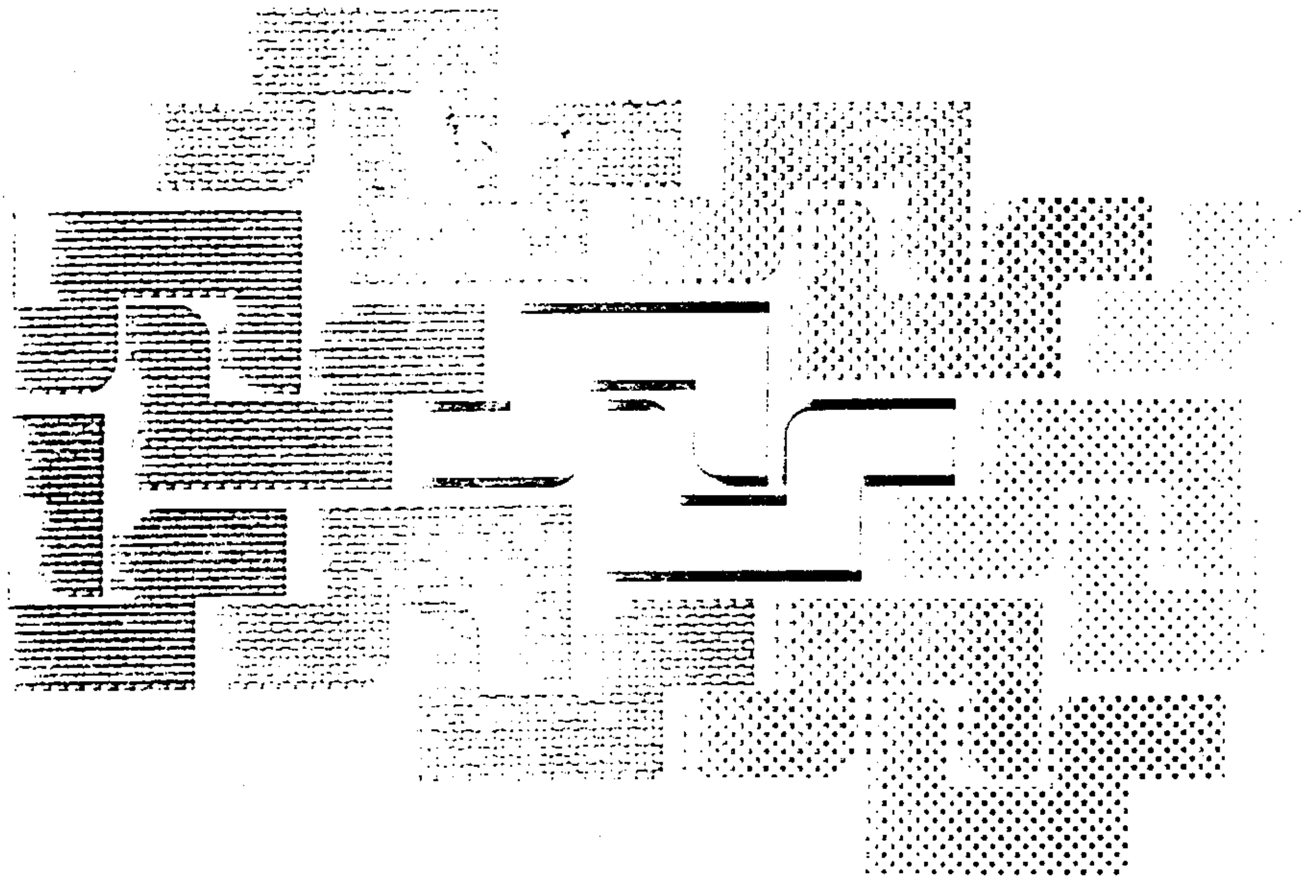

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Edited by

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Carlos A. Mota Soares

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ON THE STRENGTH OF COMPOSITE MATERIALS: VARIATIONAL BOUNDS AND COMPUTATIONAL ASPECTS.

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ABSTRACT: Bounds for the overall yield strength of composite materials are derived in terms of the strength of individual phases and of their arrangement. A general method for the numerical computation of the strength of periodic composites is outlined. The predictions of both methods, bounds and numerical simulations by the finite element method, are presented and compared for some specific examples.

1. Introduction

This paper is devoted to the prediction of the strength of a composite from the knowledge of the strengths of its individuals constituents. Its connection with the present workshop is a problem arising in the optimal design of a structure with respect to its *strength*. For simplicity, the strength of the individual phases is governed by the Von Mises criterion. Therefore, the results to be presented apply more specifically to ductile composites, such as metal matrix composites, rather than to brittle composites.

1.1. A MODEL PROBLEM

Consider a fixed domain Ω subjected to body forces λg_0 proportional to a load parameter λ and fixed on its boundary. Assume that the material occupying Ω has a limited strength governed by the Von Mises criterion, with yield stress $k(x)$. Then the maximal load (limit load) which can be supported by Ω is:

$$\bar{\lambda} = \text{Sup} \left\{ \lambda \text{ such that there exists } \sigma(x) \text{ satisfying: } \atop \text{div}(\sigma(x)) + \lambda g_0(x) = 0,\ \sigma_{eq}(x) \leqslant k(x) \text{ for every } x \text{ in } \Omega \right\} \quad (1.1)$$

σ_{eq} is the Von Mises equivalent stress:

$$\sigma_{eq} = \left(\frac{3}{2} s_{ij} s_{ij}\right)^{1/2}, \quad s_{ij} = \sigma_{ij} - \frac{\text{Tr}(\sigma)}{3}\delta_{ij}.$$

M. P. Bendsøe and C.A. Mota Soares (eds.), Topology Design of Structures, 355–374.

$\bar{\lambda}$ can alternatively be defined by the following variational problem (TEMAM (1985), SALENCON (1983)):

$$\bar{\lambda} = \operatorname*{Inf}_{v} \left(\frac{\int_\Omega k(x)\epsilon_{eq}(v)\ dx}{\left| \int_\Omega g_0 v\ dx \right|} \right) , \ \mathrm{div}(v) = 0 \ in\ \Omega, \ v = 0 \ on\ \partial\Omega, \qquad (1.2)$$

where $\epsilon_{eq} = \left(\frac{2}{3}\epsilon_{ij}\epsilon_{ij}\right)^{1/2}$ is the equivalent strain. The model problem is that of the optimal lay-out in Ω of two materials in given proportions c_1 and c_2, $c_1 + c_2 = 1$, with yield stresses k_1 and k_2. If ω denotes the domain occupied by phase 1, χ its characteristic function, $k(x) = k_1\chi(x) + k_2(1-\chi(x))$ and $\bar{\lambda}(\omega)$ the limit load given by (1.1) or (1.2) with this definition of k(x), the model problem reads:

$$\operatorname*{\mathit{Maximize}}_{\omega}\ \bar{\lambda}(\omega)\ \textit{among designs}\ \omega\ \textit{such that}\ |\omega| = c_1 |\Omega|. \qquad (1.3)$$

As noted by MURAT and TARTAR (1985) and by KOHN and STRANG (1986), a relaxed version of this problem has to be considered. The result is that, instead of the dichotomy phase 1-phase 2, one has to consider a family of composites made up of mixtures of both phases. Consequently one has to predict the strength of these composites as function of the strengths of the constituents and of their volume fractions.

