On the Homogenization of 2D Porous Material with Determination of RVE

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***Abstract*-- The numerical homogenization technique is used in order to compute the effective elastic properties of heterogeneous random 2-phase composites. Differents microstructures are considered with different volume fraction.**
microstructure with random distribution of identical non-overlapping phases inclusions based on the Poisson process. (PBC), boundary conditions are applied on the representative volume element, RVE, of microstructures, for elastic modeling by finite element method. The aim of the work was to examine how spatial distribution and particles volume fraction influences the elastic properties of the composite material. The results were compared to various analytical model.

***Index Term*-- RVE, two-phase heterogeneous material, integral range, numerical homogenization, statistical approach.**

INTRODUCTION

The homogenization of a heterogeneous material and analysis of its effective properties are classical problems in the micromechanics of heterogeneous material. There are many homogenization models, such as the inclusion model based on the Eshelby's solution, the direct averaging method and the two-scale expansion method Andrievski (2001) and Cailletaud (1994). The inclusion model can predict the effective properties depending on the volume fraction, geometrical size of the inclusion and constituent's properties of composites. The the Hashin-Shtrikman model Hashin (1963) and the self-consistent scheme (SCM) Herve (1995) and Ostoja-Starzewski and Jeulin (2001) are developed along this line. They are widely applied to solve the effective properties of various kinds of inhomogeneous materials.
A different way to solve homogenization problems is to use numerical techniques and simulations on samples of the microstructure. These techniques, used to estimate the effective properties of random heterogeneous materials from the constitutive law and the spatial distribution of different components of the microstructure, are a main subject in the mechanics of random materials. It is related to the determination of the size of the representative volume element (RVE) wich has been recentely studied widely with the numerical and statistical tools (Sab, 2005a), (Tarada, 1998), (Ostoja-Starzewski and Jeulin, 2001), and (Kanit et al., 2003). The resulting apparent properties depend in fact on the choice of boundary conditions used to impose mean strain, stress. Three types of boundary conditions are classically used in computational homogenization: kinematic uniform (*KUBC*), stress uniform (*SUBC*) and Periodic boundary conditions (*PERIODIC*).
The aim of our work is firstly the evaluation of effective elastic properties of randomly distributed circular porous inclusions and using the numerical homogenization cited in (Kanit et al., 2006). Then we try to find a relationship between the integral range and morphological properties of inclusions.
A quantitative definition of the RVE size based on the notion of integral range is introduced. The *RVE* sizes found for the different properties are compared. Their dependence on the volume fraction and contrast properties is also discussed.

1 GENERATE OF MICROSTRUCTURE AND MECHANICAL PROPERTIES

Different methods are commonly used for constructing random microstructure volumes, the random sequential adsorption (*RSA*) used in [22], [24] and [25], the Monte Carlo method in [26], the molecular dynamics simulations in [20] and [27], and the random-walk methods in the work of [28].

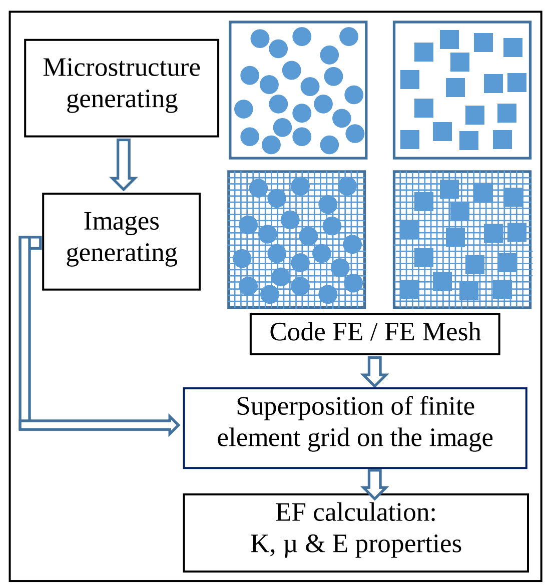

Fig. 1. Process of generating and meshing technic.

