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# On the capability of micromechanics models to capture the auxetic behavior of fibers/particles reinforced composite materials

W. L. Azoti<sup>1,2</sup>, N. Bonfoh<sup>2</sup>, P. Lipinski<sup>2</sup>, Y. Koutsawa<sup>1</sup>, S. Belouettar<sup>1</sup>

<sup>1</sup> *Centre de Recherche Public Henri Tudor, 29 Avenue John F. Kennedy, L-1855 Luxembourg, Luxembourg*

<sup>2</sup> *Laboratoire de mécanique, Biomécanique, Polymère, Structures (LaBPS), ENIM, 1 route d'Ars Laquenexy, CS65820, 57078 Metz Cedex, France.*

## Abstract

This work investigates the possibility to predict the auxetic behavior of composites consisting of non-auxetic phases by means of micromechanical models based on Eshelby's inclusion concept. Two specific microstructures have been considered: (i) the three-layered hollow-cored fibers-reinforced composite and (ii) a microstructure imitating the re-entrant honeycomb micro-architecture. The micromechanical analysis is based on kinematic integral equations as a formal solution of the inhomogeneous material problem. The interaction tensors between the inhomogeneities are computed thanks to the Fourier's transform. The material anisotropy due to the morphological and topological textures of the inhomogeneities was taken into account thanks to the multi-site approximation of these tensors. In both cases, the numerical results show that auxetic behavior cannot be captured by such models at least in the case of elastic and isotropic phases. This conclusion is supported by corresponding finite element investigations of the second microstructure that indicate that auxetic behavior can be recovered by introducing joints between inclusions. Otherwise, favorable issues are only expected with auxetic components.

**Keywords:** Microstructure, Auxetic materials, Interaction tensor, Multi-site version, Mori-Tanaka scheme

## 1. Introduction

The Poisson's ratio (PR) is one of two constants that can be used to describe the elastic behavior of isotropic solids at small strain approximation [1]. In the case of stretching test, the PR is characterized by the negative ratio of the transverse strain to the axial one. The PR's effect is so fundamentally important to the material behavior that a change in its value leads to significant effects on material's mechanical performances. In the case of isotropic materials, the PR ( $\nu$ ) ranges in the interval of  $-1 \leq \nu \leq 1/2$ , due to thermodynamic restrictions [1]. For most materials this constant remains positive.

The term "Auxetic" refers to materials with negative Poisson's ratio (NPR). Contrary to conventional ones, auxetic materials get fatter when stretched, and thinner when compressed. In 1987, Lakes [2] first discovered the negative Poisson's ratio effect in polyurethane foam with re-entrant structures, which was named anti-rubber, auxetic, and dilatational by later researchers [3].

Moreover, Lakes [4] presented a review dealing with the related advance researches and the fabrication methods of the auxetic materials, which are present across the length scales. They are ranging from the nano scale to centimeter scale or macro scale [5], and can have natural occurrence or man-made origin (see Ref. [3] for more details). Auxetic materials are also known to exhibit various physical characteristics [6] better than those of their conventional counterparts. It's specially the case of material properties with  $(1-\nu^2)$  and  $(1+\nu)$  dependency. Indeed, the indentation resistance of an isotropic material is proportional to  $E/(1-\nu^2)$ , when an indenter with a uniform pressure is assumed. The indentation resistance rapidly increases when the PR tends towards  $-1$ . Similar tendency can be observed for the shear modulus of isotropic materials. The  $(1+\nu)^{-1}$  dependency of this property assumes an increase of the static elastic shear modulus when the PR tends towards  $-1$ . These enhanced characteristics make auxetic materials perform better in many practical applications. Although the use of auxetic materials is currently limited, some potential applications [7] of the auxetic behavior for the design of innovative materials and structural elements or for new processing techniques have been outlined in the engineering sciences. In biomechanics field, the example of auxetic polytetrafluoroethylene (PTFE) flexible sheath [8] used as arterial prosthesis can be cited. These kinds of materials also have good potentials in aerospace and automotive applications where non-auxetic composites having high strength and stiffness to weight ratios are permanently sought. Indeed, carbon-fiber-reinforced epoxy composite laminate panels with in-plane and through thickness negative Poisson's ratios [8] made by Evans's group have been cited with a value of Young modulus of 60GPa and an enhanced fracture toughness and indentation resistance. Some auxetic composites are used in sensor and actuator applications. It is the case of piezoelectric composites that consist of piezoelectric ceramic rods [8] within an auxetic polymer matrix and which are used in medical ultrasonic imagers and hydrophone receivers of naval sonar (see Ref. [2, 3, 7, 8] and [9] for more applications).

It is seen that auxetic behavior is related to a highly specific microstructure or nanostructure that gives rise to this behavior [2, 10]. Indeed, most of these materials have a microstructure that induces the NPR at a macro scale [11]. In this fact, the analysis of the auxetic behavior leads to get down in the small length scale of the composite from the microstructure point of view. At the level of the structure length scale, the auxetic behavior has been studied by several investigators through a various networks as potential microstructure. In this context, much interest [12] is centered on the non convex re-entrant honeycomb microstructure which seems to be the right geometry exhibiting a NPR. Several analytical and FE models [10, 13, 14] and experimental measurements [11, 15, 16] had showed that this non convex-shaped (re-entrant) microstructure is the most understandable origin of the auxetic behavior [7]. Recently, Lira et al. [17] proposed, for a re-entrant honeycomb sandwich panel, a theoretical approach based on Voigt and Reuss bounds through theorems of minimum potential and complementary strain energies and have noticed in-plane auxetic deformations with this cellular structure. Other works (Stavroulakis [7], Gaspar et al. [10]) emphasis that, for engineering applications, auxetic effect and its dependence

on the microstructure can be studied by homogenization tools. Using auxetic inclusions, Wei et al. [16] have shown the existence of auxetic windows for composites via the mean field theory [16, 18, 19] and the two-three bodies' interaction formalism [16]. For composites reinforced with thinly-coated hollow-cored fibers, and with osteon-like fibers (modeling cortical bone tissue), Stagni [20] has found, using eigenstrain concept, subjected to uniform arbitrary remote loading and some complex potentials functions, that the effective transverse Poisson's ratio becomes negative beyond certain porosity levels, and the parity of the number of fiber layers is a significant parameter.

The main purpose of this study can be formulated in following questions: Is it possible to design auxetic composite material from non-auxetic phases? What could be the response of the micromechanical model based on kinematic integral equation on the description of the auxetic behavior? What about the impact of taking into account interactions between the re-entrant microstructure reinforcements in this description? To answer these questions, micromechanical formulations will be used in this study. Firstly, Mori-Tanaka analytical development related to a biphasic composite with spherical inclusion is studied in order to predict a theoretical domain for auxetic composite. Next, two kinds of microstructures are explored, namely the multi-coated inhomogeneity [21, 22] and the re-entrant network of reinforcements. The approaches developed here are based on the kinematic integral equation as formal solution of the inhomogeneous material problem [23]. In the multi-coated microstructure, the inhomogeneity is coated with a shell of the matrix material and the resulting material is embedded in an infinite body having the unknown properties of the homogeneous equivalent medium. This model also called the Generalized Self-Consistent scheme (GSC) has been studied by Christensen and Lo [24], Hervé and Zaoui [25], Cherkaoui et al. [26]. The obtained results are discussed with those provided by Stagni [20] to analyze the impact of kinematic integral equation without internal strains (eigenstrains) on the auxetic behavior. In the last part of this work, the re-entrant microstructure is modeled through the Eshelby's inclusion concept [27] embedded in an infinite matrix. Following Fassi-Fehri et al. [28], the interaction tensor between inhomogeneities is introduced in order to better describe this special microstructure. This allows the construction of a multi-site approximation of the integral equation. Here, the material anisotropy is taken into account on the one hand by the morphological texture that describes the shape and the orientation of the inhomogeneities and on the other hand by the topological texture that describes their relative positions. The multi-site version of Mori-Tanaka scheme [23] is developed to predict the effective material properties.

Finite Element calculations on a RVE representing the re-entrant microstructure are also performed to validate micromechanical results.

In the following, section 2 reminds micromechanical constitutive equations while section 3 deals with the micromechanical models used for the exploring design of auxetics. In this section, are discussed the numerical results from micromechanics and finite element methods. Section 4 ends this work by the conclusion.