The prediction of the yield strength of nonhomogeneous materials, polycrystals or composites, is also a relevant problem in Mechanics of Materials. Appropriate, but not exhaustive, references adressing this problem are given by DRUCKER (1959), HILL (1967), HUTCHINSON (1976), BAO, HUTCHINSON and Mc MEEKING (1991). The specific case of composites with a periodic micro-structure has been considered by LE NIZERHY (1977), SUQUET (1983) , DE BUHAN (1986), DE BUHAN and TALIERCIO (1991). In the case of an arbitrary disposition of phases, a new direction of research was opened by WILLIS (1989) (1991) and PONTE CASTANEDA (1991) who proposed new variational principles to obtain bounds on the effective properties of nonlinear composites. We propose here another method, simpler in the specific case under consideration, to obtain these bounds and new results on the strength domain of a composite.

1.2. OVERALL STRENGTH OF COMPOSITE MATERIALS

To begin, consider the case of a periodic composite, the micro-structure of which is specified on a unit cell V. It has been established (SUQUET (1983) , BOUCHITTE and SUQUET (1987) (1991)) that the overall strength domain of the composite is given by the convex set:

$$P^{hom} = \Big\{ \Sigma \in \mathbb{R}^9_s \ , \ \exists\ \sigma(x)\ \textit{such that:}\ \langle\sigma\rangle = \Sigma,\ \sigma.n\ \textit{anti-periodic on}\ \partial V \\ \mathrm{div}(\sigma(x)) = 0 \ , \ \sigma_{eq}(x) \leqslant k(x),\ \forall\ x \in V \Big\} , \qquad (1.4)$$

where $\langle . \rangle$ denotes the volume average over the unit cell V. P^{hom} can be alternatively determined by its support function:

$$\Pi^{hom}(E) = \underset{u \in \mathcal{E}_{per}}{\mathrm{Inf}} \langle \pi(x,\epsilon(u)) \rangle, \tag{1.5}$$

$$\mathcal{E}_{per} = \{ u = E.x + u^*,\ \mathrm{div}(u) = 0,\ \ u^* \text{ periodic}\}.$$

$\pi(x,.)$ is the support function of the local strength domain:

$$\pi(x,\epsilon) = k(x)\epsilon_{eq} \quad \text{if } \mathrm{Tr}(\epsilon) = 0,\ \pi(x,\epsilon) = +\infty \text{ otherwise.}$$

When the micro-structure of the composite is not periodic, some of these results can formally be adopted as definitions. Let V be a representative volume element of the composite containing a large number of heterogeneities of small size. The macroscopic dissipation function Π^{hom} is the average of the microscopic dissipation function π:

$$\Pi^{hom}(E) = \underset{u \in \mathcal{E}}{\mathrm{Inf}} \langle \pi(x,\epsilon(u)) \rangle, \tag{1.6}$$

$$\mathcal{E} = \{ u = E.x + u^*,\ \mathrm{div}(u) = 0,\ \ u^* = 0 \text{ on } \partial V \ \}.$$

It is readily checked that Π^{hom} is a convex lower semi-continuous function which is positively homogeneous of degree 1 with respect to E. Therefore, it is the Legendre transform of the indicator function of a closed convex set P^{hom}, which is the *macroscopic strength domain*:

$$P^{hom} = \left\{ \Sigma \in \mathbb{R}^9_s \ ,\ \exists\ \sigma(x) \text{ such that: } \langle\sigma\rangle = \Sigma, \\ \mathrm{div}(\sigma(x)) = 0\ ,\ \sigma_{eq}(x) \leqslant k(x),\ \forall\ x \in V \right\} \tag{1.7}$$

Remark: Instead of the boundary conditions of uniform strain on ∂V in (1.6), boundary conditions of uniform stresses could be considered in (1.7). It may be expected that both boundary conditions are equivalent in the limit of a large representative volume element. However, as pointed out by DE BUHAN (1986) and discussed further in BOUCHITTE and SUQUET (1991), that is not the case in the present context of strength properties.

2. Bounds

2.1. ARBITRARY DISTRIBUTION OF PHASES

In this subsection, no assumptions are made on the distribution of the phases which can be arbitrary.

2.1.1 Dissipation potential: A fictitious linear composite, that is incompressible and isotropic with shear modulus $\mu(x)$ at point x and occupies the same volume element V than the given real nonlinear composite, is introduced. Then,

$$k(x)\ \epsilon_{eq}(u(x)) = \left(\frac{3}{2}\mu(x)\ \epsilon^2_{eq}(u(x)) \right)^{\frac{1}{2}} \left(\frac{2k^2(x)}{3\mu(x)}\right)^{\frac{1}{2}},$$

and

$$\langle\ k(x)\ \epsilon_{eq}(u(x))\ \rangle = \operatorname*{Inf}_{\mu(x) \geq 0} \left\langle \frac{3}{2}\mu(x)\ \epsilon_{eq}^2(u(x)) \right\rangle^{\frac{1}{2}} \left\langle \frac{2k^2(x)}{3\mu(x)} \right\rangle^{\frac{1}{2}}. \quad (2.1)$$

Indeed, it follows from Cauchy-Schwarz inequality that the left hand side of (2.1) is smaller than its right hand side. Moreover, equality is obtained with

$$\mu(x) = \frac{2}{3}\frac{k(x)}{\epsilon_{eq}(u(x))}. \quad (2.2)$$

The infimum of $\langle\ k(x)\ \epsilon_{eq}(u(x))\ \rangle$ over all admissible fields u, can be computed from (2.1) by interchanging the order of the infima:

$$\Pi^{hom}(E) = \operatorname*{Inf}_{\mu(x) \geq 0}\ \operatorname*{Inf}_{u \in \mathcal{E}} \left\langle \frac{3}{2}\mu(x)\ \epsilon_{eq}^2(u(x)) \right\rangle^{1/2} \left\langle \frac{2k^2(x)}{3\mu(x)} \right\rangle^{1/2}. \quad (2.3)$$

The infimum over u in (2.3) amounts to solving a homogenization problem for a *linear composite*. Finally

$$\Pi^{hom}(E) = \operatorname*{Inf}_{\mu(x) \geq 0} (W^{hom}(\mu,E))^{1/2} \left(\left\langle \frac{2k^2(x)}{3\mu(x)} \right\rangle\right)^{1/2}, \quad (2.4)$$

where
$$W^{hom}(\mu,E) = \operatorname*{Inf}_{u \in \mathcal{E}} \left\langle \frac{3}{2}\mu(x)\ \epsilon_{eq}^2(u(x)) \right\rangle \quad (2.5)$$

The exact evaluation of the infimum over $\mu(x)$ in (2.4) requires the knowledge of the homogenized (quadratic) energy W^{hom} for arbitrary moduli $\mu(x)$. This exact information is not available except in very specific situations (laminates), but for any choice of the field μ, (2.4) will provide an upper bound for Π^{hom}:

$$\Pi^{hom}(E) \leq (W^{hom}(\mu,E))^{1/2} \left(\left\langle \frac{2k^2(x)}{3\mu(x)} \right\rangle\right)^{1/2} \textit{ for any positive field } \mu(x). \quad (2.6)$$

Therefore, even if it is not possible to compute W^{hom} for arbitrary $\mu(x)$, it is possible to use available expressions or upper bounds on W^{hom} for a class of specific fields $\mu(x)$.

