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THE PROBLEM OF ELASTIC INCLUSIONS AT FINITE CONCENTRATION

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Abstract—This paper is aimed at determining the overall properties and the local stresses of a composite material. The material is constituted of elastic ellipsoidal inclusions suspended in a homogeneous elastic matrix. An analytical approximate method is proposed to account for the interaction between the inclusions at finite concentration. This approach is based on a formulation of the problem of heterogeneous elasticity proposed by Zeller, R. and Dederichs, P. H. (1973). Elastic constant of polycrystals, *Phys. Status Solidi B* **55**, 831–842. The zero order approximation of our scheme, coincides with the Mori–Tanaka method when the inclusions are spherical, but improves significantly this method when higher order approximations are considered. The morphological and spatial distribution of the inclusions is accounted for in our scheme. Through different examples, it is shown how our results compare to existing analytical or numerical solutions. Copyright © 1996 Published by Elsevier Science Ltd.

1. INTRODUCTION

This paper is aimed at determining the overall elastic properties and local stresses of a composite material. The material considered is constituted by elastic ellipsoidal homogeneous inclusions, possibly of different phases, distributed in a homogeneous elastic matrix. Our objective is to derive a simple analytical approximate method that provides a mean to account for the interaction between the inclusions at finite concentrations.

The pioneer work of Eshelby (1957) on the elastic inclusion is the basis of several of the methods developed to analyse the response of a composite material of the type considered here. Among these methods, the 1-site self consistent scheme (Budiansky, 1965; Hershey, 1954; Kröner, 1958), has been successful in obtaining the effective properties at a low concentration of inclusions. However this scheme is symmetric in the sense that the different phases are equally treated, no distinction being made between the inclusions and the matrix. Furthermore an inclusion feels the surroundings (i.e., the other inclusions and the matrix) through the homogeneous equivalent medium, and therefore the interaction between the inclusions is not well described at finite concentration. The differential scheme, Boucher (1974), McLaughlin (1977), Norris (1985), Hashin (1988), Christensen (1990), provides a method that accounts for the fact that one phase is suspended in a matrix of another phase. The results of Zimmerman (1991) concerning an elastic material with hard spherical inclusions or spherical voids are in good agreement with experimental results up to a concentration of inclusions of 50%. The composite sphere model of Christensen and Lo (1979) and the model of Mori and Tanaka (1973) (equivalent to the Hashin–Shtrikman upper (respectively lower) bound in the case of spherical soft (respectively hard) inclusions) give an evaluation of the effects of the dispersive phase, with the restriction that this phase has an isotropic spatial repartition. These models improve the quality of the evaluation of the effective properties of composites with inclusions at large concentrations.

Our approach is based on the work of Zeller and Dederichs (1973), who formulated the problem of heterogeneous elasticity in terms of an integral equation, similar to the Lippman–Schwinger–Dyson equation of Quantum Mechanics. From that integral equation, and by taking the homogeneous matrix as a reference medium, we obtain the average stresses and strains in the inclusions as solutions of a linear system of equations. The number of unknowns is finite in the case of a periodic spatial distribution of inclusions.

Some randomness can be accounted for by considering a representative volume with a large number of inclusions. This representative volume is then reproduced by periodicity so as to cover the whole three-dimensional space. Different realizations of the distribution of the inclusions can be analysed to get statistical information.

The approach developed here has some relation to that presented by Molinari *et al.* (1987), Ahzi *et al.* (1987) and Canova *et al.* (1992) in the case of polycrystalline materials. To account for a better description of the interaction of a grain with its neighbours, a cluster self consistent scheme was developed in these papers. The classical 1-site self consistent scheme, where the grain is embedded in the homogeneous equivalent medium, was extended in the following way. A grain is embedded in a cluster constituted by several layers of neighbouring grains. The cluster is itself suspended in the homogeneous equivalent medium. The present work, although it relies on similar ideas, has a different context since the matrix has to take here a previlegious role.

The problem of the interaction of elastic inclusions at finite concentration has also been considered recently by Rodin (1993) with a different approach based on the eigenstrain method. The results obtained by Rodin (1993) for a regular periodic arrays of spheres are in good agreement with finite element calculations. Note also that the multiparticle problem was considered by Buryachenko and Kreher (1995) in a statistical approach.

The cluster method developed here is quite general. It applies for ellipsoidal inclusions and arbitrary spatial distributions. The results presented are restricted to spherical inclusions. The accuracy of the cluster scheme is tested by comparison with existing analytical or numerical calculations. In the case of a two phase material, where the inclusions are spherical, the cluster scheme is shown to coincide with the Mori–Tanaka method, at the first-order, i.e., when the cluster is reduced to a single inclusion. When the size of the cluster is increased, the interaction effects between inclusions are shown to be well accounted for.

2. FORMULATION OF THE PROBLEM

The local linear elastic behavior is described by the Hooke's law

$$\boldsymbol{\sigma}_{ij}(\mathbf{x}) = C_{ijkl}(\mathbf{x})\boldsymbol{\varepsilon}_{kl}(\mathbf{x}) \tag{1}$$

where C_{ijkl} is the tensor of elastic moduli, $\mathbf{x}$ is the position vector, and where $\boldsymbol{\sigma}_{ij}$ and $\boldsymbol{\varepsilon}_{ij}$ designate the Cauchy stress and the infinitesimal strain tensor, respectively, the latter defined by

$$\boldsymbol{\varepsilon}_{ij}(\mathbf{x}) = \tfrac{1}{2}(u_{j,i}(\mathbf{x})),$$

where $\mathbf{u}$ is the displacement vector. The subscript j designates the partial derivative with respect to x_j. The convention of summation on repeated indices is adopted in this paper.

The macroscopic constitutive law reads

$$\Sigma_{ij} = C^{\text{eff}}_{ijkl}\,E_{kl}, \tag{2}$$

where Σ_{ij} and E_{ij} are the macroscopic Cauchy stress and strain tensors, respectively, and C^{eff}_{ijkl} represents the effective tensor of elastic moduli.

We consider now a homogeneous reference medium with a tensor of elastic moduli C^0_{ijkl}. The tensor of elastic moduli of the composite material is decomposed into a constant part C^0_{ijkl} and a fluctuating part δC_{ijkl}

$$C_{ijkl}(\mathbf{x}) = C^0_{ijkl}+\delta C_{ijkl}(\mathbf{x}). \tag{3}$$

A substitution of the constitutive law eqn (1) into the equilibrium equation

$$\sigma_{ij,j}(\mathbf{x}) = 0 \tag{4}$$

provides a Navier-type equation

$$C^0_{ijkl}u_{k,lj}(\mathbf{x}) + f_i(\mathbf{x}) = 0 \tag{5}$$

in which $f_i(\mathbf{x})$ is a fictitious body force defined by

$$f_i(\mathbf{x}) = [\delta C_{ijkl}(\mathbf{x})u_{k,l}(\mathbf{x})]_{,j}. \tag{6}$$

The solution of the Navier equation (5) can be expressed in terms of the Green functions G_{mi}

$$u_m(\mathbf{x}) = u^0_m(\mathbf{x}) + \int_{R^3} G_{mi}(\mathbf{x}-\mathbf{x}')f_i(\mathbf{x}')\,\mathrm{d}\mathbf{x}'. \tag{7}$$

The Green functions are associated to the reference medium of moduli C^0_{ijkl} and are assumed to match a condition of zero displacement at infinity. They are solutions of the following set of equations:

$$C^0_{ijkl}G_{km,lj}(\mathbf{x}-\mathbf{x}') + \delta_{im}\delta(\mathbf{x}-\mathbf{x}') = 0, \tag{8}$$

where $\delta(\mathbf{x}-\mathbf{x}')$ represents the Dirac function located at $\mathbf{x}'$ and the δ_{im} are the Kronecker symbols. When incorporating the definition (6) of $f_i(x)$ in eqn (7), we obtain, after derivation, integration by part and symmetrization, an integral equation (where the strain $\boldsymbol{\varepsilon}_{mn}$ is the unknown) similar to the Lippman–Schwinger–Dyson equation in Quantum Mechanics [see Zeller and Dederichs (1973)]

$$\varepsilon_{mn}(\mathbf{x}) = \varepsilon^0_{mn} + \int_{R^3} \Gamma_{mnij}(\mathbf{x}-\mathbf{x}')\delta C_{ijkl}(\mathbf{x}')\varepsilon_{kl}(\mathbf{x}')\,\mathrm{d}\mathbf{x}'. \tag{9}$$

The kernel in the integral is defined by

$$\Gamma_{mnij} = [G_{mi,nj}]_{\{mn\}\{ij\}}. \tag{10}$$

The symbols $\{mn\}$, and $\{ij\}$ indicate that the quantity has been symmetrized with respect to (m,n) and (i,j), respectively.

3. THE MULTIPLE INCLUSIONS PROBLEM

In this paragraph, we take advantage of the particular nature of the composite material considered here, which consists of elastic inclusions suspended in a homogeneous infinitely extended matrix. The tensor of elastic moduli of the matrix is denoted by $\mathbf{C}^m$. A natural choice is to take the matrix as the reference medium, therefore we have $\mathbf{C}^0 = \mathbf{C}^m$.