## 2. Kinematic Integral equation

Micromechanics describes the relationship between the continuum properties of a material and its microstructure. The transition from the micro scale to the macro scale is performed by considering a Representative Volume Element RVE like suggested by Hill [29], Kroner [30, 31] and Willis [32]. Then, the associated boundary-value problems are formulated, in terms of uniform macro field traction vector or linear displacement fields. The RVE is assumed to be in equilibrium and its overall strain compatible. Also the body forces and inertia term are absents. These general considerations are restricted to the case of a linear elastic constitutive law and the small transformation approximation [23]. For a macro homogeneous and micro heterogeneous material, through the RVE, the scale transition consists firstly, in the localization of the global strain tensor by the introduction of a fourth order strain concentration tensor  $A(\mathbf{r})$  [29] and secondly, in the homogenization process, which uses averaging techniques to approximate the macroscopic behavior. Also, it is supposed that all the constituents of the RVE are perfectly bounded together. Under these conditions one can express the effective properties of the RVE:

$$C_{ijkl}^{eff} = \frac{1}{V} \int_V c_{ijmn}(\mathbf{r}) A_{mnkl}(\mathbf{r}) dV \quad (1)$$

where  $\mathbf{c}(\mathbf{r})$  and  $V$  represent respectively, the local elastic constants tensor, and the volume of the RVE. The strain concentration tensor  $A(\mathbf{r})$  that is the unknown parameter of heterogeneous inclusion problem depends on the considered microstructure. At this level, a homogeneous reference medium of elastic constants tensor  $\mathbf{c}^R$  is introduced such as:

$$\mathbf{c}_{ijkl}(\mathbf{r}) = \mathbf{c}_{ijkl}^R + \delta\mathbf{c}_{ijkl}(\mathbf{r}) \quad (2)$$

The tensor  $\delta\mathbf{c}$  represents the fluctuation part of the local elastic properties. Substituting Eq. (2) into local equilibrium condition  $\sigma_{ij,j}(\mathbf{r}) = 0$  leads to a kind of the Navier's equation:

$$\mathbf{c}_{ijkl}^R \mathbf{u}_{k,lj} + (\delta\mathbf{c}_{ijkl}(\mathbf{r}) \mathbf{u}_{k,l})_{,j} = 0 \quad (3)$$

The solution of Eq. (3) has been proposed by Dederichs and Zeller in terms of the so-called integral equation (See Refs. [32, 33, 34]). The displacement and strain fields of the heterogeneous medium therefore rise:

$$\begin{cases} \mathbf{u}_m(\mathbf{r}) = U_m^r(\mathbf{r}) + \int_V G_{mi}(\mathbf{r}-\mathbf{r}') (\delta\mathbf{c}_{ijkl}(\mathbf{r}') \varepsilon_{kl}(\mathbf{r}'))_{,j} dV' \\ \varepsilon_{mn}(\mathbf{r}) = E_{mn}^r - \int_V \Gamma_{mnij}(\mathbf{r}-\mathbf{r}') \delta\mathbf{c}_{ijkl}(\mathbf{r}') \varepsilon_{kl}(\mathbf{r}') dV' \end{cases} \quad (4)$$

$\mathbf{G}$  represents the Green's tensor,  $\mathbf{E}^r$  and  $\mathbf{U}^r$  are respectively the reference strain and displacement field and  $\mathbf{\Gamma}$  the modified Green tensor expressed by:

$$\Gamma_{mnij}(\mathbf{r}-\mathbf{r}') = -\frac{1}{2} \{G_{mi,nj}(\mathbf{r}-\mathbf{r}') + G_{ni,mj}(\mathbf{r}-\mathbf{r}')\} \quad (5)$$

Based on the kinematic integral equation (4) and Eshelby's inclusion concept [27] for ellipsoidal inclusions, an expression of the strain concentration tensor  $\mathbf{A}(\mathbf{r})$  has been proposed by Vieville et al. [23] through an iterative procedure. The global strain concentration tensor yields as:

$$\begin{cases} \mathbf{A}(\mathbf{r}) = \mathbf{a}(\mathbf{r}) : \langle \mathbf{a}(\mathbf{r}) \rangle^{-1} \\ \langle \mathbf{A}(\mathbf{r}) \rangle = \mathbf{I} \end{cases} \quad (6)$$

where  $\mathbf{I}$  is the fourth identity tensor and  $\mathbf{a}(\mathbf{r})$  a strain concentration tensor with respect to the reference medium, such that:

$$\begin{aligned} \boldsymbol{\varepsilon}(\mathbf{r}) &= \mathbf{a}(\mathbf{r}) : \mathbf{E}^r \\ \mathbf{a}(\mathbf{r}) &= \sum_{I=0}^N \mathbf{a}^I \theta^I(\mathbf{r}) \end{aligned} \quad (7)$$

with  $\theta^I(\mathbf{r}) = \begin{cases} 1 & \text{if } \mathbf{r} \in V_I \\ 0 & \text{if } \mathbf{r} \notin V_I \end{cases}$  and  $V_I$  representing the volume of  $I^{\text{th}}$  inclusion.

The final iterative expression of the strain concentration tensor  $\mathbf{a}^I$  yields [23]:

$$\begin{cases} (\mathbf{a}^I)_0 = \mathbf{I} \\ (\mathbf{a}^I)_{i+1} = [\mathbf{I} + \mathbf{T}^{II}(\mathbf{c}^R) : \Delta \mathbf{c}^I]^{-1} : \left[ \mathbf{I} - \sum_{\substack{J=0 \\ J \neq I}}^N \mathbf{T}^{IJ}(\mathbf{c}^R) : \Delta \mathbf{c}^J : (\mathbf{a}^J)_i \right] \\ I = 0, 1, 2, \dots, N \end{cases} \quad (8)$$

where  $\mathbf{T}^{IJ} = \frac{1}{V_I} \int_{V_I} \int_{V_J} \mathbf{\Gamma}(\mathbf{r}-\mathbf{r}') dV dV'$  represents the interaction tensor in its multi-site version and  $N$  the number of constituents. (For more details on the calculation of the global strain concentration tensor, see Ref [23, 35, 36]). Knowing the strain concentration tensors of all constituents, the effective properties of the heterogeneous material can be calculated in function of constituent volume fraction  $f_I$  using the discrete version of Eq (1):

$$\mathbf{C}^{eff} = \sum_{I=0}^N f_I \mathbf{c}^I \mathbf{A}^I \quad (9)$$

### 3. Micromechanics models and results

This section investigates the suitable microstructure that could lead to the auxetic behavior at the macroscopic level. For this purpose, firstly an analytical development for a spherical biphasic isotropic composite is considered. In this case, the analytical solution for the interaction tensor is known. Through this microstructure, the validity domain of auxetic behavior is examined under the one-site Mori-Tanaka scheme.

#### 3.1. Analytical Mori-Tanaka modeling of isotropic biphasic materials

The considered microstructure consists of spherical inclusion embedded in infinite medium. In this isotropic elastic case, the analytical expression of the interaction tensor takes the form:

$$\mathbf{T}^I(\mathbf{c}^R) = \left( \frac{1}{3\kappa_R + 4\mu_R} \right) \mathbf{J} + \left( \frac{3(\kappa_R + 2\mu_R)}{5\mu_R(3\kappa_R + 4\mu_R)} \right) \mathbf{K} \quad (10)$$

where  $\kappa_R$  and  $\mu_R$  are respectively the bulk and shear moduli of the reference medium and  $\mathbf{J}$  and  $\mathbf{K}$  are the well known idempotent tensors defined by the following expressions  $J_{ijkl} = \frac{1}{3}(\delta_{ij}\delta_{kl})$ ,  $K_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl})$ . The elastic constant tensors of the isotropic phases are expressed in terms of idempotent tensors such as:

$$\begin{cases} \mathbf{c}^I = 3\kappa_I \mathbf{J} + 2\mu_I \mathbf{K} \\ \mathbf{c}^0 = 3\kappa_0 \mathbf{J} + 2\mu_0 \mathbf{K} \\ \Delta \mathbf{c}^I = 3(\kappa_I - \kappa_0) \mathbf{J} + 2(\mu_I - \mu_0) \mathbf{K} \end{cases} \quad (11)$$

where  $\kappa_I$  and  $\mu_I$  represent respectively the bulk and shear moduli of the inclusion  $I$ , and  $\kappa_0$  and  $\mu_0$  the bulk and shear moduli of the matrix. Following Mori-Tanaka formulation [23], the reference medium of elastic constant tensor is assumed to be the matrix phase of elastic constant tensor  $\mathbf{c}^R = \mathbf{c}^0$ . Substituting Eqs. (10), (11) in Eq. (8) and recasting the resulting expression in Eq. (1), one can demonstrate that the effective properties of the equivalent material can be expressed in terms of effective bulk and shear modulus as:

$$\kappa^{MT} = \kappa_0 + \frac{f(\kappa_1 - \kappa_0)(3\kappa_0 + 4\mu_0)}{3\kappa_0 + 4\mu_0 + 3(1-f)(\kappa_1 - \kappa_0)} \quad (12)$$

$$\mu^{MT} = \mu_0 + \frac{5f\mu_0(\mu_1 - \mu_0)(3\kappa_0 + 4\mu_0)}{5\mu_0(3\kappa_0 + 4\mu_0) + 6(1-f)(\mu_1 - \mu_0)(\kappa_0 + 2\mu_0)} \quad (13)$$

where  $f$  is the volume fraction of inclusion. For convenience of the analysis presented below, let's express these results in function of  $\gamma = \frac{\mu_1}{\mu_0}$  and  $\nu_0$  and  $\nu_1$ , respectively the matrix and inclusion

Poisson's ratios:

$$\bar{\kappa}^{MT} = \frac{\kappa^{MT}}{\kappa_0} = 1 + \frac{f}{(1+\nu_0)} \frac{3[\gamma(1+\nu_1)(1-2\nu_0) - (1+\nu_0)(1-2\nu_1)](1-\nu_0)}{3(1-2\nu_1)(1-\nu_0) + (1-f)[\gamma(1+\nu_1)(1-2\nu_0) - (1+\nu_0)(1-2\nu_1)]} \quad (14)$$

$$\bar{\mu}^{MT} = \frac{\mu^{MT}}{\mu_0} = 1 + f \frac{45(\gamma-1)(1-\nu_0)(1-2\nu_0)}{45(1-2\nu_0)(1-\nu_0) + 8(1-f)(\gamma-1)(4-5\nu_0)} \quad (15)$$

One can observe that the global Mori-Tanaka shear modulus does not depend on the inclusion Poisson's ratio  $\nu_0$ .