Remarks: 1. PONTE-CASTANEDA (1992) has proposed new variational principles to obtain bounds on the effective properties of nonlinear composites. When applied to the present situation, his method yields

$$\Pi^{hom}(E) = \operatorname*{Inf}_{\mu(x) \geq 0} \left(W^{hom}(\mu,E) + \left\langle \frac{k^2(x)}{6\mu(x)} \right\rangle\right), \quad (2.7)$$

and therefore for any specific choice of the field μ

$$\Pi^{hom}(E) \leqslant W^{hom}(\mu,E) + \left\langle \frac{k^2(x)}{6\mu(x)} \right\rangle . \tag{2.8}$$

The general expressions (2.4) and (2.7) are different, although they yield the same infimum $\Pi^{hom}(E)$. However, for general fields $\mu(x)$, (2.6) does better than (2.8). This is a consequence of the straightforward inequality $xy \leqslant x^2 + y^2/4$.

2. When one phase of the composite is a void (respectively, a rigid inclusion), its strength is 0 (respectively $+\infty$). Therefore the field $\mu(x)$ has to be 0 (respectively $+\infty$) in this phase.

2.1.2 Strength domain. An expression for the effective strength domain of the composite can be derived from (2.4). For a given field μ the function

$$W^{hom}(\mu,E)^{1/2} \left\langle 2k^2/3\mu \right\rangle^{1/2}$$

is positively homogeneous of degree 1 with respect to E. It is therefore the support function of a convex set $P(\mu)$ which can be determined explicitly. In this connection, recall the following duality result:

Let A be a fourth order tensor with diagonal symmetry, then $F(E) = (1/2\ A{:}E{:}E)^{1/2}$ *is the support function of the convex set*

$$K = \left\{ \Sigma,\ \ \frac{1}{2} A^{-1}{:}\Sigma{:}\Sigma \leqslant \frac{1}{4} \right\} .$$

Denoting the dual potential of W^{hom} by W_*^{hom}, we obtain:

$$P(\mu) = \left\{ \Sigma \in \mathbb{R}_s^9 \ \textit{such that:}\ \ W_*^{hom}(\mu,\Sigma) \leqslant \left\langle \frac{k^2}{6\mu} \right\rangle \right\} \tag{2.9}$$

Taking the infimum over μ in (2.4) is equivalent to taking the intersection of the sets $P(\mu)$:

$$P^{hom} = \bigcap_{\mu(x) \geqslant 0} P(\mu) . \tag{2.10}$$

This last expression can be useful when the complementary energy W_*^{hom} is easier to compute than the strain energy W^{hom}. Any choice of μ gives an estimate from the outside of P^{hom}.

2.2 LAMINATES

Consider a laminate made up of layers arranged orthogonally to direction 3. By virtue of the translation invariance of the problem, the strain fields achieving the infimum in (1.5) will not depend on x_1 and x_2. It follows from (2.2) that there is no loss of generality in restricting the minimization to fields μ depending on x_3 only. For such fields the effective energy of the fictitious linear composite is

$$w^{hom}(E) = \frac{3}{2}\frac{1}{\langle 1/\mu \rangle} E_I^2 + \frac{3}{2}\langle \mu \rangle E_{II}^2, \; \textit{for} \;\; E \; \textit{with} \;\; Tr(E) = 0$$

where $$E_I^2 = \frac{4}{3}\left(E_{13}^2 + E_{23}^2\right), \quad E_{II}^2 = \left(E_{eq}^2 - E_I^2\right).$$

Consequently (with $\Sigma_I^2 = 3\left(\Sigma_{13}^2 + \Sigma_{23}^2\right)$, $\Sigma_{II}^2 = \Sigma_{eq}^2 - \Sigma_I^2$)

$$P(\mu) = \left\{ \Sigma \in \mathbb{R}_s^9 \; \textit{such that:} \; \left\langle \frac{1}{\mu} \right\rangle \Sigma_I^2 + \frac{\Sigma_{II}^2}{\langle \mu \rangle} \leqslant \left\langle \frac{k^2}{\mu} \right\rangle \right\} \tag{2.11}$$

To compute the intersection of the sets $P(\mu)$ we rewrite (2.11) as

$$\Sigma_{II}^2 \leqslant \langle \mu \rangle \left\langle \left(k^2 - \Sigma_I^2\right)/\mu \right\rangle .$$

The intersection results in:

$$P^{hom} = \left\{ \Sigma \; , \; \Sigma_I \leqslant \inf_{x \in V} k(x_3) \; , \; \Sigma_{II} \leqslant \left\langle \left(k^2 - \Sigma_I^2\right)^{1/2} \right\rangle \right\} . \tag{2.12}$$

Similar expressions have been previously derived by different means by DE BUHAN (1983), EL OMRI (1992), PONTE-CASTANEDA and DE BOTTON (1992).

2.3 ISOTROPIC TWO-PHASE COMPOSITE

We consider in this section a composite made up of two phases in proportions c_1 and c_2 with yield stresses k_1 and k_2 (for simplicity we assume $k_1 \geqslant k_2 > 0$). We also consider a family of fictitious linear composites occupying the same configuration as the real nonlinear composite but made up of two incompressible, isotropic elastic materials with shear moduli μ_1 and μ_2. It is further assumed that the given nonlinear composite is isotropic in the sense that all the fictitious linear composites described above are macroscopically isotropic. (2.6) is applied with $\mu(x) = \mu_1$ *in phase 1*, $\mu(x) = \mu_2$ *in phase 2*, and yields the upper bound:

$$\Pi^{hom}(E) \leqslant k^{hom} E_{eq}, \; k^{hom} = \inf_{\mu_1, \, \mu_2 \geqslant 0} \left(\mu^{hom} \left(\frac{c_1 \;\, k_1^2}{\mu_1} + \frac{c_2 \;\, k_2^2}{\mu_2} \right) \right)^{1/2}, \tag{2.13}$$

where μ^{hom} is the effective shear modulus of the fictitious linear composite. The linear composite, which is isotropic by assumption, is incompressible, except when one phase is a void, in which case a separate treatment has to be applied. (2.13) means that k^{hom} is an upper bound for the yield stress of the composite.

2.3.1. Hashin and Shtrikman upper bound: The bound of Hashin and Shtrikman can be used to bound the right-hand-side of (2.6)

$$\mu^{hom} \leqslant \mu_+^{HS} \text{ , where } \mu_+^{HS} = \mu_2\left(1 + \frac{c_1}{\dfrac{1}{\Upsilon-1} + \dfrac{2(1-c_1)}{3\Upsilon+2}}\right), \quad \Upsilon = \frac{\mu_1}{\mu_2}.$$

(this explicit expression is given for $\mu_1 \geqslant \mu_2$). It is possible to work out analytically the computation of the infimum in (2.13) and the final result for the effective yield stress is:

$$\frac{k^{hom}}{k_2} \leqslant 1 + c_1 \sqrt{\frac{3}{5-2c_1}}\left(\sqrt{\left(\frac{k_1}{k_2}\right)^2 - \frac{2(1-c_1)}{5-2c_1}} - \sqrt{\frac{3}{5-2c_1}}\right). \tag{2.14}$$

This result is identical to that given by PONTE-CASTANEDA and DE BOTTON (1992).