The inclusions are assumed to be ellipsoidal. The geometry of an inclusion of label I is characterized by the principal lengths $a_\mathrm{I}, b_\mathrm{I}, c_\mathrm{I}$, three Euler angles and the position of its center. The material properties are represented by the tensor of elastic moduli $\mathbf{C}^\mathrm{I}$.

We shall assume that the stresses (and strains) are uniform in an inclusion. The uniformity of the stresses in an inclusion embedded in an infinite space has been demonstrated by Eshelby (1957). For a large concentration of inclusions, the hypothesis of stress uniformity certainly fails, but since we are mostly interested by the evaluation of the mean stresses in the different phases, it remains an interesting working assumption. That hypothesis will be tested by comparison with results obtained with numerical methods, or by other analytical means. Let us denote by $\boldsymbol{\varepsilon}^{\mathrm{I}}$ the strain in the inclusion of label I. The domain occupied by this inclusion will be noted I and its volume by V_{I}.

Considering the definition (3), it follows immediately that:

$$\delta C_{ijkl}(x) = \begin{cases} 0 & \text{when } \mathbf{x} \in \text{matrix} \\ \delta C^{\mathrm{I}}_{ijkl} = C^{\mathrm{I}}_{ijkl} - C^{0}_{ijkl} & \text{when } \mathbf{x} \in \text{inclusion I.} \end{cases} \tag{11}$$

Following the assumption of uniform strain within an inclusion, the integral equation (9) reads

$$\varepsilon_{mn}(\mathbf{x}) = \varepsilon^{0}_{mn} + \sum_{J=1}^{\infty} \left(\int_{J} \Gamma_{mnij}(\mathbf{x}-\mathbf{x}')\,\mathrm{d}\mathbf{x}' \right) \delta C^{J}_{ijkl} \varepsilon^{J}_{kl} \tag{12}$$

where the summation runs along the whole set of inclusions (possibly infinite). Note, by inspection of eqn (12), that strain uniformity is not realized in an inclusion, except when a single ellipsoidal inclusion is considered.

Therefore, in the framework of this simplified approach, to attribute a meaning to $\boldsymbol{\varepsilon}^{\mathrm{I}}_{mn}$, we shall define it as the mean strain in the inclusion I. Considering the average in I of the strain defined by eqn (12), we obtain

$$\boldsymbol{\varepsilon}^{I}_{mn} = \boldsymbol{\varepsilon}^{0}_{mn} + \sum_{J=1}^{\infty} \Gamma^{IJ}_{mnij} \delta C^{J}_{ijkl} \boldsymbol{\varepsilon}^{J}_{kl}, \tag{13}$$

where

$$\Gamma^{IJ}_{mnij} = \frac{1}{V_I} \int_I \int_J \Gamma_{mnij}(\mathbf{x}-\mathbf{x}')\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'. \tag{14}$$

Note that the interactions of the inclusion I with the other inclusions are accounted for by the fourth order tensors $\boldsymbol{\Gamma}^{IJ}$ ($J \neq I$). These interaction tensors can be calculated when the shape and the position of inclusions are known. We refer to Appendix A for explicit values of $\boldsymbol{\Gamma}^{IJ}$ when spherical inclusions are considered.

The integration constant $\boldsymbol{\varepsilon}^{0}$ that appears in eqn (12), can be related to the macroscopic strain $\mathbf{E}$ applied at infinity. We denote by $\langle f \rangle$ the average of the quantity f, defined as follows:

$$\langle f \rangle = \lim_{R \to \infty} \frac{1}{\frac{4}{3}\pi R^3} \int_{B(\mathbf{x},R)} f(\mathbf{x}')\,\mathrm{d}\mathbf{x}', \tag{15}$$

where $B(\mathbf{x}, R)$ is a sphere of center $\mathbf{x}$ and radius R. In this paper the hypothesis of statistic homogeneity is considered to be satisfied. Therefore, the definition of the average $\langle f \rangle$ does not depend on the choice of the center $\mathbf{x}$ of the sphere $B(\mathbf{x}, R)$. Averaging of the integral eqn (9) results in the following expression:

$$E_{mn} = \boldsymbol{\varepsilon}^{0}_{mn} + \langle \Gamma_{mnij} * \delta C_{ijkl} \varepsilon_{kl} \rangle, \tag{16}$$

where $*$ designates the usual convolution. The kernel $\Gamma_{mnij}(\mathbf{x}-\mathbf{x}')$ can be decomposed into the sum of a singular Dirac part having the form, $-E^{0}_{mnij}\delta(\mathbf{x}-\mathbf{x}')$ and of a function having a singularity of the form $1/|\mathbf{x}-\mathbf{x}'|^3$.

The averaging operation retains only the Dirac singularity:

$$\langle \Gamma_{mnij} * \delta C_{ijkl} \varepsilon_{kl} \rangle = -E^0_{mnij} \langle \delta C_{ijkl} \varepsilon_{kl} \rangle. \tag{17}$$

For an isotropic matrix defined by the shear and bulk moduli μ^0 and k^0, one has

$$E^0_{ijkl} = \frac{1}{15\mu^0(3k^0+4\mu^0)}\{-(3k^0+\mu^0)\delta_{ij}\delta_{kl}+9(k^0+2\mu^0)I_{ijkl}\}, \tag{18}$$

where I_{ijkl} is a unit tensor defined by

$$I_{ijkl} = \tfrac{1}{2}\{\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}\}. \tag{19}$$

The relations (13) constitute a set of equations with an infinite number of unknowns ε^J. As in Canova *et al.* (1992), the problem can be reduced to the solution of N equations with N unknowns, by considering an elementary representative cubic volume (ERV) that contains N inclusions. The ERV is reproduced by periodicity so as to cover the whole space. To each inclusion $K = 1, \ldots, N$ in the ERV is attached a family of inclusions obtained by periodicity. This family is denoted by the label K. The volumic fraction of the inclusion K in the ERV is noted f_K and is equal to the volumic fraction of the family K in the whole space. The unknowns are the strains ε^K in the inclusions ($K = 1, \ldots, N$). With these notations the constant ε^0 can be expressed by using eqns (16) and (17) as follows:

$$\varepsilon^0 = \mathbf{E}+\mathbf{E}^0 : \sum_{K=1}^{N} f_K \delta\mathbf{C}^K : \varepsilon^K, \left(\varepsilon^0_{ij} = E_{ij}+E^0_{ijmn}\sum_{K=1}^{N} f_K \delta C^K_{mnpq}\varepsilon^K_{pq}\right). \tag{20}$$

For sake of simplicity, the tensorial notation is adopted, with the double product denoted by a double dot. For clarity of the definition, the indicial notation is also given in parenthesis.

The strains ε^I are solutions of the set of linear equations

$$\varepsilon^I = \mathbf{E}+\sum_{J=1}^{\infty}\mathbf{\Gamma}^{IJ} : \delta\mathbf{C}^J : \varepsilon^J + \mathbf{E}^0 : \sum_{K=1}^{N} f_K \delta\mathbf{C}^K : \varepsilon^K. \tag{21}$$

Denoting by F_I the set of labels of the family associated to the inclusion I ($1 \leqslant I \leqslant N$), eqn (21) can be rewritten as

$$\varepsilon^I = \mathbf{E}+\sum_{J\in F_1}\mathbf{\Gamma}^{IJ} : \delta\mathbf{C}^1 : \varepsilon^1 + \cdots + \sum_{J\in F_N}\mathbf{\Gamma}^{IJ} : \delta\mathbf{C}^N : \varepsilon^N + \mathbf{E}^0 : \sum_{K=1}^{N} f_K \delta\mathbf{C}^K : \varepsilon^K. \tag{22}$$

The summations in eqn (22) involve an infinite series of inclusions. A simple approximate solution of the system (22) can be obtained in the following way. To each inclusion I we attach a sphere $S(I, R_c)$ of radius R_c having its center located at the center of the inclusion I. We denote by $C(I, R_c)$, or more briefly by C_I, the cluster of inclusions having their center in $S(I, R_c)$. The series in formula (22) can be now reduced to a finite summation that involves only the inclusions located in the cluster C_I. Defining by C_{IJ} the intersection of the cluster C_I with the family of inclusions F_J, we have

$$\varepsilon^I = \mathbf{E}+\sum_{J\in C_{I1}}\mathbf{\Gamma}^{IJ} : \delta\mathbf{C}^1 : \varepsilon^1 + \cdots + \sum_{J\in C_{IN}}\mathbf{\Gamma}^{IJ} : \delta\mathbf{C}^N : \varepsilon^N + \mathbf{E}^0 : \sum_{K=1}^{N} f_K \delta\mathbf{C}^K : \varepsilon^K \tag{23}$$

for $I = 1, \ldots, N$.

The convergence of the approximate solution to the exact solution when $R_c \to \infty$ is proved in Appendix B.

