IOSR Journal of Mechanical and Civil Engineering (IOSR-JMCE)
e-ISSN: 2278-1684,p-ISSN: 2320-334X, Volume 13, Issue 3 Ver. IV (May- Jun. 2016), PP 118-126
www.iosrjournals.org

The Effective Elastic Properties And The RVE Size By Satatistic And Numerical Approach For Porous Materials

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Abstract: *In this paper, the numerical homogenization technique and morphological analysis are used in order to compute in microscale of porous materials. The computational effective elastic properties homogenization is based on a 3D random material with cylindrical pores. Periodic boundary conditions are applied on the representative volume element (RVE) of microstructures, for effective elastic properties modeling by finite element method. The integral range is introduced for morphological characterization[1].This approach defines a RVE by establishing a connection among the RVE size, a given number of realizations, a given property and a given precision of estimation. The results prove that this approach is applicable to porous materials (lotus-type). The elastic properties estimated for the determined RVE size agree with experimental results very well according to Ichitsubo and al. [2]*

Keywords: *Porous materials, Representative volume element, Homogenization technique, Statistical-Numerical approaches, Finite element method.*

I. Introduction

Over the past few decades, porous and foamed metallic materials have become an attractive research field both from a scientific viewpoint and the prospect of industrial applications, because those exhibit many unusual combinations of physical and mechanical properties. The materials containing a number of pores or voids can be classified into a few groups. Cellular metals are materials with a high volume fraction of voids, usually more than 70 %, composed of an in-terconnected network of struts and plates. Foamed metals have polyhedral cells that may be either closed with mem- branes separating the adjoining cells, or open with no mem- branes across the faces of the cells so that the voids are inter- connected. Solid foams originating from a liquid foam are closed-cell. Some prefer to call open-cell metallic structures metal sponges. Such materials provide a distinct advantage over solid metals for energy absorption, sound absorption, vi-bration suppression, thermal management, etc.

On the other hand, porous metals have isolated, roughly spherical pores, whose volume fraction is less than 30 %. These porous metals provide various products for applications such as filtration, fluid flow control, self-lubricating bearing, battery electrodes, etc.However, these metals have a similar characteristic pore geometry, which is almost spherical, a serious weakpoint for application since spherical pores deteriorate me-chanical properties such as tensile strength and ductility.Recently a new type of porous metals whose long cylindrical pores are aligned in one direction has been fabricated by unidirectional solidification under a pressurized hydrogen or nitrogen gas.Many gas pores are evolved from insoluble hydrogen (or nitrogen) in solids while hydrogen (or nitrogen) dissolves significantly in liquids. Among them lotus-type porous metals, produced by the novel solid-gas eutectic solidification method [3] , [4]

Heterogeneous materials unlike homogeneous ones need to undergo a process called homogenization to find their effective properties. Several methods of homogenization have been created over the last century and some have attained efficient and accurate approximations of linear elastic properties of heterogeneous materials. Nowadays computational techniques are more widely used for the homogenization of heterogeneous materials. It comprises of running simulations on digital samples of the microstructure. However, to achieve this, the existence of a Representative Volume Element (RVE) is needed. An RVE [5] has many definitions butgave the classical definition which states that the RVE is a sample that is structurally typical of the whole microstructure, i.e. containing a sufficient number of heterogeneities for the macroscopic properties to be independent of the boundary conditions. However, later [6] indicated that the classical definition of an RVE is only valid when the homogenized properties tend toward those of a similar periodic medium. This implies that the RVE is independent of boundary conditions.

After various numerical simulations agreed that the RVE has to be as large as possible to facilitate the calculations. Contrary to that idea,stated that the RVE has to be the smallest volume possible where the apparent and effective properties converge and meet. Even with these slightly different definitions it is certain that the RVE of a random composite is an isotropic medium.

This study presents a method to predict the effective elastic properties of porous metals (lotus-type)within a computational homogenization framework. This approach is widely utilized in the multiscale analysis

of porous materials **[7].** For this purpose, the RVE must be defined properly. Hence, being well-defined and suitable for two-phase linear elastic heterogeneous materials, the methodology proposed by Kanit et al. [1], [10], ElMoumen et al. [7], [8] et[9] has been used in conjunction with numerical finite element simulations to determine RVE size.

II. The Microstructure Generation And The Fe Discretization

1. The microstructure generation

In this investigation we aim to study the elastic behavior of porous materials (lotus-type) with medium porosity. Microstructure information used to generate RVEs geometry is given by table 1 according to Ichitsubo and al.[2]

Table 1. Microstructural parameters used in RVE geometry generation [2].

