio $w$. In order to preserve some symmetry of the plots, the results are given as a function of $F(w)$, where $F(w) = w$ for oblate inclusions ($w \leqslant 1$) and $F(w) = 2 - 1/w$ for prolate inclusions ($w \geqslant 1$). It can be seen clearly that the lower Hashin–Shtrikman-type bounds obtained by using the matrix as reference medium in the present approach coincide with the Ponte Castañeda and Willis ones, whereas the MRP-based upper bounds strongly improve the upper Hashin–Shtrikman-type bounds proposed by Ponte Castañeda and Willis and are indeed close to the lower bounds. This latter remark provides some credit to the suggestion of Ponte Castañeda and Willis to use their analytical lower bound as a good estimate for the effective properties of the composite.

The coincidence of the present bounds and those of Ponte Castañeda and Willis, when the matrix is used as reference medium, is in fact a general result, which can be justified analytically. To do so, we consider a composite in which the aspect ratio of the inclusions $w_{\text{inc}}$ might be different from the one of the distribution $w_{\text{dis}}$. The composite inclusion problem to be solved in the MRP-based approach refers to an

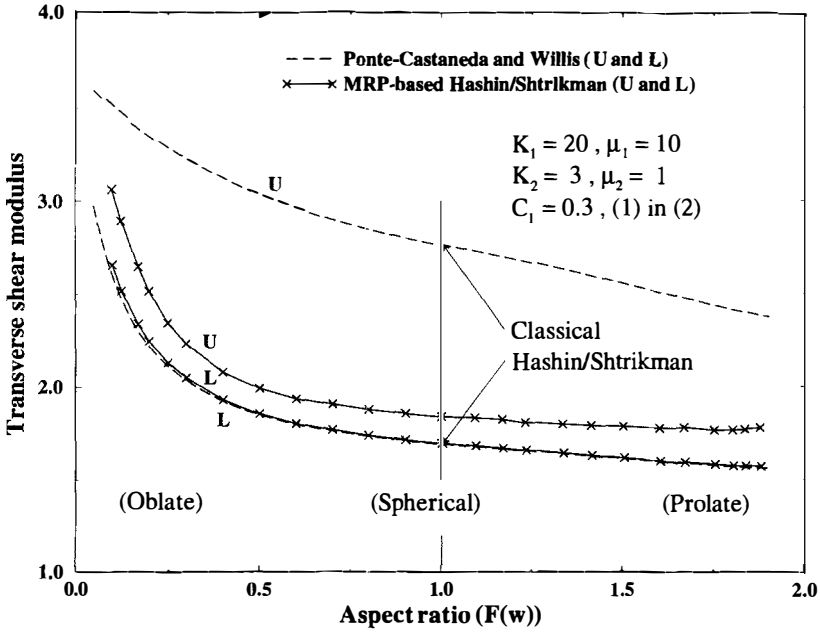



Fig. 10. Comparison between MRP-based and Ponte Castañeda and Willis upper (U) and lower (L) bounds. Composite with aligned ellipsoidal inclusions—transverse shear modulus $\mu_{xy}$.