Since the strains $\boldsymbol{\varepsilon}^I$, $I = 1, \ldots, N$, depend linearly on the overall strain $\mathbf{E}$, one can define the localization strain tensors $\mathbf{A}^I$ by solving the system (23)

$$\boldsymbol{\varepsilon}^I = \mathbf{A}^I : \mathbf{E}. \tag{24}$$

Substituting eqn (24) in eqn (23), and considering that $\mathbf{E}$ is arbitrary, a linear system of N equations is obtained where the localization tensors $\mathbf{A}^I$ are the unknowns

$$\mathbf{A}^I = \mathbf{I} + \sum_{J \in C_{I1}} \boldsymbol{\Gamma}^{IJ} : \delta\mathbf{C}^1 : \mathbf{A}^1 + \cdots + \sum_{J \in C_{IN}} \boldsymbol{\Gamma}^{IJ} : \delta\mathbf{C}^N : \mathbf{A}^N + \mathbf{E}^0 : \sum_{K=1}^{N} f_K \delta\mathbf{C}^K : \mathbf{A}^K \tag{25}$$

for $I = 1, \ldots, N$. The fourth order unit tensor $\mathbf{I}$ has been defined in eqn (19). The localization tensors $\mathbf{A}^I$ are obtained by the numerical solution of eqn (25). The matrix localization tensor, $\mathbf{A}^m$, that provides the average strain in the matrix as a function of the overall strain, is then given by

$$\mathbf{A}^m = \frac{1}{f_m}\left(\mathbf{I} - \sum_{I=1}^{N} f_I \mathbf{A}^I\right). \tag{26}$$

The overall properties results from the following relation:

$$\mathbf{C}^{\text{eff}} = \langle \mathbf{C} : \mathbf{A} \rangle = f_m \mathbf{C}^m : \mathbf{A}^m + \sum_{I=1}^{N} f_I \mathbf{C}^I : \mathbf{A}^I, \tag{27}$$

where $\mathbf{C}^m$ is the tensor of elastic moduli of the matrix.

We shall now apply this approach to various configurations, where different spatial distributions will be considered.

4. APPLICATION TO SPHERICAL INCLUSIONS

In this paragraph, the results obtained by the proposed method are compared with closed form solutions that exist for particular spatial configurations of spherical inclusions and also with approximate solutions obtained by finite element calculations. A discussion with respect to experimental results is also presented. The first example considered is that of a simple cubic periodic distribution of rigid spheres of identical radius, embedded in a linear homogeneous isotropic elastic matrix. This case has been solved analytically by Nunan and Keller (1984).

In our calculations the interaction of a sphere with the other spheres is accounted for within the simplified cluster approach described in the preceding paragraph. The representative elementary volume (called also the unit representative cell for periodic composites) is here constituted by a cube containing a single sphere at the center, Fig. 1. Therefore we have a single family F_1 of inclusions and a single unknown $\boldsymbol{\varepsilon}^1$. Equation (23) reduces to

$$\boldsymbol{\varepsilon}^1 = \mathbf{E} + \sum_{J \in C_1} \boldsymbol{\Gamma}^{1J} : \delta\mathbf{C}^1 : \boldsymbol{\varepsilon}^1 + \mathbf{E}^0 : f_1 \delta\mathbf{C}^1 : \boldsymbol{\varepsilon}^1. \tag{28}$$

When rigid inclusions are considered, eqn (28) is indeterminate, because the components of $\delta\mathbf{C}^1$ are infinite while $\boldsymbol{\varepsilon}^1$ is equal to zero. However, we can solve the problem for hard deformable inclusions. Then, the case of rigid inclusions is obtained in the limiting process where the rigidity of the inclusions is increased to infinity.

The accuracy of the approximate solution depends on the radius R_c of the cluster. A two-dimensional representation of the cluster attached to an inclusion I is shown in Fig. 2. In Fig. 3, the calculated effective shear modulus (normalized by the shear modulus of the

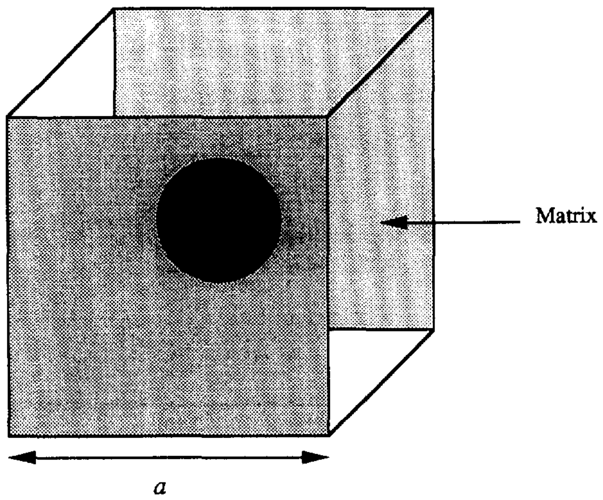

Fig. 1. Elementary representative volume (ERV) for a simple cubic distribution of spherical inclusions.

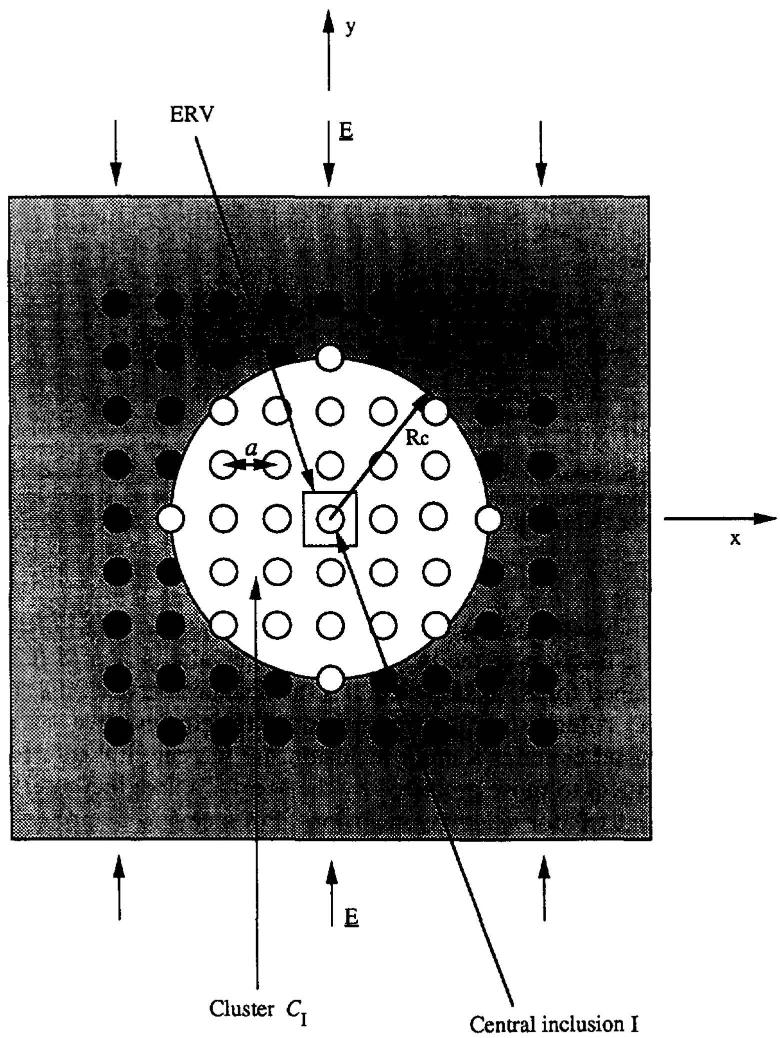

Fig. 2. Schematic representation of the cluster of radius R_c attached to an inclusion I. A simple cubic distribution of spherical inclusions is shown here. The elementary representative volume (ERV) is the small cube at the center of the figure.

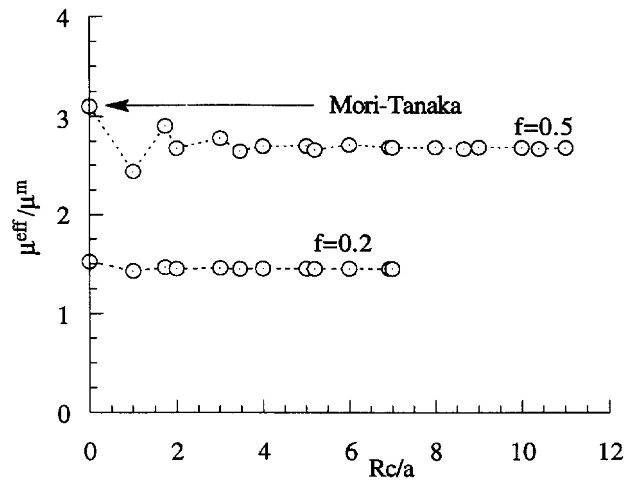

Fig. 3. Convergence of the cluster scheme for increasing values of the radius R_c of the cluster. A simple cubic distribution of rigid spheres is considered. Note that for $R_c < a$, the cluster contains a single inclusion. In that case the results are identical to those obtained with the Mori–Tanaka method.

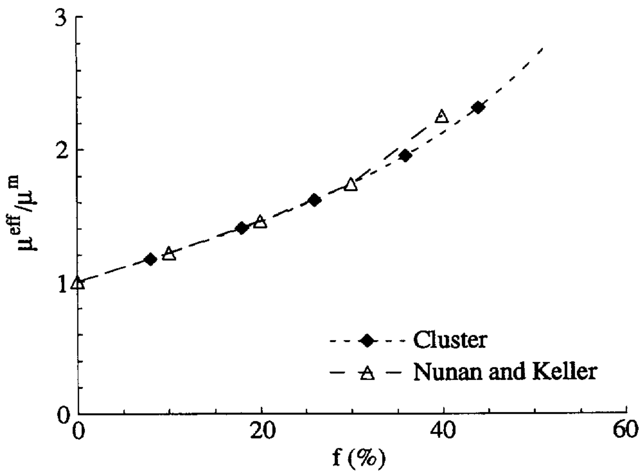

Fig. 4. Effective shear modulus (in the principal direction of cubic symmetry) as a function of the volumic fraction of rigid spheres (simple cubic distribution). The results of the cluster scheme are compared with those of Nunan and Keller and are normalized with the shear modulus μ^m of the matrix.

matrix) in the principal direction x, see Fig. 2, is represented in terms of the radius R_c of the cluster. The volumic fraction of the inclusions has the value of 0.5 or 0.2. It appears that convergence is attained for $R_c \geqslant 2a$, where a is the distance between the centers of the inclusions. For a smaller volumic fraction f of inclusions the convergence is accelerated.