In this paper the randomly distributed forms of inclusions were generated in cell unit with an algorithm implemented in Python script, see figure 1. The volume fractions of forms inclusions used in this investigation are 10%, 30% and 50%. The condition of non-overlapping inclusions is imposed here with another condition that the inclusions do not hit any face of the box. The computation numerical is used for generating images used by the Code FE software.

1.1 Material and description 1.2 Meshing

We have chosen for our work, a model of microstructure which constituted by two phases: one matrix (black color) which is the hard phase and the second phase is constituted by inclusions (in white color) (figure 2). These inclusions have a form of circles, which distributed randomly. In this object, we will use the following volume fractions: 0.10, 0.30 and 0.50 of inclusions. We have generated several realizations of microstructure for each volume fraction. These microstructures will be use to determinate effective properties of the heterogeneous material like the bulk and shear modulus.

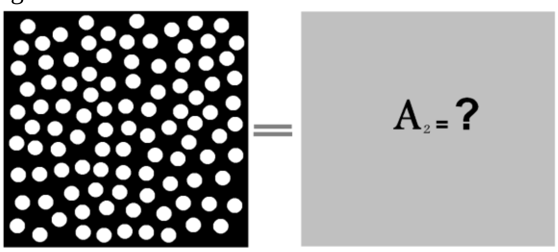

Fig. 2. Equivalent Model of the homogeneous model for two-phase

The physical properties: Young's moduli (E), Poisson ratio (ν), bulk (κ) and shear (μ) modulus of matrix and inclusions, used in the numerical simulations are given in table 1.

Table I
Physical properties of the material

Constitution	E [MPa]	ν [MPa]	k [MPa]	μ [MPa]
Matrix	1000	0.3	9615	3846
Inclusion	10^{-8}	0.49		

1.2 Meshing

The finite element mesh associated with the image of the microstructure is obtained using the method of multi-phase elements see figure 2. A regular grid of 2D finite element is superimposed on an image of material. The mesh element is the quadratic with 4 nodes and integration complet.

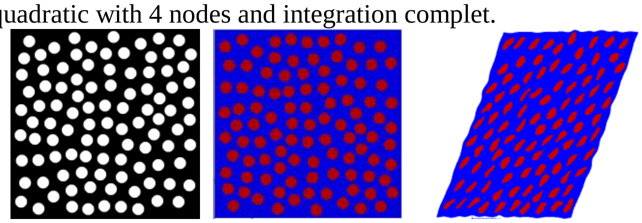

Fig. 3. *Meshing microstructures*

2 Effective Linear Elastic Properties

2.1 Numerical homogenization

The homogenization theory is used for the numerical determination of effective linear elasticity properties. A volume element of a heterogeneous material is considered. Conditions are prescribed at its boundary in order to estimate its overall properties. Two types of boundary conditions to be prescribed on individual volume element are considered:

• Kinematic uniform boundary conditions (*KUBC*): the displacement is imposed at point belonging to the boundary such that :

$$\underline{u} = E.\underline{x} \qquad \forall \underline{x} \in \partial V \tag{1}$$

E is a symmetrical second-rank tensor that does not depend on. This implies that :

$$< \varepsilon > = \frac{1}{V}\int_V \varepsilon dV = E \tag{2}$$

The symbol means equals by definition to. The macroscopic stress tensor is then defined by the spatial average:

$$\Sigma = < \sigma > = \frac{1}{V}\int_V \sigma dV \tag{3}$$

• Periodicity conditions (PERIODIC): the displacement field over the entire volume V takes the form :

$$\underline{u} = E.\underline{x} + \underline{\upsilon} \tag{4}$$

where the fluctuation $\underline{\upsilon}$ is periodic. It takes the same values at two homologous points on opposite faces of V. The traction vector $\underline{t} = \underline{\sigma}.\underline{n}$ takes opposite values at two homologous points on opposite faces of V. By applying either macroscopic strain or stress, The local behaviour at every integration point inside each grain in the simulation is described by the fourth-rank linear elasticity tensor c :

$$\sigma(\underline{x}) = c(\underline{x}) : \varepsilon(\underline{x}) \tag{5}$$