The effective Poisson's ratio can be deduced from these results using the relation:

$$\nu^{MT} = \frac{3\kappa^{MT} - 2\mu^{MT}}{2(3\kappa^{MT} + \mu^{MT})} \quad (16)$$

Assuming positive values for the effective bulk and shear moduli, the NPR can therefore be achieved if and only if  $3\kappa^{MT} - 2\mu^{MT} < 0$ . The line of effective Poisson's ratio  $\nu^{MT} = 0$  separates the domain of  $\nu_0$  and  $\nu_1$  variation into two sub-domains of negative and positive PR. This line is defined by the equation:

$$3\bar{\kappa} = 2\bar{\mu} \frac{\mu_0}{\kappa_0} = 3\bar{\mu} \frac{1-2\nu_0}{1+\nu_0} \quad (17)$$

Using expressions (14) and (15) the above equation becomes:

$$\frac{[\gamma(1+\nu_1)(1-2\nu_0) - (1+\nu_0)(1-2\nu_1)]}{3(1-2\nu_1)(1-\nu_0) + (1-f)[\gamma(1+\nu_1)(1-2\nu_0) - (1+\nu_0)(1-2\nu_1)]} = \frac{15(\gamma-1)(1-2\nu_0)(1-2\nu_0)}{8(1-f)(\gamma-1)(4-5\nu_0) + 45(1-2\nu_0)(1-\nu_0)} - \frac{\nu_0}{f(1-\nu_0)} \quad (18)$$

and can be solved with respect to  $\nu^1$  leading to:

$$\nu_1 = \frac{N(\nu_0, f, \gamma)}{D(\nu_0, f, \gamma)} \quad (19)$$

where

$$\begin{aligned} N(\nu_0, f, \gamma) &= (1-f) \left\{ f(5\nu_0-3)(\gamma-1)(1+\nu_0-\gamma+2\gamma\nu_0) - \nu_0(\gamma+2) [5\nu_0(1+2\gamma)-7-8\gamma] \right\} \\ D(\nu_0, f, \gamma) &= f^2(5\nu_0-3) [2\nu_0(\gamma-1)-\gamma-2] (\gamma-1) + \nu_0(\gamma-4) [5\nu_0(1+2\gamma)-7-8\gamma] + \\ &\quad f \left\{ 10(\nu_0)^2(1+\gamma-2\gamma^2) - 3[\gamma(\gamma+16)-2] + \nu_0[\gamma(19\gamma+58)-32] \right\} \end{aligned}$$

It appears from this solution that, whatever the values of the volume fraction  $0 \leq f \leq 1$  and quotient  $\gamma \geq 0$ , to obtain the auxetic effective material with non auxetic matrix ( $\nu_0 \geq 0$ ) the inclusion Poisson's ratio should be negative. Indeed, for the matrix Poisson's ratio  $\nu_0 = 0$  the expression of  $\nu_1$  becomes:

$$\nu_1|_{\nu_0=0} = \frac{3f(f-1)(1-\gamma)(\gamma-1)}{3f^2(\gamma+2)(\gamma-1) - 3f[\gamma(16+\gamma)-2]} \leq 0 \quad (20)$$

The similar conclusion can be written in the case for which the inclusion Poisson's ratio tends to zero. The corresponding expression of  $\nu_0$  takes the form:

$$\begin{aligned} \nu_0|_{\nu_1=0} &= \frac{f(1-\gamma)(2-11\gamma) - \gamma(23+8\gamma) - 14}{10[f(\gamma-1) - \gamma - 2](1+2\gamma)} + \\ &\quad \frac{\sqrt{f^2(1-\gamma)^2(8+\gamma)^2 + (2+\gamma)^2(7+8\gamma)^2 + 2f(1-\gamma)(2+\gamma)[16+7\gamma(13+4\gamma)]}}{10[f(\gamma-1) - \gamma - 2](1+2\gamma)} \leq 0 \end{aligned} \quad (21)$$

This last inequality indicates that the NPR is achieved for non-negative inclusion Poisson's ratio if and only if the matrix Poisson's ratio becomes negative. The above conclusions are illustrated by Figures 1 and 2 depicting respectively the evolution of the auxeticity domain in function of volume fraction  $f$  and quotient  $\gamma$ .

Results of this preliminary analytical approach suggest that it seems impossible to model, through a simple inclusion one-site (OS) micromechanical formulation, an auxetic behavior of composite materials consisting of non auxetic phases. To definitely tackle this problem, more complex micromechanical approaches are used in the following sections. First, the microstructure studied by Stagni [20] is analyzed. To this end, the model of multi-coated inhomogeneity is used to identify its impact on the description of auxetic behavior. For this microstructure, a comparison is made with results provided by Stagni [20].

### 3.2. Ellipsoidal multi-coated inhomogeneity model

The topology of the multi-coated inhomogeneity problem (see Fig. 3) consists of an ellipsoidal phase occupying a volume  $V_1$ , the behavior of which is described by the elastic moduli tensor  $\mathbf{c}^1$ . Surrounding this inhomogeneity are  $N-1$  layers of coatings of other materials with elastic properties defined by moduli tensor  $\mathbf{c}^i$ . The corresponding volumes of these coatings are denoted  $V_i$ ,  $i \in \{2, 3, \dots, N\}$ . This multi-coated inhomogeneity is then embedded in the reference medium defined by its elastic moduli tensor  $\mathbf{c}^R$ . The main objective is to determine the equivalent properties of this kind of micro-heterogeneous materials. Initial works carried out by Christensen and Lo [24], Hervé and Zaoui [25, 37] were more dealing with the spherical or cylindrical and isotropic inhomogeneities. Many attempts have been undertaken to generalize these solutions to the case of ellipsoidal and anisotropic inhomogeneities. The present developments are based on results of Lipinski et al [22] concerning the elastic multi coated ellipsoidal inhomogeneities. Note that the generalized self consistent scheme can be derived from such a modeling considering the coating  $N$  as a shell of the matrix material and embedding the resulting composite inclusion into the effective medium with unknown properties, Bardhadi et al [38].

Let's define the composite inclusion as the inhomogeneity with its surrounding layers  $i$ ,  $i \in \{2, 3, \dots, N\}$ . Also are introduced the following concentration tensors:

- $A^I$  is the tensor of strain localization in the composite inclusion  $I$  with respect to macroscopic strain  $\mathbf{E}$ :  $\boldsymbol{\varepsilon}^I = \mathbf{A}^I : \mathbf{E}$ ;
- $A^j$  ( $j=1, 2, \dots, N$ ) represents the tensor of strain localization in the layer  $j$  with respect to macroscopic strain  $\mathbf{E}$ :  $\boldsymbol{\varepsilon}^j = \mathbf{A}^j : \mathbf{E}$ ;
- $\mathbf{a}^j$  represents the tensor of strain localization in the layer  $j$  with respect to the composite inclusion strain  $\boldsymbol{\varepsilon}^I$ :  $\boldsymbol{\varepsilon}^j = \mathbf{a}^j : \boldsymbol{\varepsilon}^I$ .

Based on the kinematic integral equation Eq.(4), the strain concentration tensor  $A^I$  can be expressed as [22]:

$$\mathbf{A}^I = \left[ \mathbf{I} + \mathbf{T}^H(\mathbf{c}^R) : \left( \sum_{j=1}^N f_j \Delta \mathbf{c}^j : \mathbf{a}^j \right) \right] \quad (22)$$

where  $f_j$  represents the volume fraction of the phase  $j$  with respect to the composite inclusion volume  $V_j$ :

$$f_j = \frac{V_j}{V_j} \quad (23)$$

Obviously  $V_J = \bigcup_{j=1}^N V_j$  where  $V_j$  is the volume of the phase  $j$ .

