MODELING THE SIZE EFFECT IN THE MECHANICAL BEHAVIOR OF NANOCOM-POSITES

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1. Introduction

With the development of smart materials [1] and the constant search for mass reduction, the use of nanocomposites is constantly growing. Indeed, for very low volume fraction of reinforcements and contrary to classical composites, nanocomposites offer remarkable properties, especially mechanical ones. These remarkable properties can be explained by a size effect induced by the nanometric dimension of the reinforcements. The local phenomena present at the matrix-inclusion interface, which are negligible in the case of classical composites, are no longer so in nano-reinforced materials where the ratio (matrix-inclusion interface surface) / (material volume) becomes much larger. However, taking into account the size effect in the modeling of the behavior of nanocomposites remains a great challenge at the present time. In the context of linear elasticity, many works, taking into account a size effect of nano-fillers, have been carried out by means of analytical approaches [2, 3, 4] using micromechanical models. Compared to classical micromechanical model like the Mori-Tanaka scheme or the Hashin-shtrikman bounds, a coherent interface is introduced on the matrix-inclusion interface and the equilibrium of this interface is taken into account. The behavior of this interface is generally governed by an elastic law as presented by Bottomley et al [5]:

$$\sigma_{\mathbf{s}} = \mathbb{C}^{\mathbf{s}} : \varepsilon_{\mathbf{s}} \tag{1}$$

where $\mathbb{C}^s$ is the surface stiffness tensor of the interface, $\sigma_{\mathbf{s}}$ is the surface tangent stress on the interface and ε_s is the surface strain tensor on the interface given by :

$$\varepsilon_s = \mathbf{P}.\varepsilon.\mathbf{P} \tag{2}$$

P is the second order projection operator on the interface :

$$\mathbf{P} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n} \tag{3}$$

In addition to the classical bulk equilibrium, these analytical approaches take account the equilibrium of the interface through the generalized Young-Laplace equation on the matrix-inclusion interface [6, 7, 8]:

$$\mathbf{div}_s\sigma_{\mathbf{s}} + [\![\sigma]\!] \cdot \mathbf{n} = \mathbf{0} \qquad \forall \mathbf{x} \in \Gamma \text{ ; } \Gamma \text{ being the matrix-inclusion interface.} \tag{4}$$

Because of analytical difficulties, micromechanical models accounting for the size effect of the nano-inclusions are limited to spherical or cylindrical inclusions. To overcome this limitations, numerical

strategies have been developed [9, 10, 11, 12]. In this communication, we will present the finite element models we propose in the context of both elastic and non-linear behaviors.
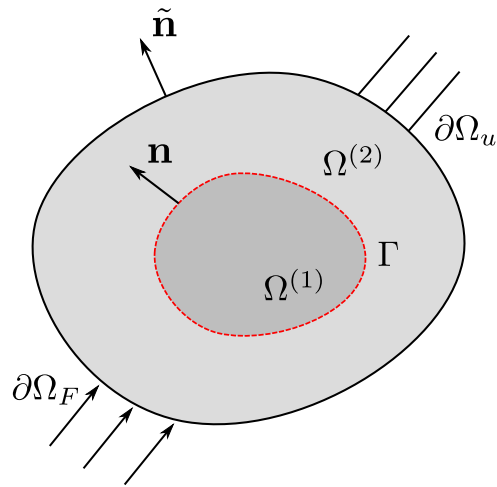
2. Problem definition

Figure 1: Two-phase material with imperfect matrix-inclusion interface.

Here we consider a bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) with boundary $\partial\Omega$ ($\partial\Omega = \partial\Omega_F \cup \partial\Omega_u$ and $\partial\Omega_F \cap \partial\Omega_u = \varnothing$). $\tilde{\mathbf{n}}$ is the outward unit normal to $\partial\Omega$. The domain Ω is made of of two phases $\Omega^{(1)}$ and $\Omega^{(2)}$ corresponding respectively to the inclusion and the matrix. These 2 domains are separated by an imperfect interface Γ (Fig.1). We note $\mathbf{n}$ the unit normal vector to Γ, chosen from $\Omega^{(1)}$ to $\Omega^{(2)}$.