We are used respectively to define the following "apparent bulk and shear modulus" (k^{app} and μ^{app}) :

$$k^{app} = < \sigma > : E_k = \frac{1}{2} trace < \sigma > = \frac{1}{2} < \sigma_{11} + \sigma_{22} > \tag{6}$$

$$\mu^{app} = < \sigma > : E_\mu = 2 < \sigma_{12} > \tag{7}$$

were <.> is the average value.

or for this case of *KUBC* and *PERIODIC* conditions prescribed to a given volume V, one takes :

$$E_k = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad and \quad E_\mu = \begin{pmatrix} 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{8}$$

2.2 Variational bounds for the effective moduli of heterogeneous

To estimate the actual mechanical properties of a heterogeneous material, there are many methods of homogenization. We have used and tested the following methods : the bounds of Voigt and Reuss bounds of Hashin-Shtrikman optimal and the self-consistent model.

Voigt and Reuss bounds give two upper and lower bounds of the behavior that justifiant equivalent behavior of the material, the Hashin-Shtrikman model (Hashin, 1963) is verified by:

$$k^{HS\pm} = k_1 + \frac{1-P}{\left(k_2-k_1\right)^{-1} + P\left(k_1+\frac{4}{3}\mu_1\right)^{-1}} \quad (9)$$

$$\mu^{HS\pm} = \mu_1 + \frac{1-P}{\left(\mu_2-\mu_1\right) + \frac{2P\left(k_1+2\mu_1\right)}{5\mu_1\left(k_1+\frac{4}{3}\mu_1\right)}} \quad (10)$$

this conditions verified the property effectif for the materiel use.

The self-consistent estimate and the upper bound of (Zaoui, 1993) are used to determine the effective properties of the porous biphasic material :

$$k^{eff} = \frac{k_1\left(\mu_1+k_2\right)+\mu_1 P\left(k_2-k_1\right)}{\left(\mu_1+k_2+P\left(k_1-k_2\right)\right)} \quad (11)$$

$$\mu^{eff} = \mu_1\left(1+\frac{P}{\frac{\mu_1}{\mu_2-\mu_1}+\frac{k_1+2\mu_1}{2\left(k_1+\mu_1\right)}\left(1-P\right)}\right) \quad (12)$$

3 Fluctuation of effective properties and determination of the integral ranges

3.1 Notion of Integral Range

We consider fluctuations of average values over different realizations of a random medium inside the domain *V*. In geostatistics, it is well known that for an ergodic stationary random function *Z*(x), one can compute the variance $D_Z^2(V)$ of its average value *Z*(x) over the volume *V* as a function of the central covariance function *Q*(h) of *Z*(x) by :

$$D_Z^2(V) = \frac{1}{V^2}\int_V\int_V Q(x-y)dxdy \quad (13)$$

For a large specimen (with V>>A_2), Eq. (13) can be expressed to the first order in *1/V* as a function of the integral range in the space R^2, A_2, by (Matheron, 1971) and (Lantuejoul, 1991) :

$$D_Z^2(V) = D_Z^2\frac{A_2}{V} \quad (14)$$

with

$$A_2 = \frac{1}{D_Z^2}\int_{R^2} Q(h)dh$$

Where D_Z^2 is the point variance of *Z*(x) and A_2 is the integral range of the random function *Z*(x).

The scaling Eq. (14) is valid for an additive combination of the variable *Z* over the region of interest *V*, when its size is such that $V > A_2$ and when A_2 is finite. For an infinite integral range, *V* can be replaced in many cases by V^α (with $\alpha \neq 1$) in Eq. (14) (Lantuejoul, 1991).