The three above concentration tensors are related each other's: [22]

$$\begin{cases} \mathbf{A}^j = \mathbf{a}^j : \mathbf{A}^I \\ \mathbf{A}^I = \langle \mathbf{A}^j \rangle = \sum_{j=1}^N f_j \mathbf{A}^j \\ \langle \mathbf{a}^j \rangle = \sum_{j=1}^N f_j \mathbf{a}^j = \mathbf{I} \end{cases} \quad (24)$$

where the strain concentration tensor  $\mathbf{a}^j$  is given by the relation:

$$\mathbf{a}^j = \mathbf{\Pi}^j : \mathbf{a}^1 \quad (25)$$

$\mathbf{\Pi}^k$  is defined by the following recurrence relation [22, 35]

$$\begin{cases} \mathbf{\Pi}^1 = \mathbf{I} ; \quad \mathbf{\Pi}^2 = \mathfrak{G}^{(1/2)} \\ \mathbf{\Pi}^j = \left( \sum_{m=1}^{j-1} f_m \right)^{-1} \sum_{m=1}^{j-1} (f_m \mathfrak{G}^{(m/j)} : \mathbf{\Pi}^m) \end{cases} \quad (26)$$

In Eq. (26),  $\mathfrak{G}^{(m/j)}$  is the strain concentration tensor between two layers  $m$  and  $j$ . It is defined by: (see Refs. [22, 33, 35] for more details in the calculation)

$$\mathfrak{G}^{(m/j)} = \mathbf{I} + \left( \mathbf{T}^{\Omega_{j-1}}(\mathbf{c}^j) - \frac{1}{f_j} \sum_{n=1}^{j-1} f_n \left[ \mathbf{T}^{\Omega_j}(\mathbf{c}^j) - \mathbf{T}^{\Omega_{j-1}}(\mathbf{c}^j) \right] \right) : \Delta \mathbf{c}^{(m/j)} \quad (27)$$

where  $\mathbf{T}^{\Omega_j}(\mathbf{c}^j)$  represents the interaction tensor in its one-site (OS) version and  $\Omega_j$  is defined as

$\Omega_j = \bigcup_{i=1}^j V_i$ . In general case of ellipsoidal inclusion embedded in anisotropic medium, this tensor

is calculated numerically using the method based on the Fourier transform  $\overline{\mathbf{G}}$  of the Green's tensor for the problem of the ellipsoidal inhomogeneity provided in [28]. Furthermore, the third equation of Eq (24) leads finally to:

$$\mathbf{a}^1 = \left( \sum_{j=1}^N \varphi_j \mathbf{\Pi}^j \right)^{-1} \quad (28)$$

So, the localization step is completed once the tensor  $\mathbf{a}^1$  is determined. Then, the effective properties can be computed through the Generalized Self-Consistent scheme (GSC) in which the reference medium  $\mathbf{c}^R$  is assumed to be the effective unknown medium  $\mathbf{c}^R = \mathbf{c}^{GSC}$ .

As it is assumed in [20], let's now consider 3-hollow-cored coated fibers reinforced composite material defined by the relative coating thickness  $k = (\rho_3 - \rho_2) / \rho_2$ , the volume fraction,  $f_I = \rho_3^2 / \rho_4^2$ , of coated fiber, the shear modulus ratios  $\gamma_m = \mu_2 / \mu_4$ ,  $\gamma_c = \mu_2 / \mu_3$  and the Poisson's ratios of each phase.  $\rho_i$  is radius ratio of phase  $i$  such as  $\rho_i = r_i / r_0$ . Here, the subscript 1 denotes the void as core, while subscripts 2, 3 and 4 indicate respectively the fiber, the coating and finally the matrix.

To compare our results with those provided by Stagni, the data used by this author are selected i.e.  $k = 0.025$ ,  $f_I = 0.7$ ,  $\nu_2 = \nu_4 = 0.3$ ,  $\nu_3 = 0.4$ . The model proposed by Stagni [20] was carried out by introducing eigenstrains in a hollow cored fiber coated material and subjected to uniform arbitrary remote loading in which the elastic fields in the phases are expressed through Kolosov's complex potentials functions defined in [39]. The analysis provided by Stagni [20] is based on the GSC scheme and the solutions are established for plane-elasticity problem of multilayered hollow-cored circular inclusion. Fig. 4 illustrates the evolution of effective Poisson's ratios as a function of the material porosity. As depicted in this figure, auxetic behavior has been reached by Stagni beyond certain porosity levels with the selected values of shear modulus ratios  $\gamma_m = 0.5$ ,  $\gamma_c = 0.1$ , and  $\gamma_c = 10$ .

The present model is based on the kinematic integral equation as the formal solution of the inhomogeneity problem with Eshelby's inclusion concept [27]. The analysis developed here is carried out for three-dimensional composite material. To reproduce the plane-elasticity configuration of the problem, multilayered circular cylinder inclusions are considered. For computation, the geometrical dimensions  $(a_1, a_2, a_3)$  of the inclusions are specified like:

$$\begin{cases} a_1 = a_2 \\ \frac{a_3}{a_1} = 1000 \end{cases} \quad (29)$$

Results provided by the present model show a slight decrease of the effective Poisson's ratio versus material porosity as it can be observed in Fig. 4. but this Poisson's ratio remains positive for all porosity domain studied by Stagni.

Consequently, it seems impossible to connect the auxetic behavior obtained in [20] neither to the assumed  $\mathbf{a}^j$  eigenstrains nor to homogenization scheme. Our results are definitely in disagreement with those provided by Stagni [20].

Some investigations [7, 10, 13, 14, 17] suggested the possibility to obtain the auxetic behavior through a re-entrant microstructure. To model such a re-entrant microstructure, the multi-site (MS) approach has been developed in order to take into account the interactions between inhomogeneities in the description of the global composite behavior.

### 3.3. The re-entrant inhomogeneities model

#### 3.3.1. Micromechanical approach of the re-entrant pattern

Some specific re-entrant pattern, illustrated in Figure 5-a, is considered in this work. This pattern is defined by two parameters, namely  $L$  describing reinforcements' length and  $e$  the gap between two adjacent horizontal elements. One can note that changing the value of  $e$  three typical microstructures can be generated:

- for  $e = 2L$  the usual honeycomb architecture is obtained,
- taking  $e = L$  the rectangular grid can be created,
- for  $e = 0$  the equilateral cell is produced.

The choice of  $0 < e < L$  leads to the re-entrant pattern.

Let's introduce the ratio  $r = \frac{e}{L}$  which according to the above remarks defines the pattern type.

Let also  $T$  be the thickness of the considered cell. By simple geometric considerations the volume of the unit cell indicated by the rectangle in Figure 5-a is given by the following expression:

$$V_{cell} = \frac{\sqrt{3L^2 + 2eL - e^2}}{2} (L + e)T = \frac{TL^2}{2} (1 + r) \sqrt{3 + 2r - r^2} \quad (30)$$

The micromechanical modeling of this unit cell using ellipsoidal inclusions is shown in Figure 5-b. The elastic properties of inclusions are specified by the tensor  $\mathbf{c}^I$  and those of the matrix material by  $\mathbf{c}^0$ . The cell thickness is correlated to the third ellipsoid semi-axis by the relation  $T = 2c$ . In order to evolve the reinforcement volume fraction two additional geometric parameters are introduced linking the reinforcement length  $L$  with remaining ellipsoid semi axes.

$$\begin{cases} a = \alpha L \\ b = \beta L \end{cases} \quad (31)$$

Consequently, the volume of the three inclusions in the unit cell is given by:

$$V_T = 4\pi abc = 2\pi\alpha\beta L^2 T \quad (32)$$

and the total volume fraction of these inclusions can be expressed as:

$$f_T = 3f_I = \frac{V_T}{V_{cell}} = \frac{4\pi\alpha\beta}{(1+r)\sqrt{3+2r-r^2}} \quad (33)$$

where  $f_I$  is the volume fraction of an individual inclusion. For this analysis, the parameter  $\alpha$  remains constant while the parameter  $\beta$  varies with the volume fraction  $f_T$ . This means that parameter  $\beta$  is connected with the resize of the inclusion's dimension  $b$  when the volume fraction  $f_T$  changes.

In order to take into account the interaction of reinforcements each others in this microstructure, the multi-site (MS) version of the Mori-Tanaka scheme is used to compute the effective properties. So, the strain concentration tensor  $\mathbf{A}^I$  is computed for inclusion  $I$  by the taken into account the influence of its ten (10) neighbors (see Fig. 6).

Also, in this scheme, the strain concentration tensor in Eq. (8) remains implicit. For more numerical stability, the first approximation  $(\mathbf{a}^I)_0$  of the concentration tensor  $\mathbf{a}^I$  is considered to be that of the one-site version. It means that:

$$(\mathbf{a}^I)_0 = [\mathbf{I} + \mathbf{T}^{II}(\mathbf{c}^0) : \Delta \mathbf{c}^I]^{-1} \quad (34)$$

Therefore, an iterative algorithm, presented in Appendix, is used to compute the approximate properties [23]:

$$\mathbf{C}^{MT} = \left( f_0 \mathbf{c}^0 + \sum_{I=1}^N f_I \mathbf{c}^I \mathbf{a}^I \right) : \mathbf{A}^0 \quad (35)$$

In Eq.(35),  $\mathbf{A}^0$  is the strain concentration tensor of the matrix with respect to the prescribed macroscopic strain  $\mathbf{E}$  :

$$\mathbf{A}^0 = \left( f_0 \mathbf{I} + \sum_{I=1}^N f_I \mathbf{a}^I \right)^{-1} \quad (36)$$

- Influence of the thickness  $T$

The influence of the thickness is studied by the variation of the parameter  $T$  for two values. The first deals with a value of  $T = 0.1$  that can represent a plane-stress configuration (see Fig. 7-a) while the second represents a plane-strain configuration with  $T = 10$  (see Fig. 7-b). Fig. 8 depicts

the evolution of the approximate Poisson's ratio  $\nu$  versus the inclusions volume fraction  $f_T$  with respect to the thickness  $T$  and for  $r = 0.1$ . The predictions of the multi-site (MS) model are compared with those provided by a one-site (OS) version approximation for material properties presented in the table 1. The parameter  $T$  has a significant impact on the approximate Poisson's ratio. Indeed, the Poisson's ratio value  $\nu_{12}^{MS}$  increases with  $f_T$  while the values  $\nu_{13}^{MS}$ ,  $\nu_{23}^{MS}$ , which are closed, decrease asymptotically to the reinforcement Poisson's ratio but remains positive.