2.3.2. Hashin's spheres assemblage: The Hashin and Shtrikman bound, and consequently (2.14), are valid under the only assumptions that the phases are isotropic and arranged isotropically. In several cases of practical importance, one phase (phase 1) is dispersed in the other phase. A model morphology accounting for this additional information has been proposed by Hashin. It consists in the piling up of composite spheres and is referred to as the Hashin's assemblage of spheres. A bound, which is sharper than the general Hashin and Shtrikman bound, has been established for this model composite by HERVE, STOLZ and ZAOUI (1991), improving a previous result of HASHIN (1962) under the additional assumption that the assemblage of spheres is isotropic (this assumption was not used by HASHIN). Their result reads (when $\mu_1 \geqslant \mu_2$):

$$\mu^{hom} \leqslant \mu_+^{HSZ} = \mu_2(1 + c_1 F(c_1, \Upsilon, \Upsilon)) \text{ with } \Upsilon = \frac{\mu_1}{\mu_2}, \text{ and,} \tag{2.15}$$

$$F(c,\Upsilon,\Upsilon_0) = \left(\frac{2}{5}(1-c) + \frac{1}{\Upsilon-1} - \frac{c(1-c^{2/3})^2}{\dfrac{10}{21}\dfrac{19(1-\Upsilon)}{16+19\Upsilon}c^{7/3} + \dfrac{10}{21} + \dfrac{25}{24(\Upsilon_0-1)}}\right)^{-1}.$$

In this case, it is no longer possible to work out analytically the infimum in (2.13), but this can done numerically (cf section 4).

2.3.3 Three-phase estimate. Estimates (and not bounds) on the effective yield strength of the composite may also be obtained from (2.13) by inserting any expression of μ^{hom} relevant to the morphology of the composite under consideration. For instance, for the case of a dispersion of spherical particles of phase 1 in a connected matrix of phase 2, the generalized self-consistent scheme of CHRISTENSEN and LO can be used. The shear modulus $\mu_{3\varphi}^{hom}$ predicted by this three-phase model is obtained by solving the implicit equation (cf HERVE *et al* (1991)):

$$\frac{\mu_{3\varphi}^{hom}}{\mu_2} = 1 + c_1 F\left(c_1, \gamma, \frac{\mu_{3\varphi}^{hom}}{\mu_2}\right) . \tag{2.16}$$

With this, the optimization problem (2.13) is solved numerically to obtain a corresponding estimate for $k_{3\varphi}^{hom}$.

2.3.4 Rigid inclusions: When phase 1 is a rigid phase ($k_1 = +\infty$), the above predictions simplify to:

$$\Pi^{hom}(E) \leqslant \left(W^{hom}(E)\ k_2\ (1 - c_1)\right)^{1/2} , \tag{2.17}$$

where W^{hom} is the effective energy of a fictitious incompressible linear composite made up of a matrix with shear modulus $\mu_2 = 2k_2/3$ containing rigid inclusions in proportion c_1. The upper bound derived from the Hashin-Shtrikman theory is $+\infty$, while the upper bound for the Hashin's spheres assemblage is:

$$k^{hom} \leqslant k_2 \left\{(1-c_1)\left[1 + c_1 \left(\frac{2}{5}(1 - c_1) - \frac{c_1\left(1 - c_1^{2/3}\right)^2}{-\frac{10}{21} c_1^{7/3} + \frac{10}{21}}\right)^{-1}\right]\right\}^{1/2} . \tag{2.18}$$

On the other hand, the corresponding three-phase estimate is obtained from (2.17), where

$$W^{hom}(E) = \frac{3}{2}\mu_{3\varphi}^{hom} E_{eq}^2, \quad \frac{\mu_{3\varphi}^{hom}}{\mu_2} = 1 + c_1 F\left(c_1, +\infty, \frac{\mu_{3\varphi}^{hom}}{\mu_2}\right), \quad \mu_2 = \frac{2}{3} k_2 \tag{2.19}$$

2.4 ABOUT DRUCKER'S REMARK

A simple remark which goes back to DRUCKER (1959), throws light on the fact that, in general there is no reason for which the optimal field $\mu(x)$ in (2.4) should be constant on domains conforming to the geometric arrangement of the phases. The remark is that when it is possible to pass a plane of shear inside the weakest phase of the composite, the strength of the composite in the corresponding direction is equal to the strength of the weakest phase. It is instructive to derive this result from the above theory. Consider a volume element V subjected to a macroscopic shear Σ_{xy} containing a plane of shear (and therefore a small layer of width δ) passing through the weakest phase (phase 2). The layer is denoted by II and V-II is denoted by I (Figure 1). Set:

$$\mu(x) = \epsilon \quad if \quad x \in II, \ \mu(x) = 1/\epsilon \ if \quad x \in I, \quad E = \frac{1}{2}(e_x \otimes e_y + e_y \otimes e_x)$$

Then, by definition of Π^{hom}: $\Sigma_{xy} = \Sigma : E \leqslant \Pi^{hom}(E) \leqslant \left(W^{hom}(\mu, E) \left\langle \frac{2k^2}{3\mu} \right\rangle \right)^{1/2}$.

The effective energy of the fictitious linear composite is (cf §2.2):

$$W^{hom}(E) = \frac{1}{2} \frac{1}{\langle 1/\mu \rangle} = \frac{1}{2} \frac{\epsilon}{c_I \epsilon^2 + c_{II}},$$

and a straightforward computation leads to

$$\Pi^{hom}(E) \leqslant \left(\frac{1}{3} \frac{c_I \langle k^2 \rangle_I \epsilon^2 + c_{II} k_2^2}{c_I \epsilon^2 + c_{II}} \right)^{1/2}.$$

Letting now ϵ tend 0 in this last expression, we obtain $\Sigma_{xy} \leqslant k_2/\sqrt{3}$. $k_2/\sqrt{3}$ is the shear strength of phase 2 (weakest phase) and is also a trivial lower bound for the shear stress of the composite, which is therefore equal to $k_2/\sqrt{3}$. It is clear from this example that the optimal field μ in (2.4) does not conform to the geometry of the composite but to the strain distribution in the nonlinear composite (see (2.2)).

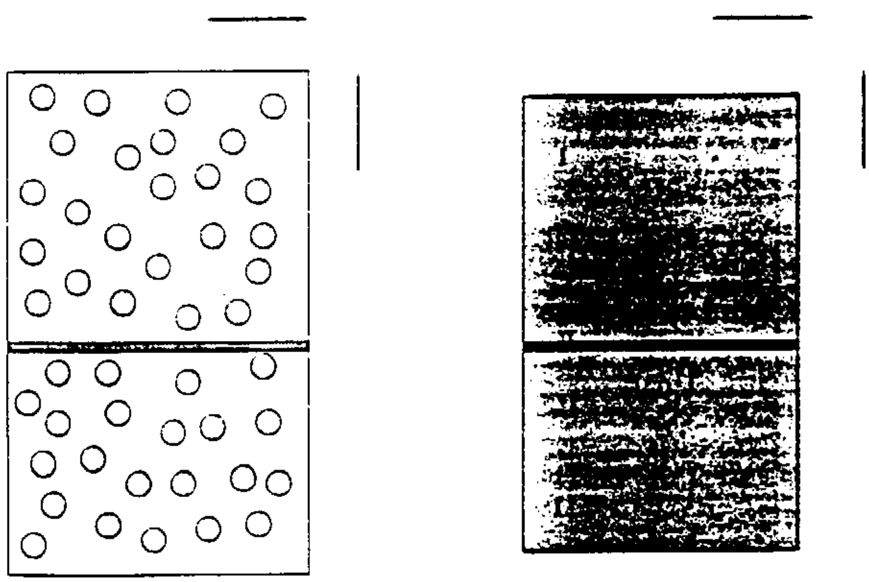

Figure 1: An illustration of DRUCKER's remark. a): real composite with a shear plane passing through the weakest phase. b): fictitious linear composite and distribution of the field μ.