For $R_c < a$, the cluster contains a single inclusion. In that case it is interesting to note that the results are identical to those predicted by the Mori–Tanaka method. This result is demonstrated in Appendix C for spherical inclusions, but seems to be no longer valid for ellipsoidal inclusions.

Note that for a large cluster size, the results are significantly improved by the proposed method, which better accounts for the particle interactions than the Mori–Tanaka method.

The results in Fig. 4 represent the effective shear modulus in the principal direction x, (normalized by the shear modulus of the matrix) as a function of the volumic fraction of the spheres. The Poisson ratio of the matrix has a value of $v = 0.3$. It appears that the results of our cluster scheme are in close agreement with the results by Nunan and Keller (1984) up to a volumic fraction of 0.4.

In addition the results of the 1 site symmetric self consistent scheme are reproduced in Fig. 5, as well as those given by the three phase model of Christensen and Lo (1979), and

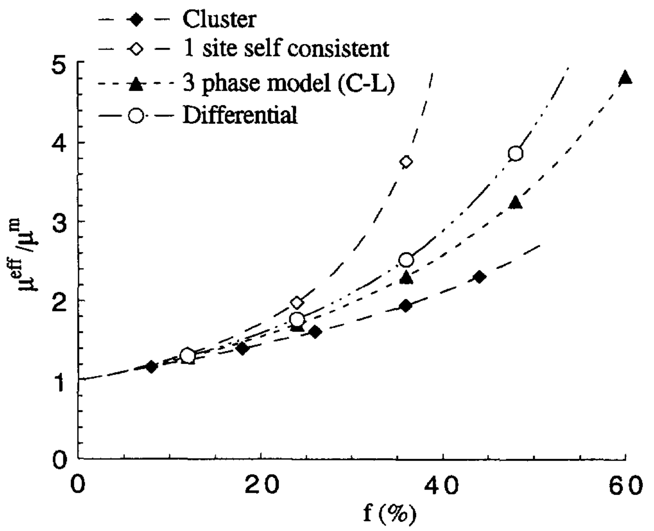

Fig. 5. Comparison of the results of the cluster approach to those of the classical one site self consistent scheme, of the three phase model and of the differential scheme. A simple cubic distribution of rigid spheres is considered.

by the differential scheme. In these methods, no assumption of periodic distribution of the spheres is made. From the results of Fig. 5, it is clear that the 1 site self consistent scheme is not adapted to the material considered here, as it does not account for the connectivity of the matrix. On the other hand, the three phase model and the differential scheme do account for the connectivity and their results are closer to that of the cluster approach. However, these two models are well suited for an isotropic distribution of the spheres, while a cubic distribution is considered here. The observation that the deviation with respect to the cluster scheme is not too large, should be attributed to the fact that the cubic anisotropy is a mild deviation of isotropy. The definite advantage of the cluster approach when compared with the three phase and the differential model is that it can be easily applied to any kind of spatial distribution of inclusions. Moreover, ellipsoidal or parallelipedic inclusions can be easily treated in the cluster scheme, while it is much more difficult in the three phase model.

In Fig. 6, it appears that the results provided by the Mori–Tanaka method overestimate the effective shear modulus, when rigid inclusions are considered. Note that the Mori–Tanaka results coincide with the Hashin–Shtrikman lower bound in the case of an isotropic

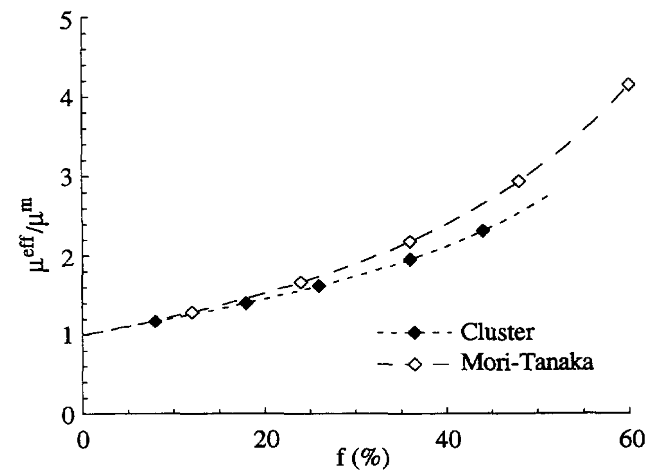

Fig. 6. Comparison of the cluster approach with the Mori–Tanaka method for a simple cubic distribution of rigid spheres.

distribution of rigid inclusions. Since a simple cubic distribution is considered here, the Mori–Tanaka method does not provide a lower bound as it is clear in Fig. 6.

The same type of results are represented in Fig. 7 for a simple cubic distribution of spherical voids. The results of our cluster scheme are in close agreement with those obtained by Nemat-Nasser *et al.* (1982) with a Fourier expansion method, Fig. 7(a). The results of Sangani and Lu (1987) based on the method of singularity distribution seem to overestimate the shear modulus, Fig. 7(a). In Fig. 7(b), it is shown that the cluster scheme is also in very good agreement with the analytical results of Rodin (1993), and the finite element calculations of Rodin (1993) and of Brockenbrough (1992).

Also, for sake of comparison, the cluster results are compared with other homogenization schemes in Fig. 8. Note that the remarks made for Fig. 5, concerning the adequacy of these homogenization schemes, are also valid here. Note also, that the percolation threshold predicted at a volumic fraction of 0.5 by the 1 site self consistent scheme, is not reproduced by the other methods.

It is interesting to compare the prediction of the cluster scheme with experimental data. In Fig. 9, the data of Walsh *et al.* (1965) for the bulk modulus of a sintered glass are compared with the differential scheme, as in the work of Zimmerman (1991), and also with the cluster approach for a simple cubic lattice of voids. Although the exact spatial distribution of voids in the real material is not known (and certainly is not exactly of the type considered in the cluster calculation), the agreement with the experiments is good, specially when compared with the 1 site self consistent scheme. Note that the largest volumic fraction of spherical voids with equal radius is equal to $f = 0.52$ for a simple cubic lattice. That

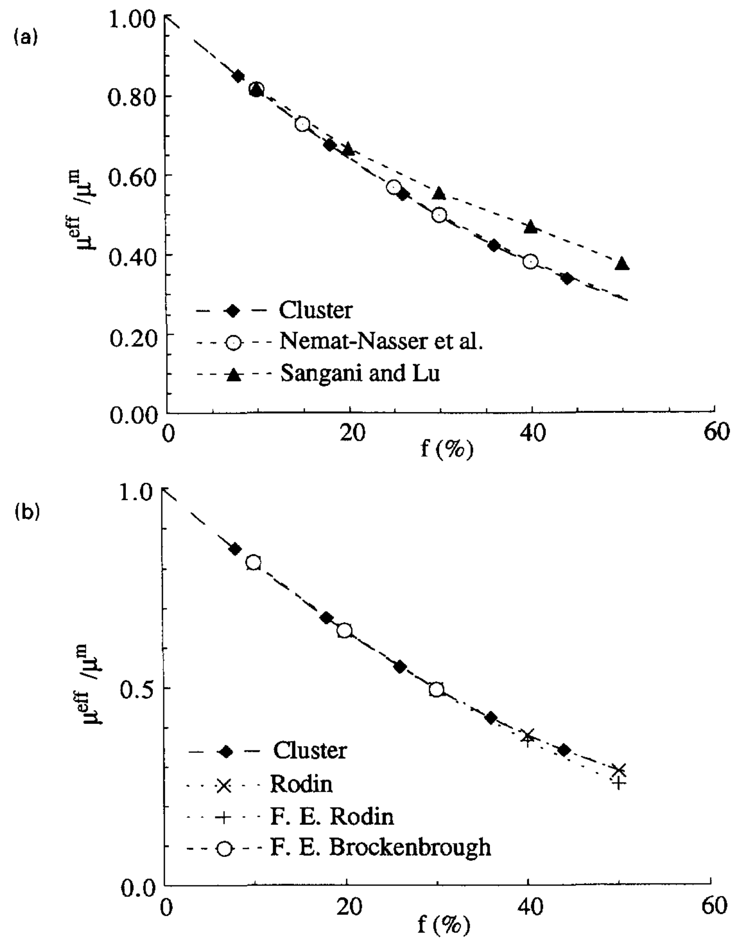

Fig. 7. Effective shear modulus in the principal direction of cubic symmetry for a simple cubic distribution of spherical voids. The results of the cluster approach are compared with those of Nemat-Nasser *et al.* (1982) and Sangani and Lu (1987), Fig. 7(a), and with the analytical results of Rodin (1993) and the finite element results of Rodin (1993) and Brockenbrough (1992).