Also, it can be observed that, the multi-site version solutions are closed to those obtained by the one-site approximation for plane-strain configuration (Fig. 8-b). However, all these Poisson's ratios remain positive. So, the auxeticity isn't reached by the model of re-entrant microstructure that takes into account the interactions between the inclusions each other's by the thickness  $T$  variation.

- Influence of the parameter  $r$

The influence of the parameter  $r$  is studied for  $0 < e < L$  that characterizes the re-entrant pattern and for  $T = 10$ . The material properties are presented in table 1. Fig. 9-a depicts the evolution of the multi-site approximate Poisson's ratio  $\nu_{12}^{MS}$  for different value of the parameter  $r$  that have a significant impact on them. Indeed, it can be observed that the approximate  $\nu_{12}^{MS}$  increases in general with the inclusions volume fraction  $f_T$ . For value of the parameter  $r$  such as  $r \geq 0.3$ , a low local decrease is noticed for the volume fraction  $f_T \leq 0.01$ . Also, it is seen that the approximate  $\nu_{23}^{MS}$  decreases with increasing  $r$ , which is related with the gap of the unit cell.

Concerning the evolution of the approximate  $\nu_{23}^{MS}$ , it is seen that the parameter  $r$  hasn't significant impact on it variation. In fact, for the different values of  $r$ , solutions remains very closed and seem to take an asymptotic value corresponding to the inhomogeneity Poisson's ratio. All these Poisson's ratios remain positive. So, the auxeticity isn't reached by the model of re-entrant microstructure that takes into account the interactions between the inclusions each other's and by the parameter  $r$  variation.

Results of the above simulations tend to show that the design space of an auxetic material using non-auxetic local phases and the micromechanics formulations remains difficult. To verify this point, a Finite Element approach of this microstructure is provided in the next subsection to confront the micromechanical response.

### 3.3.2. Finite element approach of the re-entrant microstructure

The Finite Element approach of the re-entrant microstructure is performed to validate the predictions of the previous micromechanical model. It consists of a RVE as a cube in which are embedded the ellipsoidal inhomogeneities (Fig. 10-a). Due to the symmetry of the problem, only a quarter of the RVE is considered for analysis. As regards to the inhomogeneities volume

fraction defined in Eq.(33), the semi-axis of the ellipsoidal inhomogeneities are related to the volume fraction by:

$$\begin{cases} a = \alpha L \\ b = \beta L \text{ where } \beta = \frac{f_T}{4\pi\alpha}(1+r)\sqrt{3+2r-r^2} \\ c = \frac{T}{2} \end{cases} \quad (37)$$

Also, on the remaining faces of the RVE, are applied two periodic boundaries conditions. The model was later meshed using the HyperMesh 10 software package (Altair, Troy, Michigan, USA). All calculations are performed by the MSC/MARC 2005 software package (MSC Software, Santa Ana, California, USA). The model is composed of 35 808 elements of classes PENTA(6) (Fig. 10-b). All these elements have an aspect ratio less than 3.52, and the maximum skew angle is 37.63. The RVE is subjected to an axial displacement in X (1) direction. The average values of engineering strains are determined and then, the Poisson's ratio  $\nu_{ij}$  is computed according to the expression:

$$\nu_{ij} = -\frac{\varepsilon_{jj}}{\varepsilon_{ii}} \quad (38)$$

In Eq.(38), there is no summation on repeated indices. Obtained results depicted in Fig 11, show that the RVE is deformed like conventional material. It gets thinner during a stretching test. Fig. 12 shows the evolution of Poisson's ratio versus the volume fraction of the inhomogeneity. Finite elements calculations are compared to the predictions of the previous micromechanical model.

This numerical simulation confirms the previous conclusion: even for this specific microstructure, the macroscopic RVE is definitely non-auxetic material.

However, it is well known that real re-entrant microstructure leads to the auxetic behavior. Consequently, we have also explored the case of the mechanism of re-entrant microstructure creating joints (pivots) between inclusions. Through plane-strain numerical simulations, an auxetic behavior is noticed in the expected Poisson's ratio direction as shown in Fig. 13. The RVE gets fatter when stretched. This observation is illustrated in Fig.14 in which it is noticed a decrease of the Poisson's ratio  $\nu_{12}$  with increasing ratio of inclusion and matrix Young's moduli  $\frac{E_i}{E_m}$ . According to the selected model parameters, a negative value of the Poisson's ratio is observed for  $\nu_{12}$ .

The auxetic behavior is only achieved when the inhomogeneities are tied. Unfortunately, the micromechanical approaches, up to know, are not able to take into account these tied inclusions.

#### **4. Conclusion**

In this work, mainly, three kinds of microstructures are investigated to explore the design space of auxetic materials through a micromechanical multi-scale analysis.

First, analytical micromechanical developments for isotropic spherical elastic inclusion embedded in an infinite elastic medium are provided. The main objective here was to analyze the existence of a potential auxetic domain for composite material within the usual thermodynamical restrictions for elastic materials. The results clearly showed that auxetic behavior can arise at macroscopic level only if at least one of the local phases is auxetic. Then, the multi coated inhomogeneity model suggested among others by Stagni was analyzed. It appeared that such a microstructure could no more predict the auxetic behavior in the case of non-auxetic constituents. Finally, the re-entrant microstructure has been reproduced by the cluster of ellipsoidal inclusions. The multi-site version of interaction tensors has been computed in order to take into account its specific topological and morphological textures. As in both previous cases, the overall Poisson's ratios of resulting composite remained positive for non-auxetic matrix and reinforcements.

Results of finite element simulations confirmed the conclusions of micromechanical modeling predictions. Moreover, it has been shown, via the FE analysis, that it is possible to obtain auxetic macroscopic behavior of the considered re-entrant structure introducing joints between inclusions reproducing omega-shaped reinforcements.

Fatefully, micromechanical models taking into account such mechanisms are not available yet.

#### **Acknowledgements**

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#### **Appendix**

Mori-Tanaka scheme programming algorithm (Fig. A.1)

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## Figure Captions

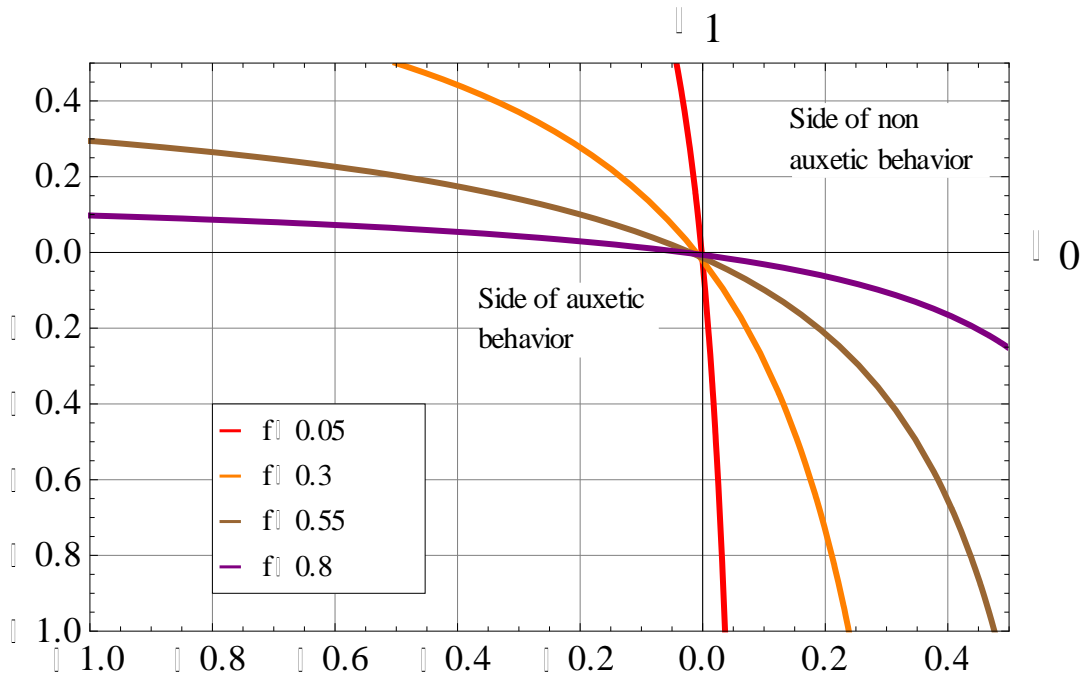


Figure 1. Auxeticity borderline evolution versus inclusion volume fraction  $f$  for  $\gamma = 2$