As considered in analytical micromechanical model accounting for the size effect of nano-inclusions, the interface is assumed to be coherent, which means that the surface stresses are related to the jump of the traction vector across the interface.

The equilibrium of the 2 phases $\Omega^{(1)}$ and $\Omega^{(2)}$ is given by the equation:

$$\mathbf{div}\sigma^{(l)} + \mathbf{b} = \mathbf{0} \quad \text{in} \quad \Omega^{(l)}, \, l = 1, 2 \,, \tag{5}$$

where σ is the bulk Cauchy stress tensor and $\mathbf{b}$ is a volume force.

The Neumann and Dirichlet boundary conditions are applied on $\partial\Omega$:

$$\sigma \cdot \tilde{\mathbf{n}} = \boldsymbol{F} \quad \text{sur } \partial\Omega_F \quad \text{et} \quad \mathbf{u} = \bar{\mathbf{u}} \quad \text{sur } \partial\Omega_u \,, \tag{6}$$

The equilibrium of the coherent interface Γ is governed by the gereneralized Young-Laplace equation written in eq. (4).

3. Linear and non-linear behavior estimations

Using eq. (5) to eq. (4), assuming Γ closed and without any debonding between matrix and inclusions, the weak form of the problem presented in section 2. can be expressed:

$$\forall \delta\mathbf{u} \qquad \int_{\Omega\backslash\Gamma} \nabla^s\delta\mathbf{u} : \sigma d\Omega + \int_{\Gamma} \nabla^s_s\delta\mathbf{u}_{|\Gamma} : \sigma_{\mathbf{s}} d\Gamma - \int_{\Omega\backslash\Gamma} \delta\mathbf{u} \cdot \mathbf{b} d\Omega - \int_{\partial\Omega} \delta\mathbf{u} \cdot \sigma \cdot \tilde{\mathbf{n}} dS = \mathbf{0} \,. \tag{7}$$

where $\nabla^s_s\{\bullet\} = \nabla^s\{\bullet\}\mathbf{P}$,
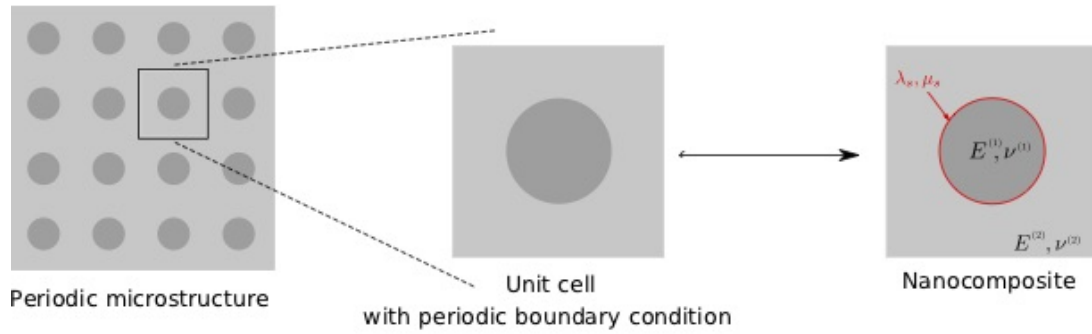$\nabla^s\{\bullet\}$ being the symmetric gradient operator.

Figure 2: Representative Volume Element (in plan $(\mathbf{e}_1, \mathbf{e}_2)$)

On a Representative Volume Element (RVE) (fig. 2) corresponding to the two-phase material problem presented in section 2., using finite element method in plane strain with interface elements, Xfem/level set method or embedded-FEM, the weak form given in eq. (7) will be solved by considering linear and non-linear behaviors in the bulk and elastic behavior on the matrix-inclusion interface. Different diameters of the cylindrical inclusions will be considered to study the impact of their size on both macroscopic and microscopic response of the material. These results and first developments considering several physics will be presented during the conference.

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