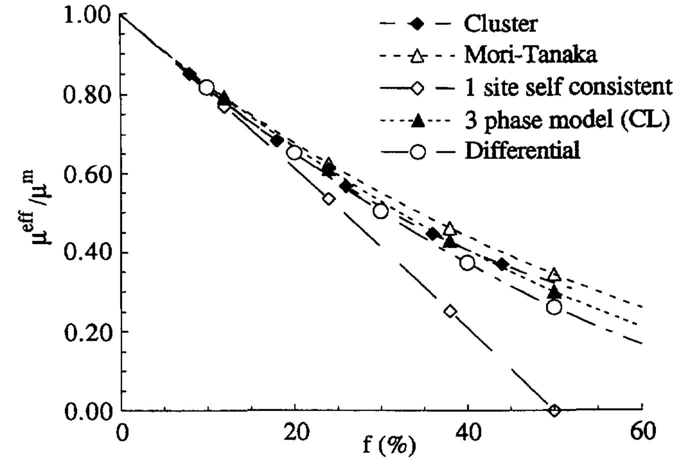

Fig. 8. Comparison of the results of the cluster approach with other homogenization models. A simple cubic distribution of spherical voids is considered.

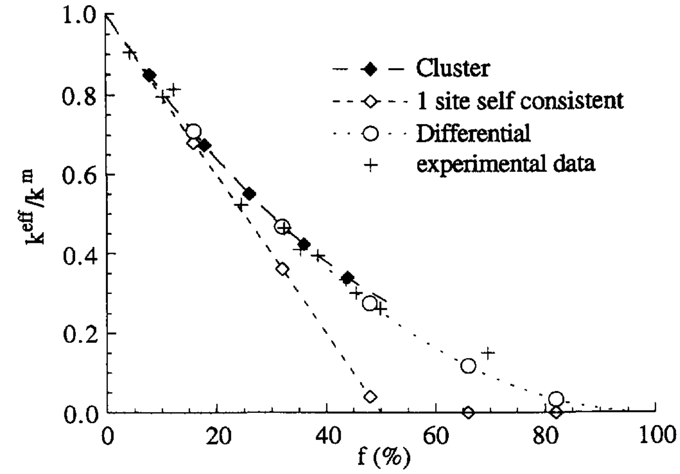

Fig. 9. Comparison of the results of the cluster scheme with experimental data obtained for a sintered glass. The results are also compared with those of the one site self consistent scheme and of the differential scheme.

restriction limits the comparison between the cluster results and the experimental data. Concerning the convergence of the cluster scheme, it has been checked that increasing the size of the cluster beyond $R_c = 2a$ does not improve the results for a simple cubic distribution of spherical voids.

Another example is that of a three phase material, where a BCC distribution of spheres is considered, half of them being voids, the others being rigid inclusions, Fig. 10. For that centered cubic symmetry, the elementary representative volume is a cube containing a sphere at the center and one eighth of a sphere at each corner of the cube, see Fig. 11. Two families of inclusions F_1 and F_2 have to be considered and the equation system (23) reduces to

$$\boldsymbol{\varepsilon}^1 = \mathbf{E} + \sum_{J\in C_{11}} \boldsymbol{\Gamma}^{1J} : \delta\mathbf{C}^1 : \boldsymbol{\varepsilon}^1 + \sum_{J\in C_{12}} \boldsymbol{\Gamma}^{1J} : \delta\mathbf{C}^2 : \boldsymbol{\varepsilon}^2 + \mathbf{E}^0 : \sum_{K=1}^{2} f_K \delta\mathbf{C}^K : \boldsymbol{\varepsilon}^K \tag{29}$$

$$\boldsymbol{\varepsilon}^2 = \mathbf{E} + \sum_{J\in C_{21}} \boldsymbol{\Gamma}^{2J} : \delta\mathbf{C}^1 : \boldsymbol{\varepsilon}^1 + \sum_{J\in C_{22}} \boldsymbol{\Gamma}^{2J} : \delta\mathbf{C}^2 : \boldsymbol{\varepsilon}^2 + \mathbf{E}^0 : \sum_{K=1}^{2} f_K \delta\mathbf{C}^K : \boldsymbol{\varepsilon}^K. \tag{30}$$

The particular case where all the spheres are voids will be also analyzed. Then

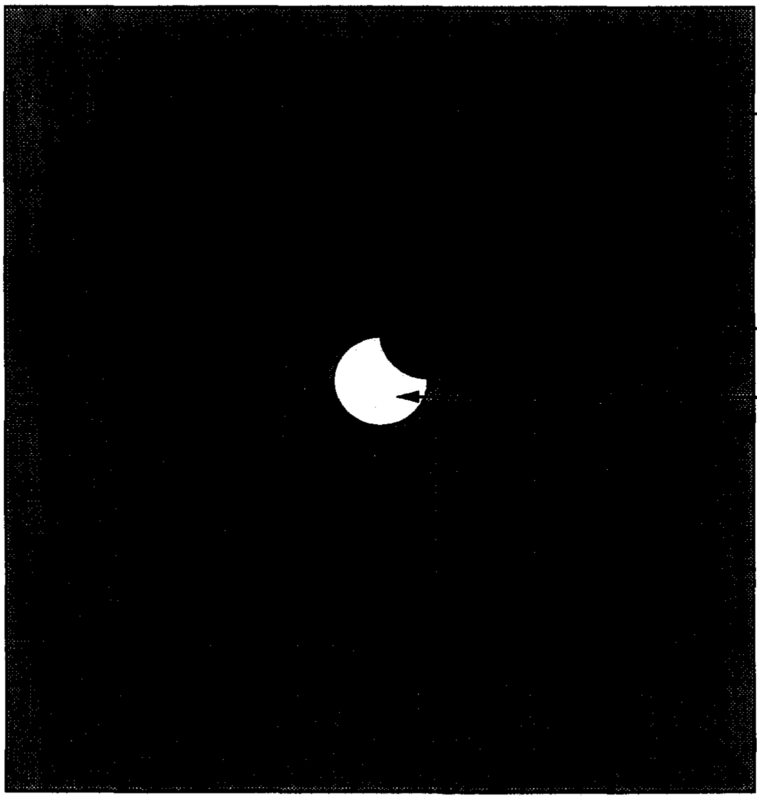

Fig. 10. Body centred cubic distribution of the spherical inclusions.

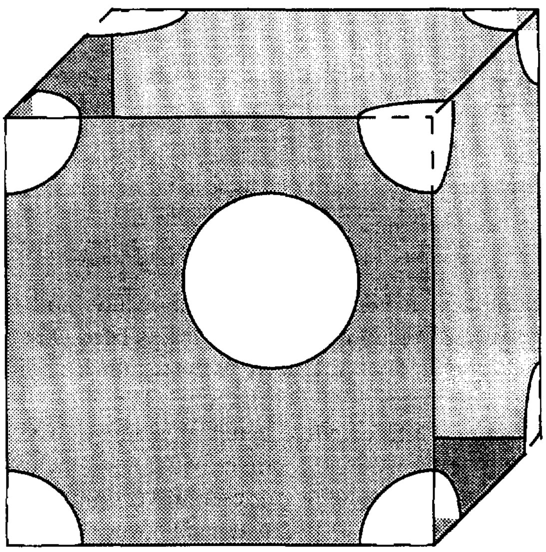

Fig. 11. Representative elementary volume for the BCC distribution of Fig. 10.

$\delta \mathbf{C}^1 = \delta \mathbf{C}^2$, and due to the symmetry of the problem we have $\boldsymbol{\varepsilon}^1 = \boldsymbol{\varepsilon}^2$. This results in a single equation to solve

$$\boldsymbol{\varepsilon}^1 = \mathbf{E} + \sum_{J \in C_1} \boldsymbol{\Gamma}^{1J} : \delta \mathbf{C}^1 : \boldsymbol{\varepsilon}^1 + \mathbf{E}^0 : f_1 \delta \mathbf{C}^1 : \boldsymbol{\varepsilon}^1 \tag{31}$$

C_1 being the cluster defined in section 3, and f_1 the volumic fraction of voids.

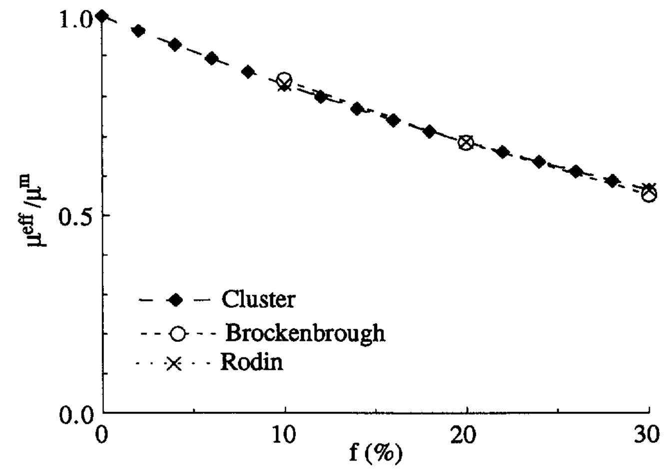

Fig. 12. Comparison of the cluster scheme with the analytical results of Rodin (1993) and numerical results of Brockenbrough (1992). A body centred cubic distribution of spherical voids is considered.