3. Periodic composites : numerical determination of the strength domain

Recall that, in the case of a periodic micro-structure with unit cell V, P^{hom} or alternatively Π^{hom} are given by (1.4) and (1.5). The minimization problem (1.5) is non-smooth in the sense that the function to be minimized is not differentiable at the origin. Although this minimization problem could be attacked directly (MAGHOUS (1991)), we approach the problem differently.

3.1. ELASTIC PLASTIC ALGORITHM

In the point of view that we have adopted, the strength domain is computed via the resolution of a sequence of evolution problems for an elastic ideally plastic material, with yield stress k(x) and elastic compliance s(x) (stiffness c(x)). This evolution problem reads:

$$\left.\begin{array}{c} \forall\, x \in V,\ \epsilon(\dot{u}) = s{:}\dot{\sigma} + \dot{\epsilon}^{p}\ ,\ \dot{\epsilon}^{p}_{ij} = \dot{\lambda}\,\dfrac{3s_{ij}}{2\sigma_{eq}},\ \sigma_{eq} \leqslant k\ ,\ \dot{\lambda} \geqslant 0 \\ \mathrm{div}(\sigma) = 0,\ \sigma.n \textit{ anti-periodic} \\ \dot{u} = \dot{E}.x + \dot{u}^{*}\ ,\ \dot{u}^{*} \textit{ periodic} \end{array}\right\} . \qquad (3.1)$$

Given the macroscopic strain-rate $\dot{E}$, the variational formulation (in terms of stresses) of this problem is:

$$\left.\begin{array}{c} \textit{Find}\ \ \sigma(t) \in \mathcal{K},\ \textit{such that:} \\ \langle s\dot{\sigma}(t){:}(\hat{\sigma} - \sigma(t))\rangle \geqslant \dot{E}{:}(\hat{\Sigma} - \Sigma(t)) \quad \forall\, \hat{\sigma} \in \mathcal{K} \end{array}\right\} \qquad (3.2)$$

where $\mathcal{K} = \{\sigma,\ \mathrm{div}(\sigma) = 0,\ \sigma.n \textit{ anti-periodic},\ \sigma_{eq}(x) \leqslant k(x),\ x \text{ in } V\}$,

Σ and $\hat{\Sigma}$ are the volume averages of the fields σ and $\hat{\sigma}$. It is readily seen that when $\sigma(t)$ attains asymptotically a limit $\sigma(\infty)$ as t approaches ∞, the associated macroscopic stress $\Sigma(\infty)$ satisfies:

$$(\dot{E},\ \hat{\Sigma} - \Sigma(\infty)) \leqslant 0\ ,\ \forall\, \hat{\Sigma} \in P^{hom}.$$

Therefore, $\Sigma(\infty)$ is on the boundary of P^{hom} and $\dot{E}$ is an outer normal vector to P^{hom} at $\Sigma(\infty)$.

3.2. PRESCRIPTION OF OVERALL STRAINS OR STRESSES

Independently of the specific constitutive law of the constituents, the local problem to be solved so as to complete the homogenization procedure has two specific features.

The first one is the periodicity condition that should be satisfied by part of the displacement field. Sometimes, symmetry considerations can be invoked to reduce these periodicity conditions to usual boundary conditions. However, multiaxial overall stress states, such as combined tension and shear, do not satisfy the required symmetries and the periodicity conditions cannot be done away with. The linear relations between the degrees of freedom of the problem, as derived from the periodicity requirement, can be accounted through several methods such as replacement of unknown variables, penalty methods, Lagrange multipliers. The replacement method has been adopted hereafter.

The second feature is that the loading to be applied to the unit cell is not prescribed through boundary conditions, but through an average condition along prescribed paths in the space of overall strains or overall stresses. A method which permits to go along paths in both spaces is presented. For simplicity, the method is illustrated in the context of linear elasticity, but its generalization to incremental laws is straightforward.

3.2.1. Prescribed overall strain: Consider first the case where the overall strain E (or strain rate $\dot{E}$) is prescribed: $E = \bar{E}$. The decomposition

$$u = E.x + u^*, \ u^* \ \textit{periodic}, \tag{3.3}$$

suggests that the problem for u^*, the periodic part of u, be solved with E as a prescribed initial strain. The variational formulation of the (elastic) problem is:

$$\left.\begin{array}{c} \textit{Find } u^* \textit{ periodic such that, for every periodic } v^* \\ \langle c:\epsilon(u^*):\epsilon(v^*)\rangle = -\langle c:\bar{E}:\epsilon(v^*)\rangle \end{array}\right\} . \tag{3.4}$$

Upon discretization, the unknowns are denoted by the vector $\{u^*\}$ and the following matrices are introduced

$$\left.\begin{array}{l} [K] = \sum_e [k^e], \textit{ where } [k^e] = \frac{1}{|Y|}\int_e [B]^T[c]\,[B]\,dx \\ [\bar{K}] = \sum_e [\bar{k}^e], \textit{ where } [\bar{k}^e] = \frac{1}{|Y|}\int_e [B]^T[c]\,dx \end{array}\right\}. \tag{3.5}$$

The matrix [B] relates strains and displacements, i.e. $\{\epsilon^*\} = [B]\{u^*\}$. The linear system to be solved reads:

$$[K]\{u^*\} = -[\bar{K}]\{\bar{E}\} \quad . \tag{3.6}$$

3.2.2. Prescribed overall stresses: The above method needs to be modified when overall stresses, rather than overall strains, are prescribed. In this new problem, the overall strain E is an unknown while the average of the stress field is given. The unknowns of the problem are the periodic field u^* (or the discrete unknowns $\{u^*\}$) together with the 6 independent components of the overall strain E.

These new unknowns are incorporated into the discrete formulation of the problem and the 6 generalized forces associated with them are the components of the overall stress Σ. Let v be a displacement field in the form (3.3), associated with a macroscopic strain $\tilde{E}$ and a periodic displacement field v^*. The principle of virtual work, applied to the unit cell V, yields:

$$\langle \sigma : \epsilon(v) \rangle = \Sigma : \tilde{E} \quad i.e. \quad \{v^*, \tilde{E}\} \begin{Bmatrix} \sum_e \frac{1}{|V|} \int_e [B]^T \{\sigma\} \, dx \\ \sum_e \frac{1}{|V|} \int_e \{\sigma\} \, dx \end{Bmatrix} = \{v^*, \tilde{E}\} \begin{Bmatrix} 0 \\ \Sigma \end{Bmatrix} . \qquad (3.7)$$

for every periodic field $\{v^*\}$ and every constant strain $\tilde{E}$ in $\mathbb{R}^6$. After due account of the elastic law, we obtain:

$$\begin{Bmatrix} \sum_e \frac{1}{|V|} \int_e [B]^T \{\sigma\} \, dx \\ \sum_e \frac{1}{|V|} \int_e \{\sigma\} \, dx \end{Bmatrix} = \begin{bmatrix} K & \bar{K} \\ \bar{K} & \bar{\bar{K}} \end{bmatrix} \begin{Bmatrix} u^* \\ E \end{Bmatrix}, \quad i.e. \quad \begin{bmatrix} K & \bar{K} \\ \bar{K} & \bar{\bar{K}} \end{bmatrix} \begin{Bmatrix} u^* \\ E \end{Bmatrix} = \begin{Bmatrix} 0 \\ \Sigma \end{Bmatrix} \qquad (3.8)$$

where $[\bar{\bar{K}}]$ is defined as: $[\bar{\bar{K}}] = \langle [c] \rangle$. Equation (3.8) displays the true nature of the degrees of freedom $\{u\}$ on the unit cell. The periodic unknowns $\{u^*\}$ capture the local fluctuations of the actual displacement field, while the 6 global d.o.f. $\{E\}$ describe the average deformation of the unit cell. Formulation (3.8) is much more versatile than (3.6) in the sense that $\{E\}$, $\{\Sigma\}$, or a combination of the components of both quantities, can be prescribed as standard d.o.f. or forces. Prescribing averaged stresses or strains amounts to imposing forces or displacements, once the identification of the averaged strains with the 6 macroscopic degrees of freedom of the unit cell E and of the averaged stresses Σ with the 6 corresponding forces has been performed.

For practical purposes these additional degrees of freedom are accounted for through the introduction of an additional node (macroscopic node) that belongs to each mesh element. The array of unknowns at the element level (subscript e) and the classical matrix [B] are replaced by

$$\{u_e\} = \begin{Bmatrix} u_e^* \\ E \end{Bmatrix} , \qquad [\hat{B}] = [B, \mathbb{I}] , \quad \{\epsilon_e\} = [\hat{B}]\{u_e\} = [B]\{u_e^*\} + \{E\}$$

where $\mathbb{I}$ is the 6x6 identity matrix. The elementary stiffness matrix and the elementary force are respectively replaced by:

$$\left[\hat{k}_e\right] = \frac{1}{|V|}\int_e [\hat{B}]^T[c][\hat{B}]\,dx, \quad \left\{\hat{f}_e\right\} = \left\{\frac{1}{|V|}\int_e [\hat{B}]^T\{\sigma\}\,dx\right\}$$

At the global (assembled) level, the last 6 components of the generalized forces vector are precisely the 6 components of the average of the stresses over the unit cell.

3.3. INTEGRATION SCHEME FOR THE ELASTIC-PLASTIC PROBLEM

3.3.1 Equilibrium iterations. Newton scheme with control of the overall stresses. The direction of the overall stresses is often to be imposed (simple tension at the macroscopic level for instance). Constant loading steps can induce large displacements steps. So as to accurately compute the the limit load, load steps have to be carefully controlled in the vicinity of the asymptote. A possible strategy could be to control the deformation steps whenever the overall direction of strain rate is known in advance. This is not the case when the overall stress direction is prescribed. A mixed procedure is thus proposed; the direction of the overall stresses is prescribed, $\Sigma_t = \lambda_t\ \Sigma^0$,but the amplitude λ_t is an unknown of the problem which is evaluated requiring that: $\Sigma^0 : E_t = t$.
Let us assume that the state variables of the problem are known at time t, namely the array $\{u^*\}_t$ of the periodic local displacement, the array $\{E\}_t$ of the overall strains and the array $\{\sigma\}_t$ of the local stresses at each integration point. The principal unknowns at time $t+\Delta t$ are:

$$\{u^*\}_{t+\Delta t} = \{u^*\}_t + \{\Delta u^*\}\ , \quad \{E\}_{t+\Delta t} = \{E\}_t + \{\Delta E\}\ .$$

For a given Δt, the incremental scheme amounts to finding increments $\{\Delta u^*\}$ and $\{\Delta E\}$ such that the unbalanced forces vanish at time $t+\Delta t$:

$$\{v^*,\bar{E}\}.\left\{\hat{F}_{int}\right\}_{t+\Delta t} = 0,\ \forall\ v^*\ \textit{periodic},\ \forall\ \bar{E}\in\mathbb{R}^9_s\ \textit{with}\ \ \{\bar{E}\}.\{\Sigma^0\} = 0, \quad (3.9)$$

with:
$$\left\{\hat{F}_{int}\right\}_{t+\Delta t} = -\left\{\sum_e \frac{1}{|V|}\int_e [\hat{B}]^T\{\sigma\}_{t+\Delta t}\,dx\right\}$$

$\{\sigma\}_{t+\Delta t}$ depends on the initial conditions $\{\sigma\}_t$ and on the increments $\{\Delta u^*\}$ and $\{\Delta E\}$. (3.9) is a nonlinear equation. An iterative Newton scheme is proposed. At the ith iteration of the step $t+\Delta t$, the procedure goes as follows:

Assume that $\{\Delta u^*\}^{i-1}_{t+\Delta t}$, $\{\Delta E\}^{i-1}_{t+\Delta t}$ *are known, with* $\{\Sigma^0\}:\{\Delta E\}^{i-1}_{t+\Delta t} = \Delta t$

i) Compute $\{\sigma\}^{i-1}_{t+\Delta t}$ *at each integration point of each element (following the procedure described at point 3.3.2 below),*

ii) if the convergence criterion is not met, solve the linear system

$$[\hat{K}]^{i-1}_{t+\Delta t}\{\hat{\delta}\}^{i}_{t+\Delta t} = \left\{\hat{F}_{int}\right\}^{i-1}_{t+\Delta t}\ ,$$

$$\{\hat{\delta}\}^{i}_{t+\Delta t} = \begin{Bmatrix} \delta u^* \\ \delta E \end{Bmatrix}^{i}_{t+\Delta t}, \quad \{\delta u^*\}^{i}_{t+\Delta t} \; periodic \quad , \quad \{\Sigma^0\} : \{\delta E\}^{i}_{t+\Delta t} = 0 \qquad (3.10)$$

iii) Update $\{\Delta u^*\}^{i}_{t+\Delta t}$ *and* $\{\Delta E\}^{i}_{t+\Delta t}$ *for the next iteration by*

$$\{\Delta u^*\}^{i}_{t+\Delta t} = \{\Delta u^*\}^{i-1}_{t+\Delta t} + \{\delta u^*\}^{i}_{t+\Delta t}, \quad \{\Delta E\}^{i}_{t+\Delta t} = \{\Delta E\}^{i-1}_{t+\Delta t} + \{\delta E\}^{i}_{t+\Delta t}. \quad (3.11)$$

(3.10) involves linear constraints on the variables $\{\delta u^*\}^{i}_{t+\Delta t}$, $\{\delta E\}^{i}_{t+\Delta t}$. Classical transformations on $\{\delta E\}^{i}_{t+\Delta t}$ and modifications of $[\hat{K}]^{i-1}_{t+\Delta t}$ and $\left\{\hat{F}_{int}\right\}^{i-1}_{t+\Delta t}$ account for this constraint. Several choices of the stiffness matrix $[\hat{K}]^{i-1}_{t+\Delta t}$ are possible. All the examples presented in section 4 were solved with a constant stiffness strategy, the stiffness matrix being the initial stiffness formed once and for all at the beginning of the loading process and with the initial elastic moduli. This method turns out to be computationaly inexpensive and rapidly converging. The typical convergence rate is between 3 and 15 iterations, under the only condition that the increments $\{\Delta u^*\}^0$ and $\{\Delta E\}^0$ at the beginning of each step be initialised with the values of the increments at convergence of the previous step. The net forces are computed and the iteration procedure typically terminates when the ratio between the maximal unbalanced force and the maximal resisting force is less than 10^{-3}.