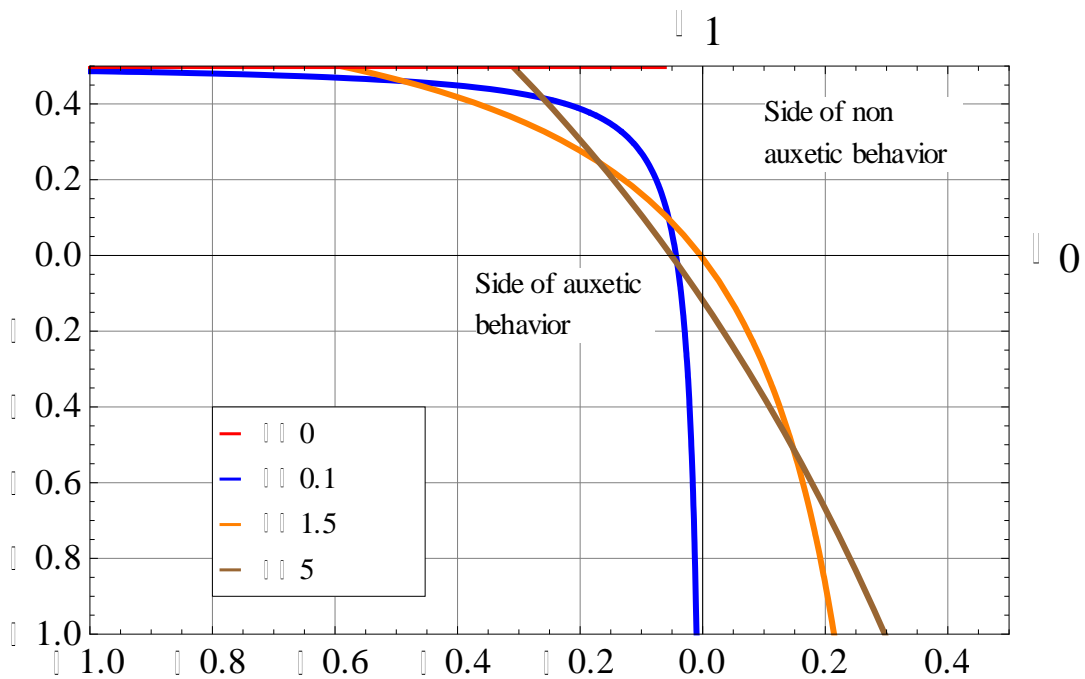


Figure 2. Auxeticity borderline evolution versus quotient  $\gamma$  for  $f = 0.3$

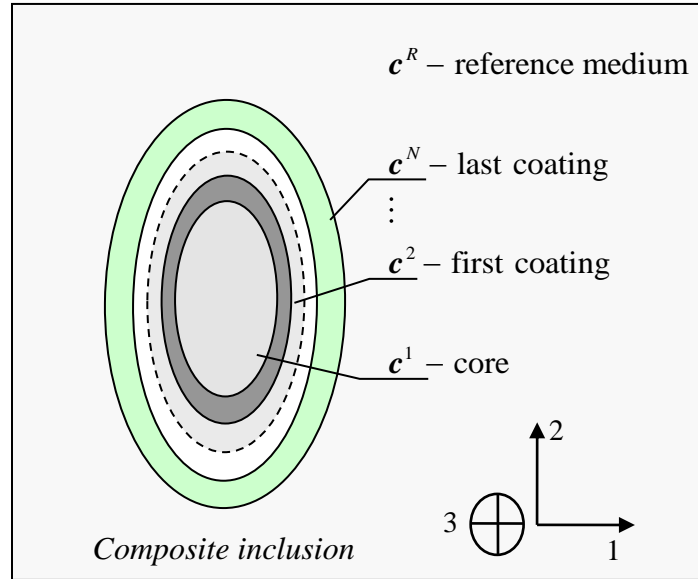


Figure 3. Topology of the multi-coated inhomogeneity model

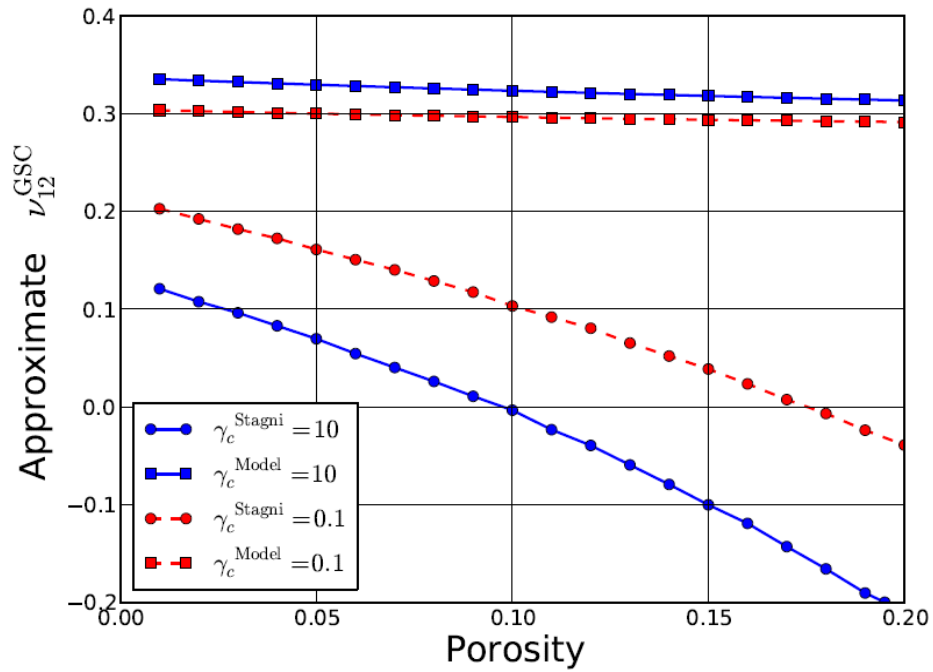


Figure 4. Effective Poisson's ratio versus porosity for  $\gamma_m = 0.5$ ,  $\gamma_c = 0.1$  and  $\gamma_c = 10$

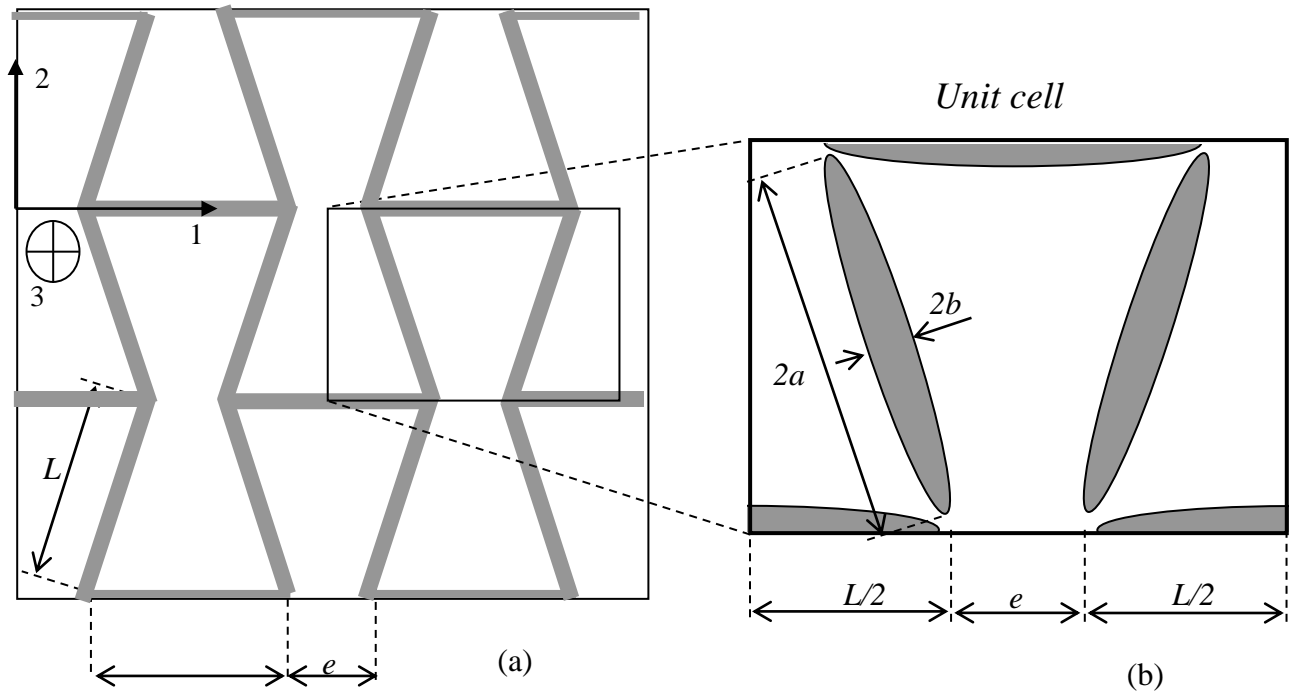


Figure 5. Topology of the re-entrant microstructure

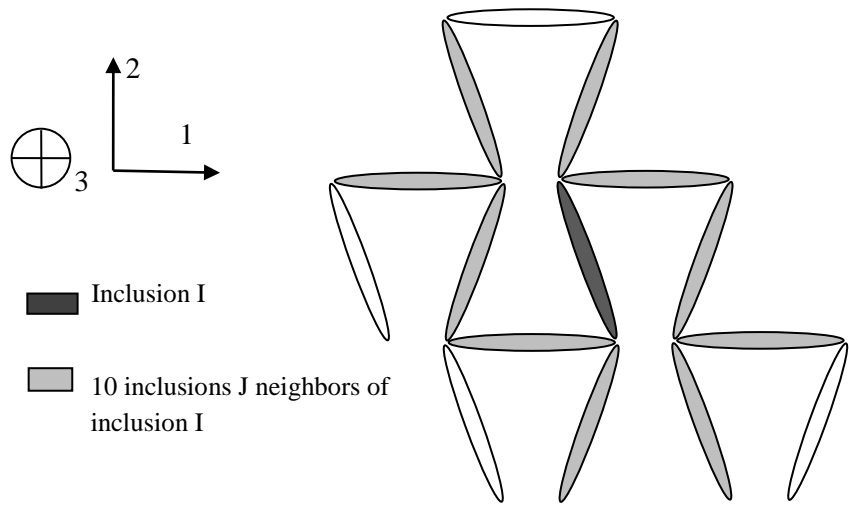
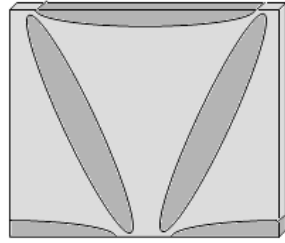
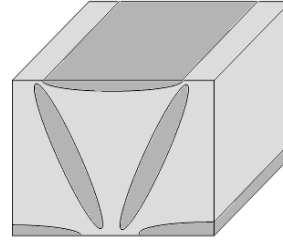