As the composition of elastic moduli in the change of scale is not additive in general, relation (14) cannot be applied. Instead we propose, as (Cailletaud et al., 2003), to test a power law according to the relation :

$$D_Z^2(V) = D_Z^2\left(\frac{A_2}{V}\right)^\alpha \quad (15)$$

A similar relation was proposed and tested by (Cailletaud et al., 1994) and (Kanit et al., 2003). In the case of a two-phase material with elastic property Z_1 for phase 1 and Z_2 for phase 2, the point variance D_Z^2 of the random variable Z is given by :

$$D_Z^2 = P(1-P)(Z_1-Z_2)^2 \quad (16)$$

with:

- *P* and (*1-P*) are the volume fraction of inclusions and matrix respectively
- Z_1 and Z_2 are the properties elastic (*k* or μ)of inclusions and matrix respectively

The Eq. (16) becomes :

$$D_Z^2(V) = P(1-P)(Z_1-Z_2)^2.\frac{A_2}{V} \quad (17)$$

3.2 Dispersions of physical Properties

The numerical simulations based on the finite element method are carried out for two different boundary conditions: kinematic uniform boundary conditions (*KUBC*) and the periodic boundary conditions (*PERIODIC*). The studied volume fraction of inclusion phase is (*P =0.10, P =0.30, P =0.50*) and the number of realizations for each volume is one realization. which is the wanted effective modulus.

It can be noticed that the mean value given by the periodic boundary conditions varies slightly as a function of the size of the domain, as compared to the other boundary conditions. Figures 4, 5 and 6 gives the corresponding confidence intervals $[\overline{Z}-2D_Z, \overline{Z}+2D_Z]$, where Z is one of the apparent moduli, $\overline{Z}$ its mean value and $D_Z^2(V)$ its variance. This three curves for the case of periodic boundary condition and *SCM* model.

The obtained mean values generally depend on the volume size, but also on the type of boundary conditions. For each modulus, the values converge towards the same limit for large volumes *V* (*V* is the numbre of inclusions), which is the wanted effective modulus. The values k^{eff}, μ^{eff} and E^{eff} found for large volume sizes are reported in table. II and compared to the Voigt-Reuss (upper bound and lower bound), Hashin-Shtrikman's bounds (*HS+* and *HS-*) and (*SCM*) (Christensen, 1979a), also given in table II :

Table II
Values of numerical resultants, VR Bounds, HS Bounds and SCM for effective elastic properties of two phase heterogeneous porous material

Properties	*Simul.*	*Voigt*	*HS+*	*SCM*
k(P = 0.10)	2822	8653	7287	6923
μ(P = 0.10)	2917	3461	3221	2933
k(P = 0.30)	3725	6730	4307	3846
μ(P = 0.30)	1633	2692	2223	1748
k(P = 0.50)	1922	4807	2481	2136
μ(P = 0.50)	526	1923	1401	1012

Table III
Integral range for k and μ modulus

	$A(k)$	$A(\mu)$
P = 0.10	0.0039	0.0045
P = 0.30	0.0017	0.0021
P = 0.50	0.00027	0.00018