In Fig. 12, the effective shear modulus of a two phase composite, where all the spheres are voids distributed in a BCC array, is represented as a function of the volumic fraction of the spheres. The Poisson ratio of the matrix has a value of $v = 0.3$. Our results are compared in Fig. 12 with the analytical results obtained by Rodin (1993), and the numerical results of Brockenbrough *et al.* (1992). In Fig. 13, the convergence of the cluster approach is shown to be satisfactory for $R_c \geqslant 2a$.

The results in Fig. 14(a), correspond to a three phase material with a BCC distribution of spheres, half of them being voids, the others rigid inclusions, see Fig. 15. The variation in the volumic fractions is obtained by changing the radius of the spheres. The variation of the effective shear modulus in a principal direction of cubic symmetry is considered in terms of the volumic fraction of voids, and for different volumic fractions of rigid spheres. The effect of the voids in decreasing the shear modulus is shown to be much more sensitive for a large volumic fraction of rigid spheres. The results in Fig. 14(b) correspond to a simple cubic distribution of inclusions, and illustrate, when compared to Fig. 14(a), the effects of the spatial distribution of inclusions.

These effects are illustrated again in Fig. 16, where two phase materials are considered. In Fig. 16(a), we have a simple cubic (SC), a body-centred cubic (BCC) and a face centred cubic (FCC) distribution of voids. The spatial distribution is shown to have an important effect as for the SC distribution the shear modulus can be reduced by 20%. Similar results are presented on Fig. 16(b) for rigid spheres. These results can be compared with those of

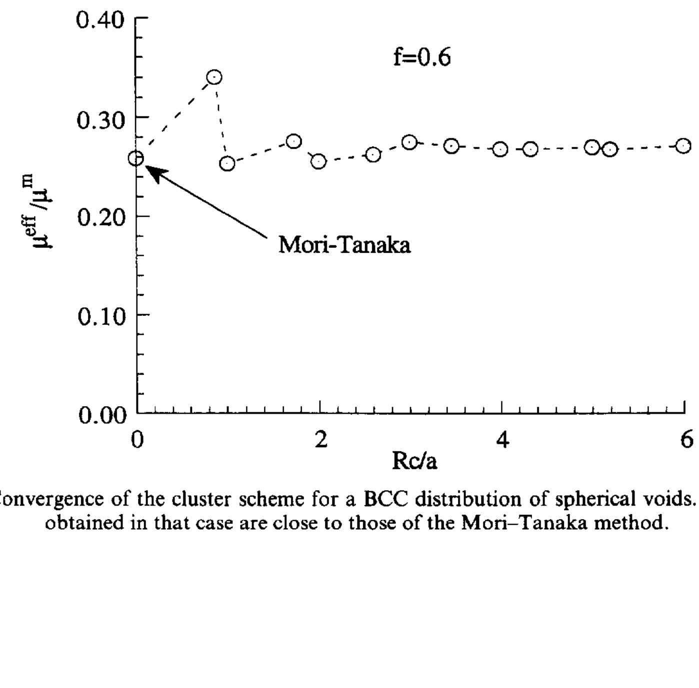

Fig. 13. Convergence of the cluster scheme for a BCC distribution of spherical voids. The results obtained in that case are close to those of the Mori–Tanaka method.

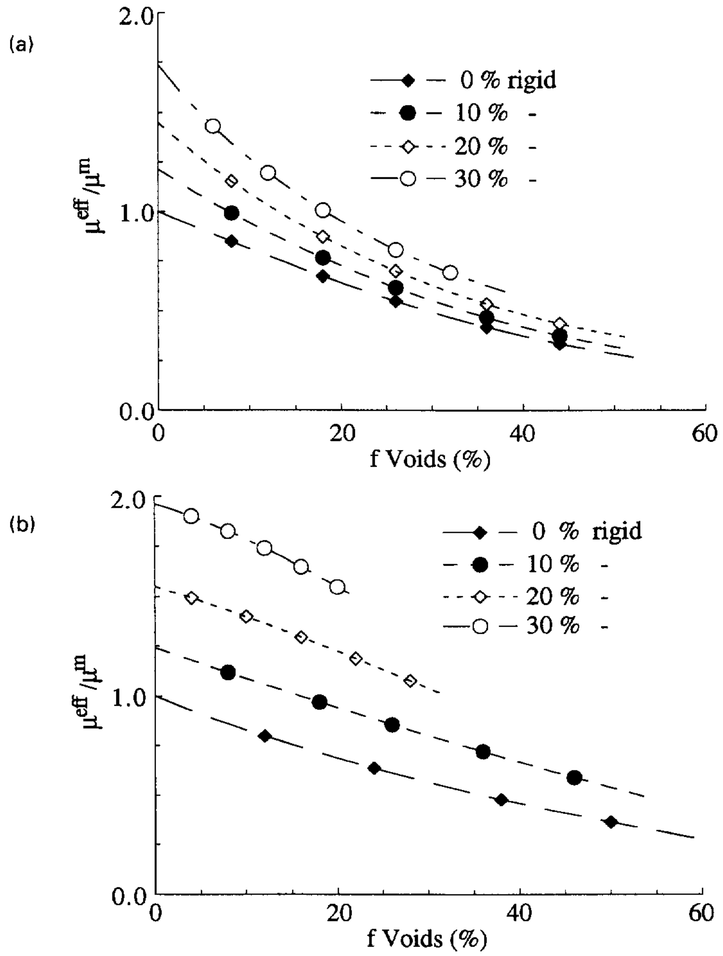

Fig. 14. Effective shear modulus (in the principal direction of cubic symmetry) for a three phase material constituted by a BCC distribution of spherical voids and of rigid spheres, Fig. 14(a), and by a simple cubic distribution, Fig. 14(b).

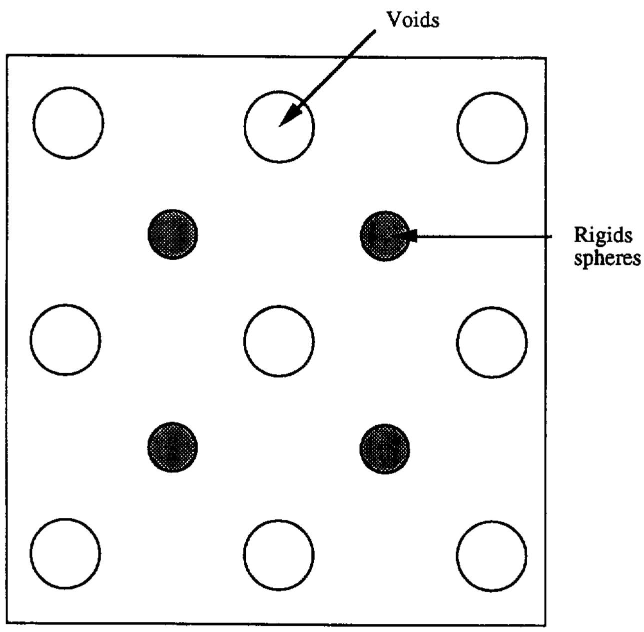

Fig. 15. Schematic two-dimensional representation of the BCC distribution of spherical voids and rigid spheres.

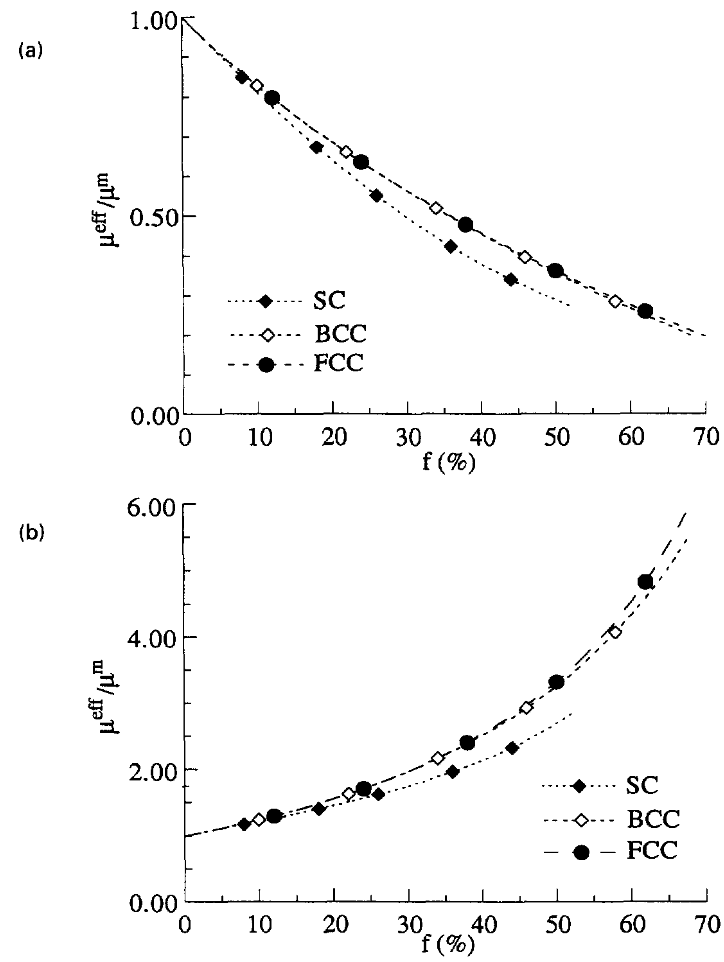

Fig. 16. Illustration of the effects of the spatial distribution of inclusions. Simple cubic, BCC and FCC distributions of spherical voids, Fig. 16(a), and of rigid spheres, Fig. 16(b).