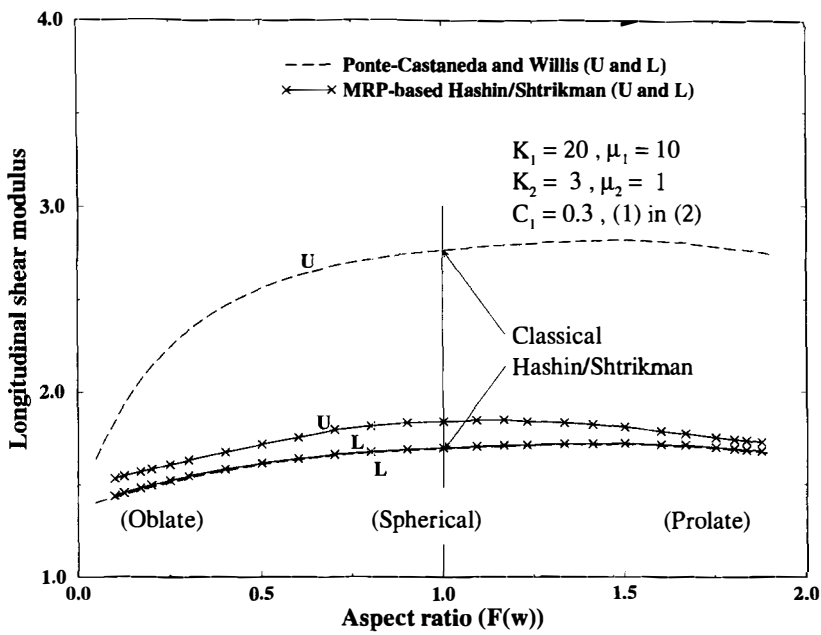



Fig. 11. Comparison between MRP-based and Ponte Castañeda and Willis upper (U) and lower (L) bounds. Composite with aligned ellipsoidal inclusions—longitudinal shear modulus $\mu_{xz}$.

ellipsoid $\Omega_{inc}$ of material 1, embedded in another ellipsoid $\Omega_{dis}$ of material 2, itself embedded in an infinite medium with properties $C_2$, subjected to homogeneous strain $E^0$ at infinity. This problem is in fact the classical Eshelby problem, so that the strain in $\Omega_{inc}$ is uniform and such that

$$\varepsilon_1 = E^0 - \int_{\Omega_{inc}} \Gamma^2_\infty(x-y)\,dy : (C_1 - C_2) : \varepsilon_1 \tag{49}$$

$$= E^0 - P^2_{inc} : (C_1 - C_2) : \varepsilon_1 \tag{50}$$

The strain in $\Omega_{dis}$ is not uniform but its average is given by

$$\langle \varepsilon \rangle_{\Omega_{dis}} = E^0 - \frac{1}{|\Omega_{dis}|} \int_{\Omega_{dis}} \int_{\Omega_{inc}} \Gamma^2_\infty(x-y)\,dy : (C_1 - C_2) : \varepsilon_1 \tag{51}$$

$$= E^0 - c_1 P^2_{dis} : (C_1 - C_2) : \varepsilon_1, \tag{52}$$

by the use of Fubini's relation and since $\Omega_{inc} \subset \Omega_{dis}$ and $|\Omega_{inc}|/|\Omega_{dis}| = c_1$. The average strain in the matrix is then

$$\varepsilon_2 = \frac{|\Omega_{dis}| \langle \varepsilon \rangle_{\Omega_{dis}} - |\Omega_{inc}| \varepsilon_1}{|\Omega_{dis}| - |\Omega_{inc}|} \tag{53}$$

$$= E_0 - \frac{c_1}{c_2} (P^2_{dis} - P^2_{inc}) : (C_1 - C_2) : \varepsilon_1. \tag{54}$$

The average stress over $\Omega_{dis}$ can be computed according to

$$\langle \sigma \rangle_{\Omega_{dis}} = c_1 C_1 : \varepsilon_1 + c_2 C_2 : \varepsilon_2. \tag{55}$$

The definition $\langle \sigma \rangle_{\Omega_{dis}} = C^{HS-} : \langle \varepsilon \rangle_{\Omega_{dis}}$ leads then to result (47), after some simple manipulations.

These results may be generalized to composites with inclusions of several different types such as those considered in Ponte Castañeda and Willis (1995). In the case of ellipsoidal inclusions, the Hashin–Shtrikman-type estimates obtained when the matrix is used as reference medium is identical to the corresponding MRP-based bound, but the upper and lower MRP-based Hashin–Shtrikman-type bounds are always sharper than the ones derived through the Ponte Castañeda and Willis approach, because at least for one of the bounds the use of *non-piecewise constant* polarization field improves the optimal choice of this field. In a sense, more local point-to-point interactions are included in the MRP-based bounds. But one should also keep in mind that the MRP-based bounds are valid only for a generalized Hashin's assemblage microstructure. The case of inclusions with non-ellipsoidal shapes can also be addressed by Ponte Casteñeda and Willis by means of a numerical computation of tensor $P^1_{inc}$. In this case too, the polarization field used in the MRP-based approach is *not* piecewise constant, even when the matrix is used as reference medium. The MRP-based bounds are then always better.