Figure 6. Description of interaction between inclusion I and its neighbors J

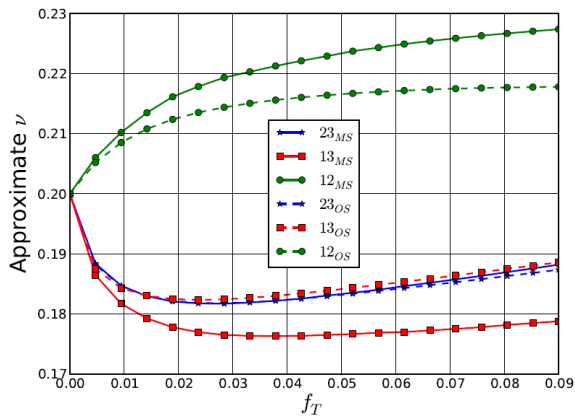


a.  $T = 0.1$

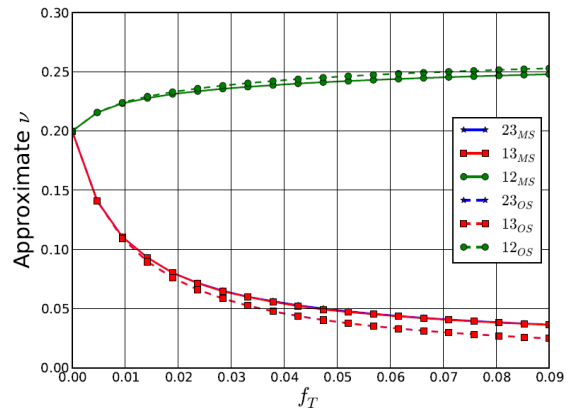


b.  $T = 10$

Figure 7. (a) Plane-stress configuration, (b) Plane-strain configuration.

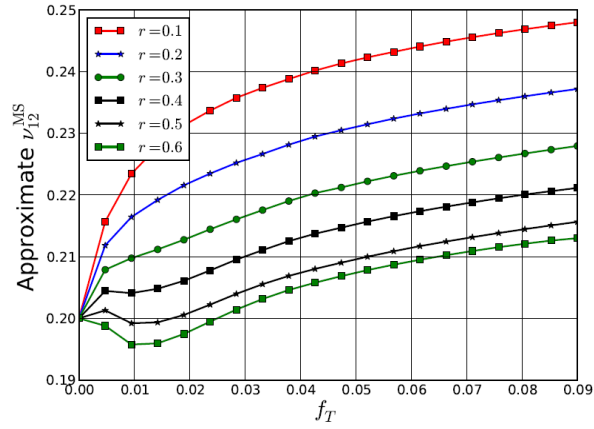


a.  $T = 0.1$

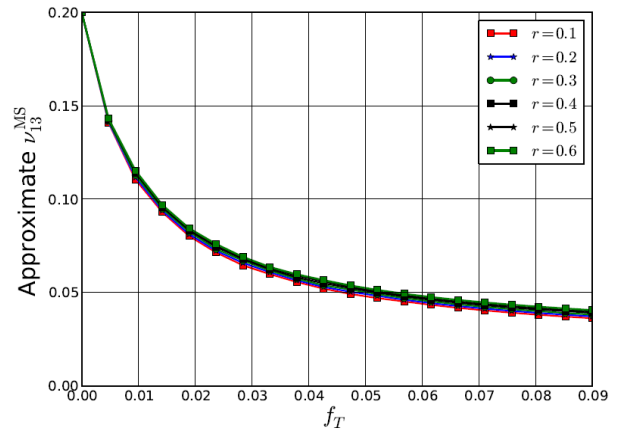


b.  $T = 10$

Figure 8. Approximate Poisson's ratio  $\nu$  versus  $f_T$  for different values of  $T$  and  $\alpha = 0.4$

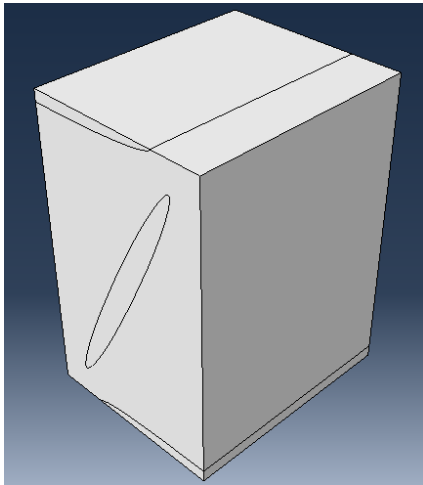


a.

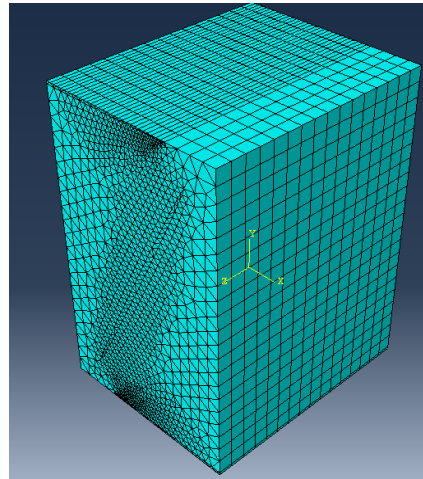


b.

Figure 9. Approximate Poisson's ratio versus  $f_T$  for different values of  $r$ ,  $\alpha = 0.4$ ,  $T = 10$



a. Numerical model



b. Meshed model

Figure 10: Finite Element model of the re-entrant microstructure

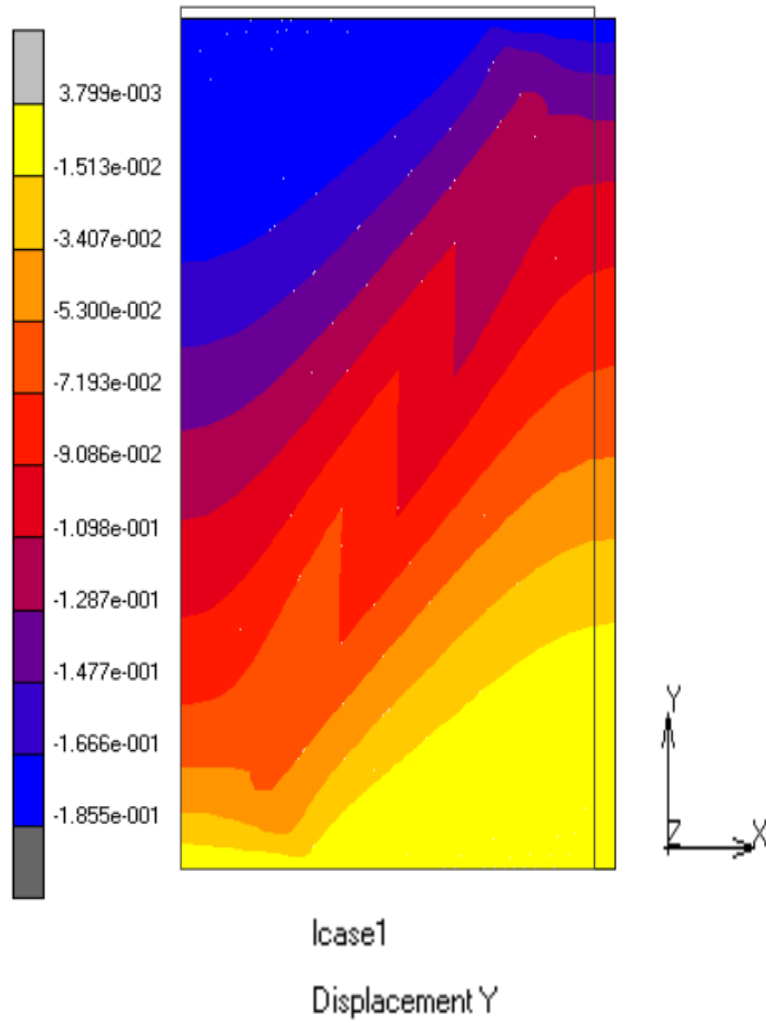


Figure 11: RVE deformation under stretching in 3-D analysis

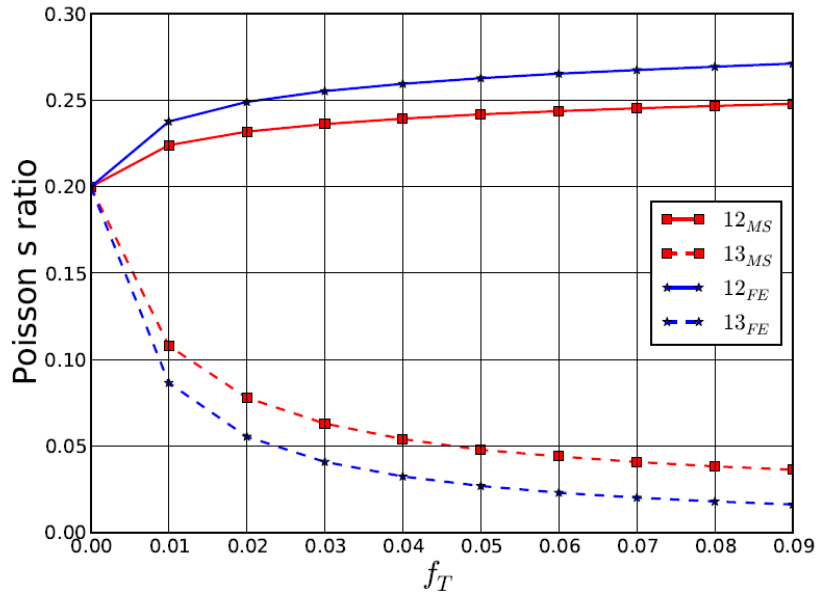


Figure 12. Poisson's ratio evolution versus inclusions volume fraction: FE and micromechanics solutions for  $\alpha = 0.4$ ,  $T = 10$ ,  $r = 0.1$