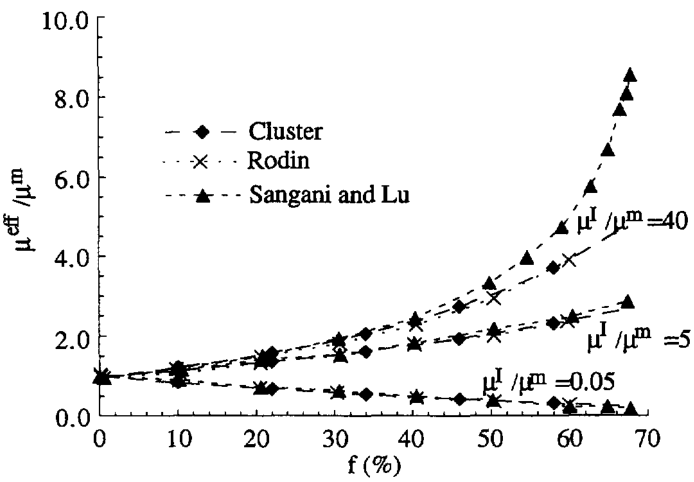

Fig. 17. Comparison of results of the cluster scheme to those of Rodin (1993) and Sangani and Lu (1987), for a BCC distribution of elastic spheres, with different values of the ratio μ^I/μ^m (0.05, 5, 40).

Fig. 14, considering the fact that zero percent of voids corresponds to a SC distribution of rigid spheres in Fig. 14(a), and to a FCC distribution in Fig. 14(b).

In Fig. 17, we have compared our results with those of Rodin (1993) and Sangani and Lu (1987) for a BCC distribution of elastic spheres. Three different values are considered

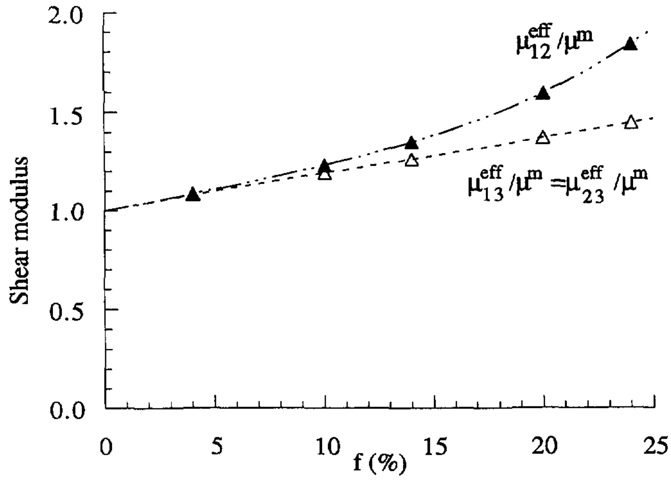

Fig. 18. Effective shear moduli (in the principal directions of symmetry) for an orthorhombic distribution of rigid spheres ($c = 2a = 2b$).

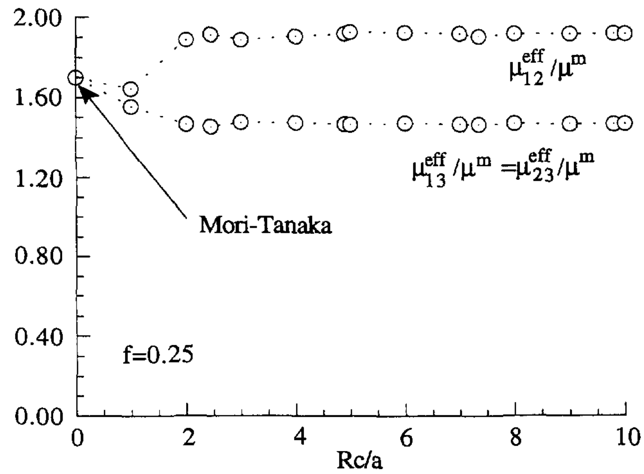

Fig. 19. Convergence of the cluster scheme for increasing values of radius R_c of the cluster. An tetragonal distribution of rigid spheres is considered ($c = 2a = 2b$). Note that the Mori–Tanaka results are retrieved when $R_c \to 0$.

of the ratio μ^I/μ^m of the shear modulus of the inclusions with the shear modulus of the matrix. The results of the cluster scheme are very close to those of Rodin.

Finally we have considered an tetragonal distribution of rigid spheres with $c = 2a = 2b$. In Fig. 18, the effective shear moduli μ_{12}^{eff}, and $\mu_{13}^{eff} = \mu_{23}^{eff}$ are compared (the indices 1, 2, 3 refer to the directions a, b, c, respectively). It is shown how the anisotropic global behaviour is enhanced when the volumic fraction of the voids is increased. The convergence of the cluster approach is checked in Fig. 19. Note that the Mori–Tanaka results (that are retrieved when $R_c \to 0$) cannot account for the anisotropic global response.

5. CONCLUSION

In this paper, a general cluster scheme has been presented that accounts for the elastic interactions between ellipsoidal inclusions embedded in an elastic matrix. When two families of spherical inclusions distributed on a regular array are considered, it has been demonstrated that the proposed cluster approach coincides with the Mori–Tanaka method, in the limiting case of the radius R_c of the cluster tending to zero.

When the radius of the cluster is increased, the results of the cluster scheme were shown to converge. Simple analytical solutions were obtained for a single family of spherical inclusions regularly distributed.

The results of the cluster scheme were shown to agree with other analytical or numerical solutions. In addition, the flexibility of the proposed method allows applications to more complex situations. As an example, a tetragonal distribution of spherical inclusions was treated. Further developments with ellipsoidal inclusions will be presented in another paper.

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APPENDIX A
EVALUATION OF Γ^{IJ}

The calculation of the tensor Γ^{IJ} given by the relation (14) is complex when the matrix is not isotropic. In this case the Green's tensors cannot be explicitly calculated. A numerical method has been proposed by Kneer (1965) for the calculation of Γ^{II}, see also Laws (1977) and Ghahremani (1977). Berveiller *et al.* (1987) have used a similar method to calculate the tensor Γ^{IJ} in the case of two ellipsoidal inclusions.

In the case of spherical inclusions, the results are analytical. Let us denote by $R = (O, x_1, x_2, x_3)$ a rectangular system, with the axis Ox_3 chosen so as to contain the centers of the spherical inclusions. We denote by a, b the radius of the inclusions I and J, by $V_J = 4\pi b^3/3$ the volume of J, by R the distance between the centers and by μ, v the matrix shear modulus and Poisson ratio. The components Γ^{IJ}_{ijkl} are given by

$$\Gamma^{IJ}_{1111} = \Gamma^{IJ}_{2222} = \frac{-V_J}{16\pi R^3}\frac{1}{\mu(1-v)}(1-4v+\tfrac{9}{5}\rho^2)$$

$$\Gamma^{IJ}_{1122} = \Gamma^{IJ}_{2211} = \frac{-V_J}{16\pi R^3}\frac{1}{\mu(1-v)}(-1+\tfrac{3}{5}\rho^2)$$

$$\Gamma^{IJ}_{1133} = \Gamma^{IJ}_{2233} = \Gamma^{IJ}_{3311} = \Gamma^{IJ}_{3322} = \frac{-V_J}{16\pi R^3}\frac{1}{\mu(1-v)}(2-\tfrac{12}{5}\rho^2)$$

$$\Gamma^{IJ}_{1212} = \Gamma^{IJ}_{1221} = \Gamma^{IJ}_{2121} = \Gamma^{IJ}_{2112} = \frac{-V_J}{16\pi R^3}\frac{1}{\mu(1-v)}(1-2v+\tfrac{3}{5}\rho^2)$$

$$\Gamma^{IJ}_{1313} = \Gamma^{IJ}_{1331} = \Gamma^{IJ}_{3113} = \Gamma^{IJ}_{3131} = \frac{-V_J}{16\pi R^3}\frac{1}{\mu(1-v)}(1+v-\tfrac{12}{5}\rho^2)$$

$$\Gamma^{IJ}_{2323} = \Gamma^{IJ}_{2332} = \Gamma^{IJ}_{3223} = \Gamma^{IJ}_{3232} = \frac{-V_J}{16\pi R^3}\frac{1}{\mu(1-v)}(1+v-\tfrac{12}{5}\rho^2)$$

$$\Gamma^{IJ}_{3333} = \frac{-V_J}{16\pi R^3}\frac{1}{\mu(1-v)}(-8+8v+\tfrac{24}{5}\rho^2),$$

where

$$\rho^2 = (a^2+b^2)/R^2.$$

Note that $\Gamma^{IJ}_{ijkl} = 0$ when three of the indices are different, or when three of the indices are equal, but different from the fourth.