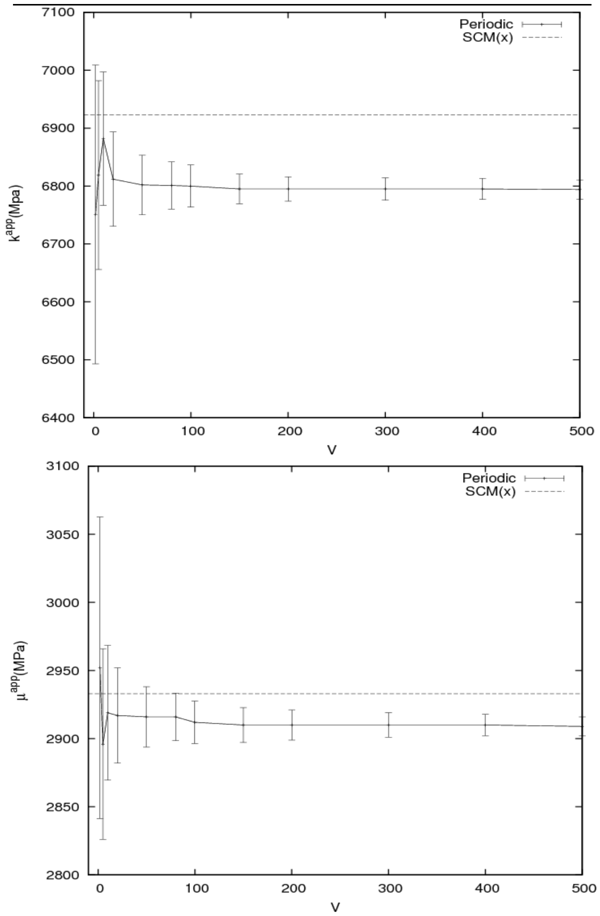

Fig. 4. *A figure title;* Convergence curve of the RVE and dispersion and mean value of the apparent elastic properties as a function of the domain size for periodic boundary conditions in the case (P=0.10) : a) evolution of k^{app}; and b) evolution of μ^{app}.

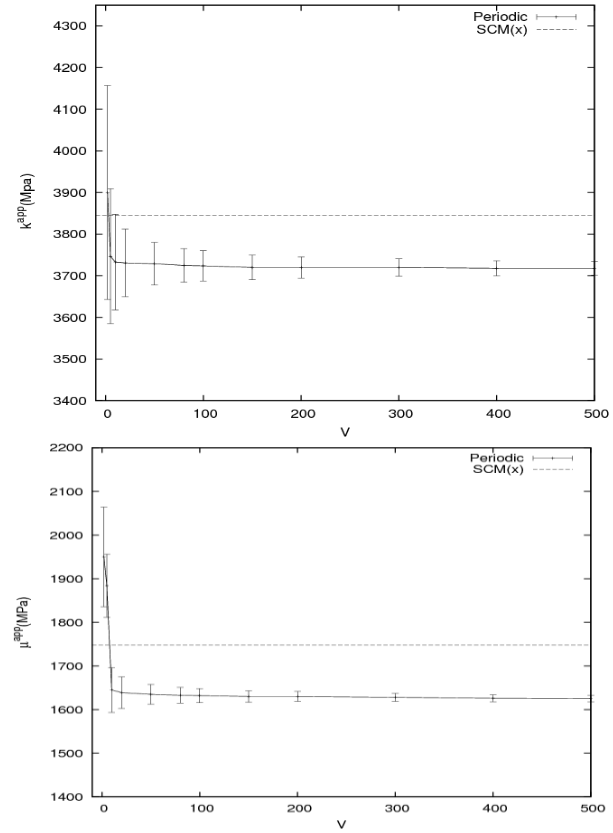

Fig. 5. *A figure title;* Convergence curve of the RVE and dispersion and mean value of the apparent elastic properties as a function of the domain size for periodic boundary conditions in the case (P=0.30) : a) evolution of k^{app}; and b) evolution of μ^{app}.