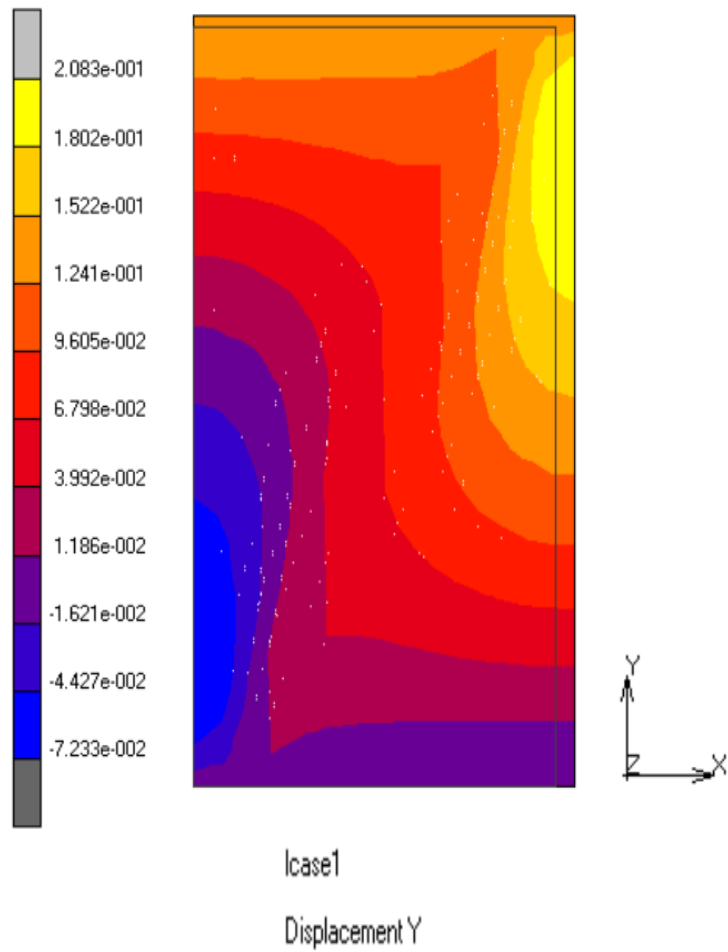


Figure 13. Finite Element modeling of tied inclusions: RVE deformation under stretching in 2-D plane strain analysis

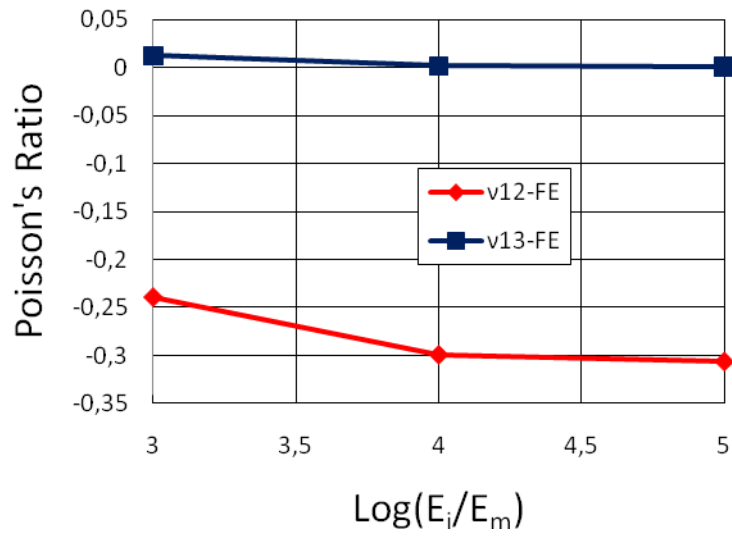


Figure 14. Finite Element modeling of tied inclusions: Poisson's ratio  $\nu_{12}$  and  $\nu_{13}$  versus Young modulus ratio  $\frac{E_{inclusion}}{E_{matrice}}$

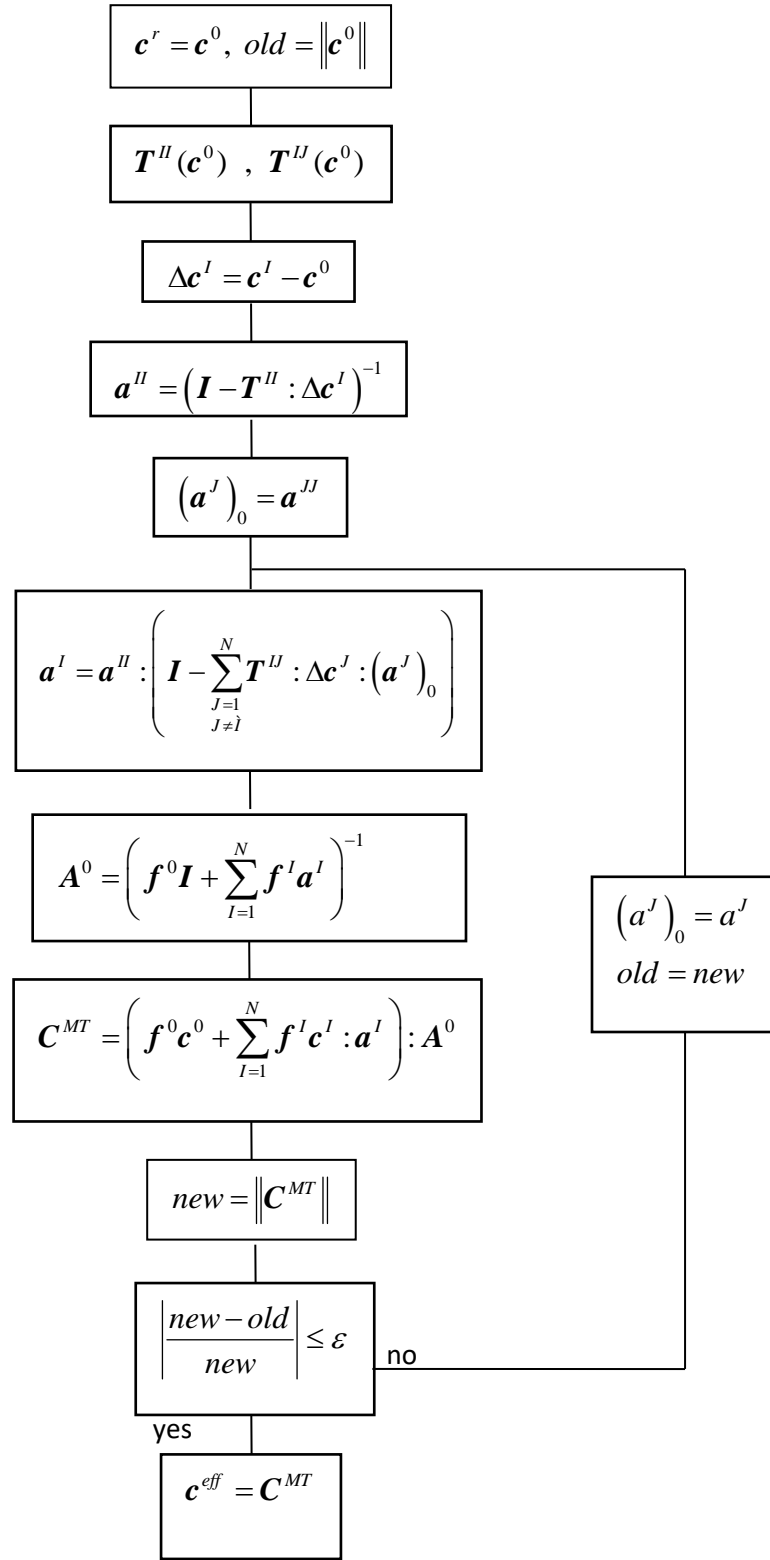


Fig. A.1. Appendix

<b>Inclusion</b>		<b>Matrix</b>	
Shear modulus $\mu$	Poisson's ratio $\nu$	Shear modulus $\mu$	Poisson's ratio $\nu$
238.095 GPa	0.05	2.083 GPa	0.2

Table 1: Materials properties used in the multi-site version approximation