APPENDIX B
CONVERGENCE OF THE CLUSTER SCHEME

For an inclusion I and a radius R_c, we consider a partition of the family F_i of inclusions into:

$$F_i = C_{Ii} \cup \hat{C}_{Ii}, \quad C_{Ii} \cap \hat{C}_{Ii} = \varnothing, \tag{B1}$$

where C_{Ii} has been defined in the paragraph 3 as the set of the inclusions of the family F_i with a center included in the sphere $S(I, R_c)$. The latter has a radius R_c and its center is identical to that of the inclusion I. Conversely the centers of the inclusions belonging to $\hat{C}_{Ii}$ are located outside $S(I, R_c)$

For large values of the cluster radius R_c, it is justified to replace the system of eqn (22) by eqn (23), providing that the terms of the form

$$\sum_{J \in \hat{C}_{Ii}} \boldsymbol{\Gamma}^{IJ} : \delta\mathbf{C}^i : \boldsymbol{\varepsilon}^i$$

can be neglected. This is of course the case if one can prove that

$$\operatorname*{Lim}_{R_c \to \infty} \sum_{J \in \hat{C}_{Ii}} \boldsymbol{\Gamma}^{IJ} = 0. \tag{B2}$$

This result comes from the following well known property satisfied by $\boldsymbol{\Gamma}(\mathbf{x}, \mathbf{x}')$:

$$\int_{S^c} \boldsymbol{\Gamma}(\mathbf{x}, \mathbf{x}')\,\mathrm{d}\mathbf{x}' = 0 \quad (\mathbf{x} \in S) \tag{B3}$$

for $\mathbf{x}$ belonging to the interior of a sphere S (the integration is made on the exterior of the sphere $S^c = R^3 - S$).

It is sufficient to prove eqn (B2) for the family F_1 of inclusions, that is for $i = 1$. Let us consider the inclusion J belonging to $\hat{C}_{11}$; its center is located outside the sphere $S(I, R_c)$. We shall note Ω_J the cube reproduced by periodicity from the ERV, that includes the inclusion J, see Fig. B1.

From eqn (14) we have

$$\Gamma^{IJ}_{mnij} = \frac{1}{V_1}\int_I\left(\int_J \Gamma_{mnij}(\mathbf{x},\mathbf{x}')\,\mathrm{d}\mathbf{x}'\right)\mathrm{d}\mathbf{x}.$$

For a large value of R_c, the following approximations are justified:

$$\Gamma^{IJ} \approx \frac{V_J}{V_I}\int_I \Gamma(\mathbf{x},\mathbf{x}_J)\,\mathrm{d}\mathbf{x} \approx \frac{1}{V_I}\frac{V_J}{\Omega_J}\int_I\left(\int_{\Omega_J}\Gamma(\mathbf{x},\mathbf{x}')\,\mathrm{d}\mathbf{x}'\right)\mathrm{d}\mathbf{x}, \tag{B4}$$

where $\mathbf{x}_J$ is the center of the inclusion J.

Since V_J/Ω_J is equal to the volumic fraction f_1 of inclusions of the family F_1, we have:

$$\sum_{J\in\hat{C}_{11}}\Gamma^{IJ} = f_1\frac{1}{V_1}\int_I\left(\int_{\hat{\Omega}}\Gamma(\mathbf{x},\mathbf{x}')\,\mathrm{d}\mathbf{x}'\right)\mathrm{d}\mathbf{x}, \tag{B5}$$

where

$$\hat{\Omega} = \sum_{J\in\hat{C}_{11}}\Omega_J$$

is close to $R^3 - S(I, R_c)$ when R_c is large. Thus $\hat{\Omega}$ can be replaced by S^c, where S is the sphere $S(I, R_c)$. Therefore the demonstration of eqn (B2) results from:

$$\sum_{J\in\hat{C}_{11}}\Gamma^{IJ} \approx f_1\frac{1}{V_1}\int_I\left(\int_{S^c}\Gamma(\mathbf{x},\mathbf{x}')\,\mathrm{d}\mathbf{x}'\right)\mathrm{d}\mathbf{x} = 0. \tag{B6}$$

This appears as a direct consequence of eqn (B3), since $\mathbf{x}\in S$.

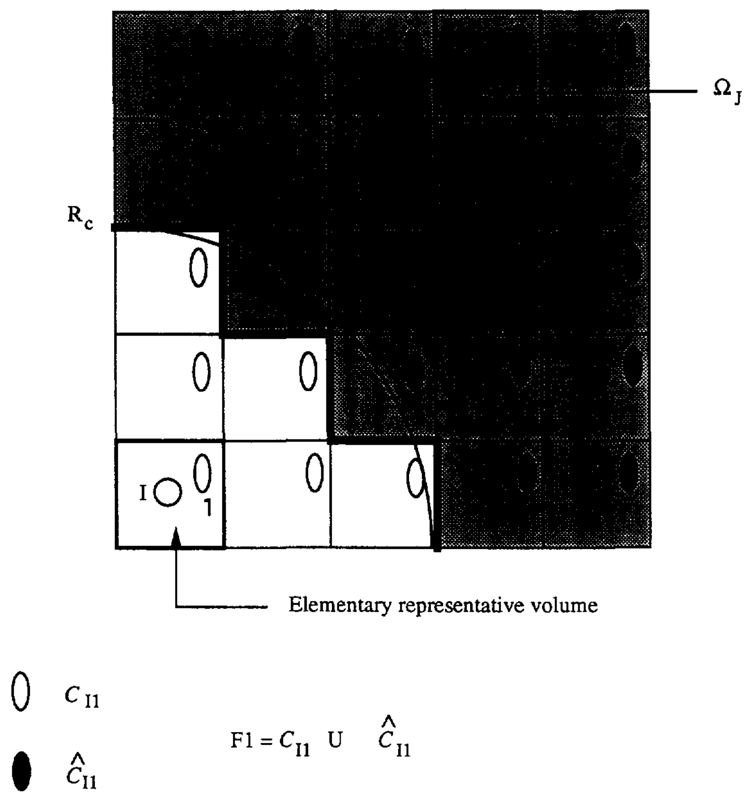

Fig. B1. Schematic representation of the partition of the family F_1 of inclusions.

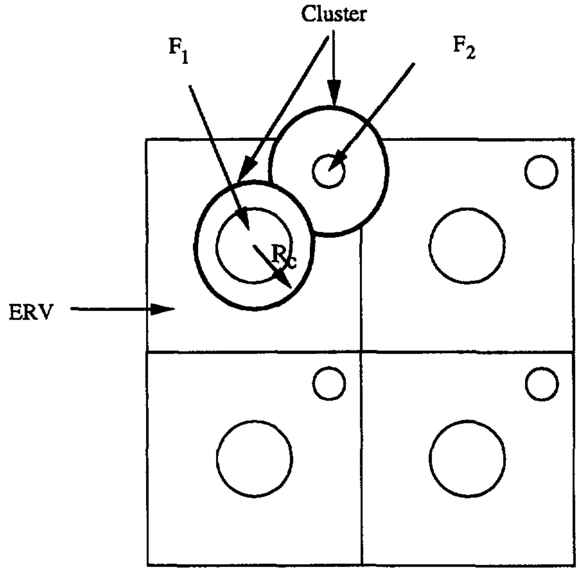

Fig. C1. Representation of a periodic spatial distribution of two families of spheres F_1 and F_2.

APPENDIX C
COMPARISON OF THE CLUSTER SCHEME WITH THE MORI–TANAKA METHOD

A population of spherical inclusions is considered. It is shown, at least when two families of inclusions are considered, that the cluster approach coincides with the Mori–Tanaka method, when the cluster size tends to zero.

In the Fig. C1, a representation is given of a periodic spatial distribution of two families of elastic spheres F_1 and F_2. Considering the fact that we have two families of inclusions, and that the cluster size is so small that a single inclusion is contained in each cluster, the relation (23) reduces to:

$$[\mathbf{I}+(1-f_1)\mathbf{E}^0:\delta\mathbf{C}^1]:\boldsymbol{\varepsilon}^1-f_2\mathbf{E}^0:\delta\mathbf{C}^2:\boldsymbol{\varepsilon}^2=\mathbf{E} \tag{C1}$$

$$-f_1\mathbf{E}^0:\delta\mathbf{C}^1:\boldsymbol{\varepsilon}^1+[\mathbf{I}+(1-f_2)\mathbf{E}^0:\delta\mathbf{C}^2]:\boldsymbol{\varepsilon}^2=\mathbf{E}. \tag{C2}$$

To obtain that results we have used the fact that $C_{12}=C_{21}=\varnothing$ $(C_{12}=C_1\cup F_2)$ and that $\boldsymbol{\Gamma}^{\mathrm{II}}=-\mathbf{E}^0$ for spherical inclusions with $\mathbf{E}^0$ defined by (18).

On the other hand, the Mori–Tanaka method provides the following relations:

$$\boldsymbol{\varepsilon}^1=\boldsymbol{\varepsilon}^m-\mathbf{E}^0:\delta\mathbf{C}^1:\boldsymbol{\varepsilon}^1 \tag{C3}$$

$$\boldsymbol{\varepsilon}^2=\boldsymbol{\varepsilon}^m-\mathbf{E}^0:\delta\mathbf{C}^2:\boldsymbol{\varepsilon}^2. \tag{C4}$$

The mean strain $\boldsymbol{\varepsilon}^m$ in the matrix is related to the macroscopic strain $\mathbf{E}$ through the relation

$$\mathbf{E}=\langle\boldsymbol{\varepsilon}\rangle=f_1\boldsymbol{\varepsilon}^1+f_1\boldsymbol{\varepsilon}^2+(1-f_1-f_2)\boldsymbol{\varepsilon}^m. \tag{C5}$$

Therefore $\boldsymbol{\varepsilon}^m$ can be eliminated in eqns (C3) and (C4) and a simple algebraic manipulation leads to a system of equations identical to eqns (C1) and (C2).