## 5. CONCLUSIONS

The main idea involved in the above proposed new approach for bounding the effective properties of elastic inhomogeneous materials lies in the consideration of finite composite subdomains, the so-called morphologically representative patterns, whose material content and spatial distribution allow to express directly some morphological properties which could hardly be described by former approaches. It has been shown how the classical Hashin–Shtrikman variational treatment can be adapted to such a description through the use of *variable* instead of *piecewise uniform* polarization fields and may yield new bounds for the overall elastic moduli. Such a bounding can be derived explicitly when adequate properties of the spatial distribution of the patterns are considered, such as the ellipsoidal distribution, which has been dealt with in this paper. Within this framework, we are left with (composite) inclusion–matrix problems which can be solved either analytically in the simplest cases or numerically otherwise. This allows treatment of anisotropic situations, such as the ones with cubic symmetry and with transverse isotropy, which have been given as illustrations of possible developments of the proposed approach and compared to Milton and Kohn's as well as Ponte Castañeda and Willis analyses, especially for the investigation of the competition between two sources for the overall anisotropy, which are associated with the pattern distribution and their material content, respectively. Finally, we would stress the fact that estimates instead of bounds could be derived from the same approach according to the generalized self-consistent point of view which has been proposed in the preliminary developments by Bornert (1996). In addition it is expected that such new bounds and estimates in the linear case could be used for the derivation of new bounds and estimates for composites with non-linear constitutive behaviour through the methods developed by Willis (1983), Ponte Castañeda (1991) or Suquet (1993).

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## APPENDIX: SYMMETRY OF $C^{HS}$

The relation $\langle \sigma_0^* \rangle = C^{HS} : E$ makes use of the linear dependence of the optimal polarization field $p_0^*$ with the loading parameter $E$, which can be checked easily. $C^{HS}_{ijkl}$ is symmetric in $(i,j)$ and $(k,l)$ from its definition. To check the $(ij,kl)$ symmetry let $E_i, i \in [1,2]$ be two applied macroscopic strains, with associated optimal polarization fields $p_{0i}^*$, generating trial fields $\varepsilon_{0i}^*$ and $\sigma_{0i}^*$. Since $\sigma_{01}^* = C_0 : \varepsilon_{01}^* + p_{01}^*$ is statically admissible and $\varepsilon_{02}^*$ kinematically admissible with $E_2$, one has

$$\langle \sigma_{01}^* : \varepsilon_{02}^* \rangle = \langle \sigma_{01}^* \rangle : E_2 \qquad \text{(A.1)}$$

$$= \langle \varepsilon_{01}^* : C^0 : \varepsilon_{02}^* \rangle + \langle p_{01}^* : \varepsilon_{02}^* \rangle. \tag{A.2}$$

The field $p_{02}^*$ is optimal so that relation (18) with $dp = p_{01}^*$ ensures $\langle p_{01}^* : \varepsilon_{02}^* \rangle = \langle p_{01}^* : H : p_{02}^* \rangle$. Finally one gets

$$\langle \sigma_{01}^* \rangle : E_2 = \langle \varepsilon_{01}^* : C^0 : \varepsilon_{02}^* \rangle + \langle p_{01}^* : H : p_{02}^* \rangle. \tag{A.3}$$

Since $C^0$ and $H$ are symmetric tensors, this relation is symmetric in subscripts 1 and 2, which proves the symmetry of $C^{HS}$. Note that this is a completely general property: no particular assumption has to be made on the subspace of the space of symmetric second order tensor fields over $\Omega$ in which the used polarization stress fields vary. It has just to be a vector space so that $dp$ varies in the same space as $p$. In particular, this property is not related to particular hypotheses on phase distributions, as it could be understood reading Ponte Castañeda and Willis (1995).