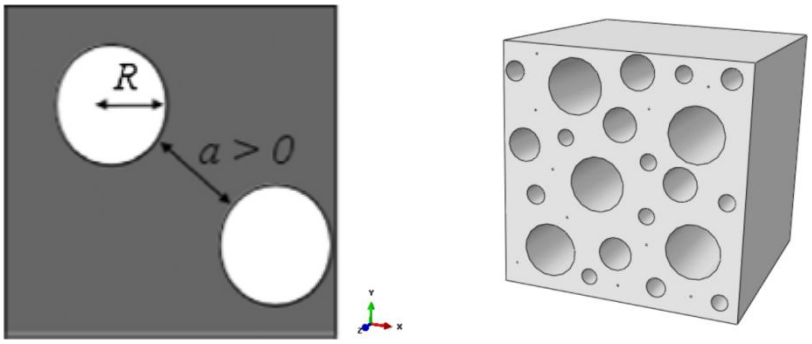
f (%)	D (µm)	D_{max}(µm)	D_{mini} (µm)
31	16.5	55	1.8

The elastic properties computations of porous materials, assumed cubic with unidirectional cylindrical pores, pores are oriented along z-axis, as is shown in Fig.1, which in practice is the solidification direction are presented.Here, elastic properties of lotus-type copper with a medium porosity of 31% is studied [Moumen]. Its microstructure is inspected by [2] and it is observed that its pores aspect ratio is of order 10-100.

RVEs are assumed cubic with unidirectional cylindrical pores. Pores are oriented along z-axis, as is shown in Fig.1, which in practice is the solidification direction. Regarding what has just been mentioned, only pores distribution is needed to be defined in a cross-section parallel to xy-plane to generate a RVE geometry. Pores number and pores diameter are calculated through an iterative process. In each iteration, a random pore diameter is generated from a given normal distribution with mean pore diameter D. The Pores diameter should lie between minimum diameter D_{min} and maximum diameter D_{max}. Eventually, planar pores distributed in the cross-section are extruded along z-axis into cylindrical pores to make a final geometry.

The relative pore positioning is proposed that the pore i of each center, with respecting a given repulsion distance a between neighboring pores, the pores are not allowed to touch each other, consequently, the center-center distance between a new pore i and each previous pore i+1 is set to :

$\frac{(D_i+D_{i+1}).1,1}{2}$ (cas : a > 0)



(a) (b)

Fig 1: (a) Relative pore positioning and repultion distance (b) RVE Geometry

According to this conditions, Five volume are genereted with n realizations (Table 2)

Table 2. The number of realizations for each RVE size.

RVE	V_1	V_2	V_3	V_4	V_5
n	250	200	150	120	100
Volume size (μm^3)	123506	292755	571787	988048	1568984

2. FE discretization and convergence of macroscopic elastic proprietes

In this part, the convergence of macroscopic elastic properties was verified. We try to get the number of FE necessary to mesh elementary volume containing N pores. For that purpose a specific 3D microstructure made of random cylindrical pores is considered. The RVEs geometry is discretized by 20-node quadratic brick with reduced integration elements.

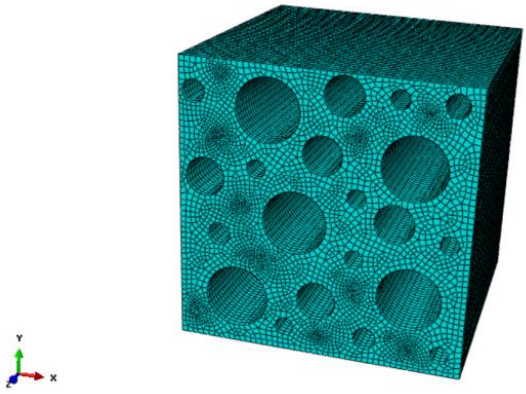


Fig 2: FiniteElementMesh

A simple uniaxial tensile is applied on the microstructure perpendicular to pores direction and the homogenized effective Young's modulus is determined.

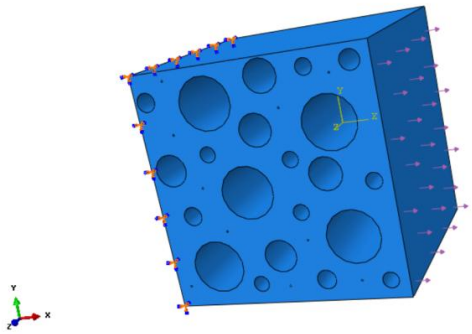


Fig 3 : Simple uniaxial tensile applied on the RVE

Fig. 4 shows the discretization of the RVE when loading is perpendicularto the pores direction (x-axis). Apparent young's moduli perpendicular to pores direction are obtained for the different mesh densities for which the number of finite elements varies from 148 to 18740 where the number of degrees of freedom varies from 2880 to 256949 The results shown in Fig. 4 represent the apparent young's modulus with respect to the number of degrees of freedom.