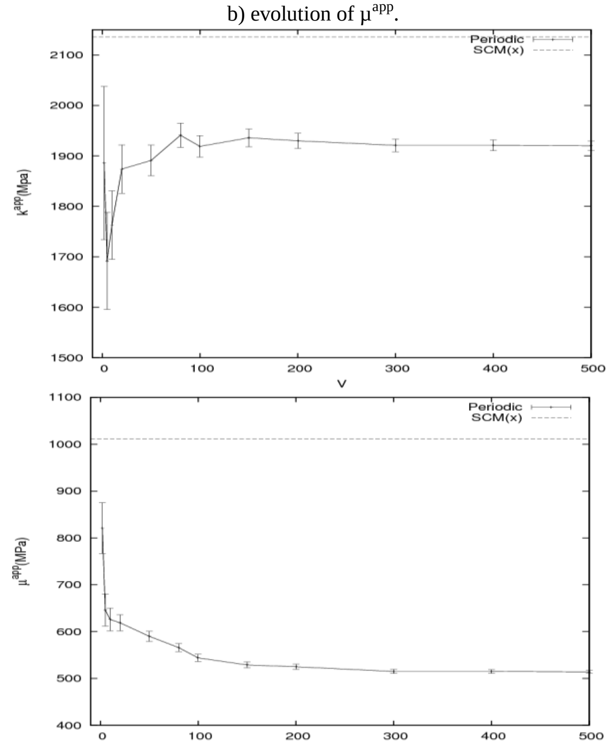

Fig. 6. *A figure title;* Convergence curve of the RVE and dispersion and mean value of the apparent elastic properties as a function of the domain size for periodic boundary conditions in the case (P=0.50) : a) evolution of k^{app}; and b) evolution of μ^{app}.

3.3 Representative Volume Elementary Size

In this part we represent the table are obtained by simulation of elastic properites volume function *V*. The results is obtained by fitting the mathematical model with the simulation curves of k^{app} and μ^{app}, or :

$$k^{eff} = \frac{2D_Z\sqrt{A_3}}{\varepsilon_{rel}\sqrt{V}} \tag{18}$$

Or D_Z is the variance of k modulus : $D_Z = D_k$ and ;

$$\mu^{eff} = \frac{2D_Z\sqrt{A_3}}{\varepsilon_{rel}\sqrt{V}} \tag{19}$$

or D_Z is the variance of μ modulus : $D_Z = D_\mu$. The numerical results of simulation of physical properties corresponds to the model mathematical (18) and (19) gives the following table.
The size of the RVE can now be defined as the volume for which for instance n = 1 realization is necessary to estimate the mean property Z with a relative error a ε = 1%, provided we now the function $D_Z(V)$:

This table shows the property A_2 for the three volume fractions in both cases (k and μ). The integral range A_2 depend only on the volume fraction of the inclusion. We have seen in all the cases studies here that the others parametrers have no relation and influence on the integral range. Integral range A_2 can be found by using the proposed relation :

$$A_2 = P/RVE \tag{20}$$

for the exemple studies in this paper, we have :

- *P=0.10*, *RVE =20* inclusions
- *P=0.30*, *RVE =100* inclusions
- *P=0.50*, *RVE =200* inclusions

Figure 6 sumarize the evolution of the RVE with the volume fraction of the inclusion.

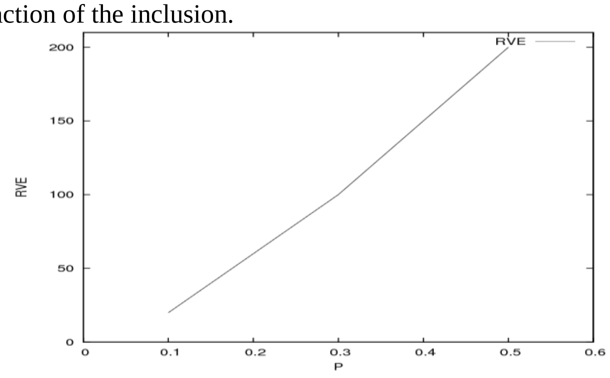

Fig. 7. Evolution of the RVE with the volume fraction

3.4 Effect of the volume fraction and contrast on the integral ranges

The apparent properties and integral ranges obtained for elasticity depend on the volume fraction of phases and the representative elementary volume (*RVE*). In this section, we come back to the variance D_z^2 of the effective properties for the two-phases elastic material, which is Eq. (17), in the two-dimensional it becomes :

$$D_z^2 = P(1-P)(k_1-k_2)^2\frac{A_2}{RVE}$$

It was found that the quantity: $A_2 = P/RVE$, implies :

$$D_k^2 = P(1-P)(k_1-k_2)^2\frac{P}{RVE^2} \tag{21}$$

and

$$D_\mu^2 = P(1-P)(\mu_1-\mu_2)^2\frac{P}{RVE^2} \tag{22}$$

so, for the contrast c = $k_2/k_1 \Rightarrow k_2 = c.k_1$
(k_1: matrix and k_2 : inclusion)
for example :
If $k_1 = 1$, (18) implies:

$$D_k^2 = P.k_1^2(1-P)(1-c)^2\frac{P}{RVE^2} \tag{23}$$

for the model is converge it is necessary that the variance D_k^2 takes the minimum (ie : $D_k^2 = 1$)
implies

$$1 = P^2.k_1^2(1-P)(1-c)^2\frac{1}{RVE^2}$$

or:

$$RVE = P.|1-c|.\sqrt{1-P} \tag{24}$$

it is the relationship between RVE and contrast (*RVE = f(c)*)
The relation : $RVE = P|1-c|\sqrt{1-P}$
equivalent of relation :

$$y = f(c) = P|1-c|\sqrt{1-P}$$

Or, to plot the three cases we study the contrast :

- *c < 1* matrix stiffer than the inclusion
- *c = 1* matrix stiffer than the inclusion
- *c > 1* inclusion stiffer than the matrix

so for *P=0.3* the curve *y = f(c)* is represented as follows:

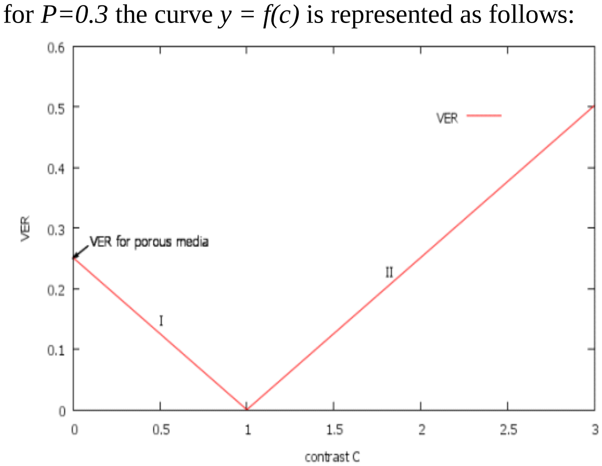

Fig. 8. *Relation between RVE in the contrast*

- when c=0 the *RVE* is equal to the value $P.\sqrt{1-P}.k_1$ or the RVE depends on the volume fraction and the property k_1 of the matrix.

when $c=1$ the $RVE=0$ that mean that the properties of the two phases are equal implies $k_2 = k_1$,

- when $RVE \in I$ implies $k_2 < k_1$, when th contrast $0 < c < 1$ and $RVE_{RPM} < RVE < 1$ (RVE_{RPM} is the *RVE* for porous media), media matrix is more compressible than for the inclusion.

- when $RVE \in II$ implies $k_1 < k_2$, when the contrast $c > 1$, the media for inclusions is more compressible than for the matrix.

CONCLUSIONS

The effective linear properties of random materials can be determined not only by numerical simulations on large volume elements of heterogeneous material, but also as mean values of apparent properties of rather small volumes, providing that a sufficient number of realizations is considered. This is very important, since computations on large volumes are usually prohibitive. This corresponds also to an enlarged definition of representative volume element. Its size mustbe considered as a function of five parameters: the physical property, the contrast of properties, the volume fractions of components, the wanted relative precision for the estimation of the effective property and the number of realizations of the microstructure associated with computations that one is ready to carry out. It depends also in fine on the special morphology of distribution of The integral range is of importance in the study of homogenization of microstructures and for the determination of effective properties of materials, this property is a quantity morphological and for the case of porous material, it depend only on volume fraction of inclusion. the proposed relation (20) for the determiantion of the value of integral range complate the methodology proposed by (Kanit et al., 2003).

The contrast between the two phases is very importante on the behaviour of the porous material, this question is investigated and developped in the last section and need to be study more.

we soulved three great point from the study of the contrast :

- contrast $c = 0 \Rightarrow$ porous material
- contrast $c \in]0, 1[\Rightarrow$ porous material
- contrast $c = 1 \Rightarrow$ RVE d'ont exist or material incompressible
- contrast $c > 1 \Rightarrow$ the behaviour of the material depend on the inclusion.

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