3.3.2. Local integration of the elasto-plastic behavior. The effective computation of $\{\sigma\}^{i}_{t+\Delta t}$, with given $\{\Delta u^*\}^i$ and $\{\Delta E\}^i$, is often referred to as the "local integration of the constitutive law". This integration is performed separately at each point of numerical integration in each element. An abundant literature exists on this subject and the following list does not attempt to be exhaustive SIMO and TAYLOR (1986), SLOAN (1987), DEBORDES and al (1987), HORNBERGER and STAMM (1989). Our choice is to consider the elasto-plastic constitutive law as a system of differential equations with respect to time. The system to be solved at each point of numerical integration reads:

$$\{\dot{\sigma}\}_{\tau} = [C_{ep}(\sigma_{\tau})] \left([B]\{\dot{u}^*\} + \{\dot{E}\}\right), \quad \tau \; in \quad [t, t+\Delta t], \qquad (3.12)$$

with initial data $\{\sigma\}_t$. $[C_{ep}]$ denotes the elasto-plastic tangent stiffness matrix. The rates $\{\dot{u}^*\}$ and $\{\dot{E}\}$ are defined as

$$\{\dot{u}^*\} = \frac{1}{\Delta t}\{\Delta u^*\}, \quad \{\dot{E}\} = \frac{1}{\Delta t}\{\Delta E\}.$$

A semi-implicit Euler scheme with variable steps is used to solve the system of differential equations (3.12). Inside a subinterval $[\tau_0, \tau_1]$ within $[t, t+\Delta t]$, a mid-point method is used:

$$\{\sigma\}_{-_1} = \{\sigma\}_{\tau_0} + (\tau_1 - \tau_0)\left[C_{ep}\left(\sigma_{\frac{\tau_1+\tau_0}{2}}\right)\right]\left([B]\{\dot{u}^*\} + \{\dot{E}\}\right), \qquad (3.13).$$

(3.13) is solved by a classical Newton-Raphson technique. The time step is chosen following HORNBERGER and STAMM (1989).

4. Examples

4.1 LAMINATES

The two-phase laminate is a test problem on which the validity of the algorithm can be checked. The laminate is submitted to a macroscopic, off-axis tensile test. θ is the angle of inclination of the direction of tension with respect to axis 1. The results of the finite element simulation agree with the analytical result deduced from (2.12) (Figure 2). There is no weakest link effect in tension. The tensile strengths in the direction of the layers and in the direction orthogonal to the layers are both equal to the average of the strengths (which is an upper bound of the macroscopic strength).

4.2 LONG FIBERS

Consider a two-phase composite made-up of elastic fibers (infinite strength) in a metal matrix composite (flow stress σ_0). The fibers are parallel to direction 3 and arranged at the nodes of a triangular lattice. The unit cell can be chosen to be hexagonal. The composite is deformed is submitted to an in plane transverse tension. θ is the angle between direction 1 and the tensile direction. For fiber volume fractions below $c_0 = \sqrt{3}\pi/8$ there exist directions for which a shear plane can be passed through the matrix. For such directions the tensile strength is $2\sigma_0/\sqrt{3}$, which is the tensile strength of the matrix under plane strains. For a significant transverse reinforcement, the volume fraction of the fibers has to be chosen above c_0.

For long fibers composites, computations should not be performed under plane strains conditions but under *generalized plane strains* conditions. A body is said to be in a state of generalized plane strains if:

$$u_\alpha = u_\alpha(x_1, x_2),\ \alpha = 1,2,\ u_3 = E_{33}x_3.$$

The 4 relevant components of the overall strain and stress are

$$\{E\} = \{E_{11},\ E_{22},\ 2E_{12},\ E_{33}\}^T, \qquad \{\Sigma\} = \{\Sigma_{11},\ \Sigma_{22},\ \Sigma_{12},\ \Sigma_{33}\}^T$$

and the unknowns fields under consideration are:

$$\{\epsilon^*\} = \left\{\epsilon^*_{11},\ \epsilon^*_{22},\ 2\epsilon^*_{12}\ ,\ 0\right\}^T, \qquad \{\sigma\} = \{\sigma_{11},\ \sigma_{22},\ \sigma_{12},\ \sigma_{33}\}\ .$$

The general methods exposed for 3-d computations in section 3.2 can be transposed to 2-d computations, after modifications of the matrix $[\hat{B}]$ which now reads as

$$[\hat{B}] = \begin{bmatrix} b_{11} & . & . & b_{1n} & 1 & 0 & 0 & 0 \\ b_{21} & . & . & b_{2n} & 0 & 1 & 0 & 0 \\ b_{31} & . & . & b_{3n} & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

where the b_{ij}'s are the components of the classical matrix $[B]$ in 2-dimensions and n is the number of local d.o.f. for each element. Once again it can be checked that:

$$\{\epsilon_e\} = \left\{\epsilon_e^*\right\} + \{E\} = [\hat{B}]\begin{Bmatrix} u_e^* \\ E \end{Bmatrix}.$$

Once these modifications are performed, the elementary stiffness matrices are assembled in a standard manner. The tangent matrix $[C_{ep}]$ has to be modified accordingly. The differential system (3.12) is now to be solved for the 4 unknowns σ_{11}, σ_{22}, σ_{12} and σ_{33}.

4.3 ISOTROPIC TWO-PHASE COMPOSITE

Consider a two-phase composite made-up of spherical particles (phase 1) dispersed in a matrix (phase 2). For comparison with finite element computations, a 3-d cell should be chosen. To avoid difficulties intrinsic to 3-d calculations, we have used an approximate axisymmetric model, similar to that of BAO, HUTCHINSON and Mc MEEKING (1991). This axial symmetry, imposed on the computed solutions, rules out the possibility of non-axisymmetric failure modes under axial tension. This is the reason for which no "DRUCKER's effect" is observed.

i) When the particles are purely elastic, they can be considered as rigid for the determination of the macroscopic flow stress. The finite elements results and the predictions of various bounds and estimates presented in section 2, are compared on Figure 4. The three-phase estimate gives the more reasonable agreement with f.e.m. calculations.

ii) At a given volume fraction of inclusions, when the ratio between the flow stress of the two phases is varied from 1 to infinity (Figure 5), the macroscopic flow stress varies from 1 to its value for rigid inclusions. This limit value is not reached asymptotically but is attained for a finite value of the ratio k_1/k_2 above which the stress in the particles never reaches the strength of the particle. Again, the prediction of the three-phase model reproduces the main trends observed in the f.e.m. calculations.

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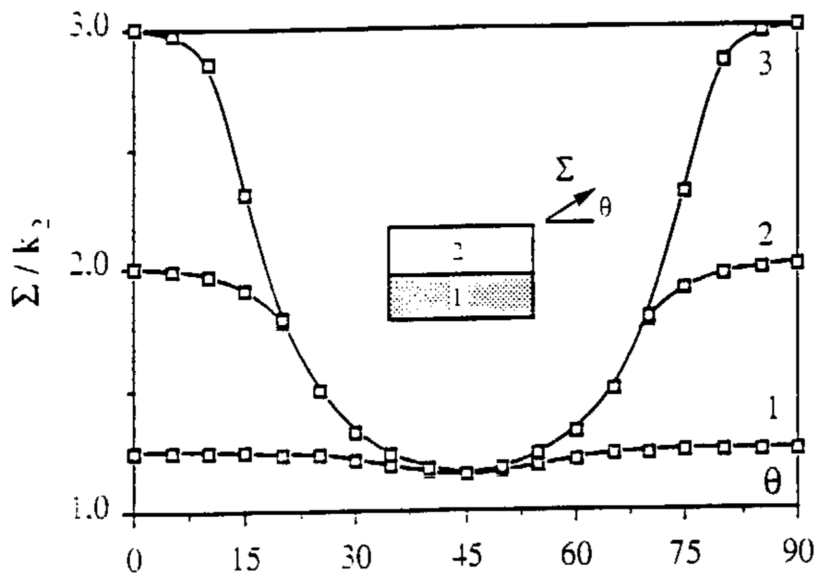

Figure 2: Two-phase laminate subjected to an off-axis tensile test. Yield stress Σ as a function of the orientation. Analytical result (solid line) and F.E.M. results (o). Different contrast ratios: (1) $k_1/k_2 = 1.5$, (2) $k_1/k_2 = 3.$, (3) $k_1/k_2 = 5.$ $c_1 = c_2 = 0.5$.

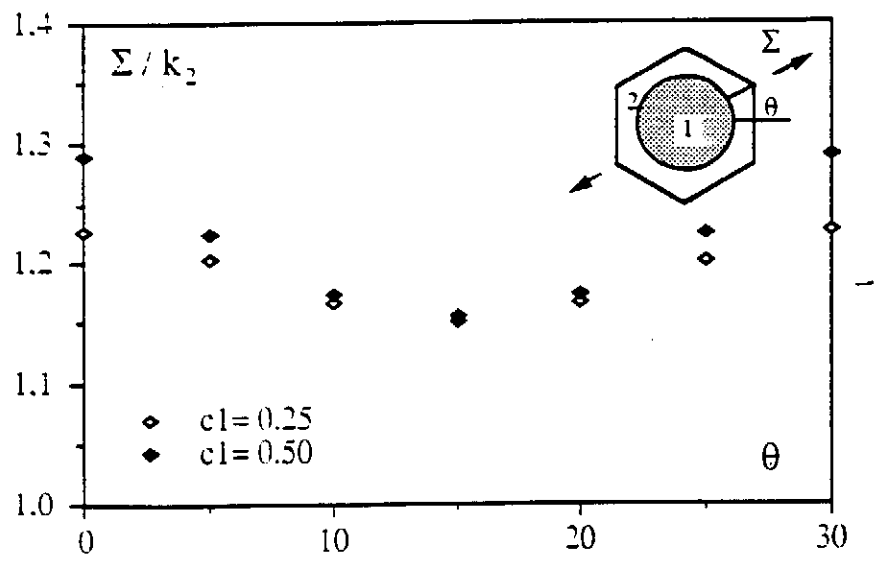

Figure 3: Two-phase composite reinforced by long fibers. Triangular lattice. Volume fractions $c_1 = 0.25$, $c_1 = 0.5$. Off-axis tensile test in the transverse plane.

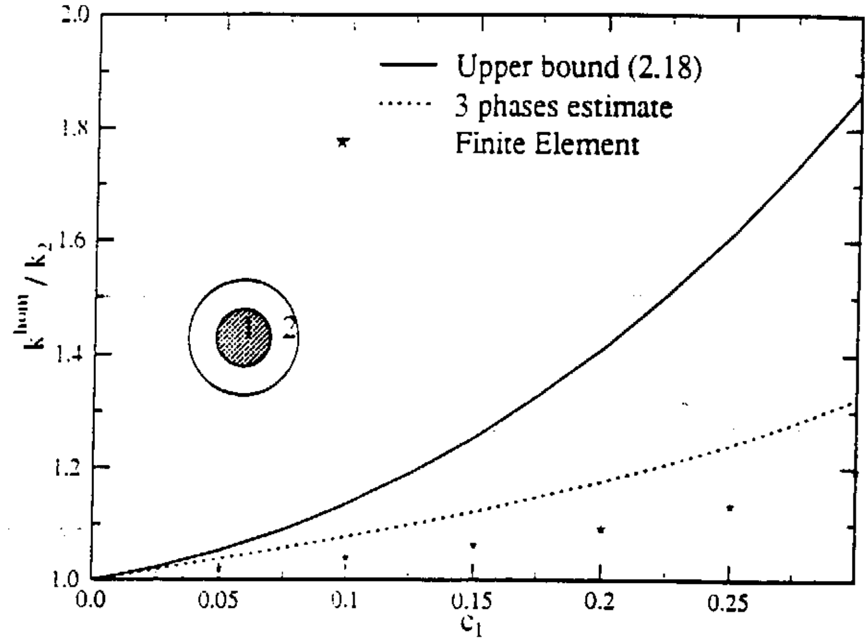

Figure 4: Macroscopic flow stress of a two-phase isotropic composite. Spherical rigid inclusions (phase 1) dispersed in a rigid plastic matrix (phase 2).

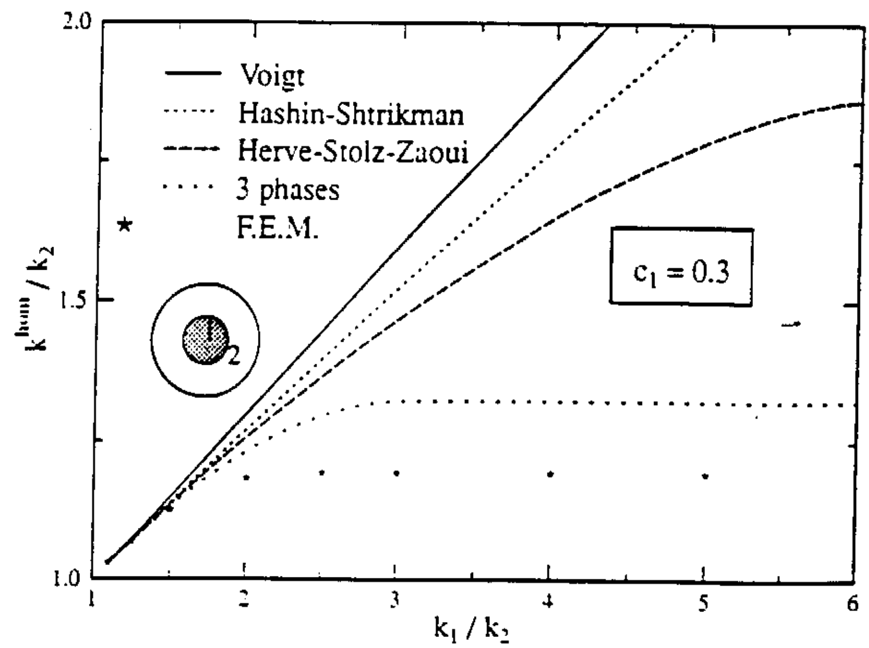

Figure 5: Macroscopic flow stress of a two-phase isotropic composite as function of the contrast ratio k_1/k_2.

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