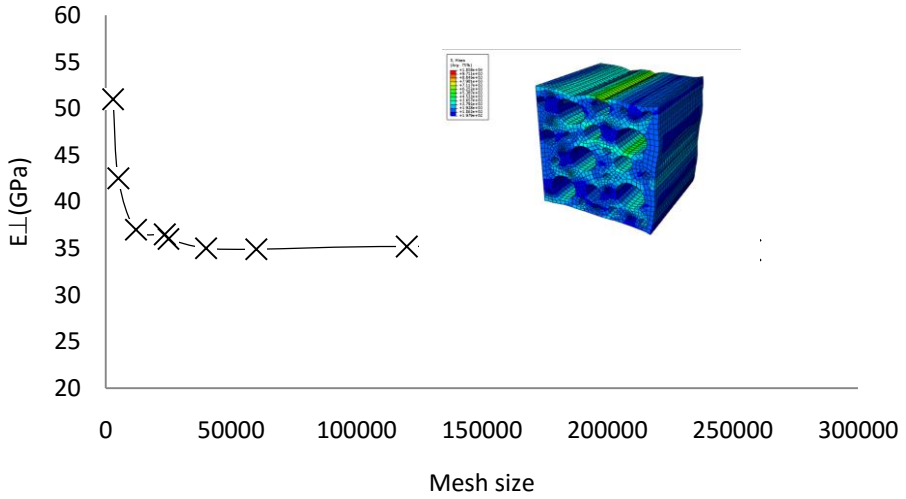


Fig 4. Effect of mesh size on the value of young's modulus $E_{\perp}$

Fig. 4 shows that the variation of the young's modulus becomes less than 1% for numbers of degrees of freedom greater than 50000. Therefore, for RVEs of volume V_3 a mesh density with around 50000 degrees of

freedom is used. Also, RVEs of other volume sizes than V3 are discretized by meshes with numbers of degrees of freedom proportional to the ratio of their volume sizes to volume V_3.

III. Governing, Constitutive Equations And Methodology

1.Effective and apparent elastic properties

For heterogeneous elastic materials admitting a RVE, the effective elastic properties can be defined by the linear constitutive equation:

$$\bar{\sigma} = C^{eff}\,\bar{\varepsilon} \qquad (1)$$

where :
C^{eff} is the effective stiffness tensor
$\bar{\sigma}$: macroscopic stress fields
$\bar{\varepsilon}$: macroscopic strain fields

in the RVE of volume V, stress and strain fields, and respectively derived using the spatial averages :

$$\bar{\sigma} = \frac{1}{V}\int_V \sigma(x)dV \qquad \forall\, x\epsilon V \qquad (2)$$

$$\bar{\varepsilon} = \frac{1}{V}\int_V \varepsilon(x)dV \qquad \forall\, x\epsilon V \qquad (3)$$

Since using numerical methods necessitates small volume elements, the apparent elastic properties is given by the relation :

$$\bar{\sigma} = C^{app}\,\bar{\varepsilon} \qquad (4)$$

The equivalence of strain energy between the macrofields and the microfields is ensured through the Hill's microhomogeneity condition:

$$\bar{\varepsilon}:\bar{\sigma} = \frac{1}{V}\int_V \varepsilon(x)dV \qquad (5)$$

The microscale geometry of the RVE is assumed periodic, therefore the best choice among these boundary conditions is periodic boundary conditions.

2.Numerical homogenization technique

The technique FEM is chosen to calculate the REV of our material given inTable 1 using the methodology explained in Kanit et al [1], [10] and ElMoumen [7], [8].The used methodology for realizations generation is based on the sub-volume technique, the principle of this technique consists to use several independent block volumes Vi smaller than the larger volume V by keeping the same pores volume fraction. Each volume contains a specific number N of pores, which are ranging from 2 until the convergence of macroscopic properties of studied porous materials. The convention is made that increasing the volume size, the pore number is increased. So, each block Vi contains a specific number N of pores. This technique is explained and presented in Fig. 9 for five sub-volume and already used in [11] for composites and [12] for geomaterials. Table 2 gives n realisations for every volume size.

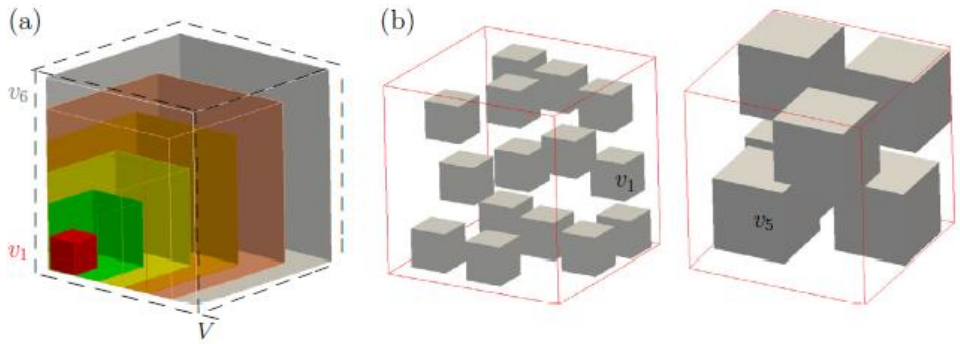


Fig 5 : Methodology of realizations generation: (a) different block sizes, and (b) some n realizations randomly distributed in V.

For a reliable homogenization, each sub-volume v_i must randomly cover the total volume v, as explaining in Fig.5.Finally, the PBC are applied on each block in order to determine the macroscopic (apparent)

effective propperties and morphological properties. The size of the volume increases until the convergence of the macroscopic properties. The obtained results by set realizations are used to identification of statistical parameters and todetermine RVE size for porous materials so that the effective elastic properties

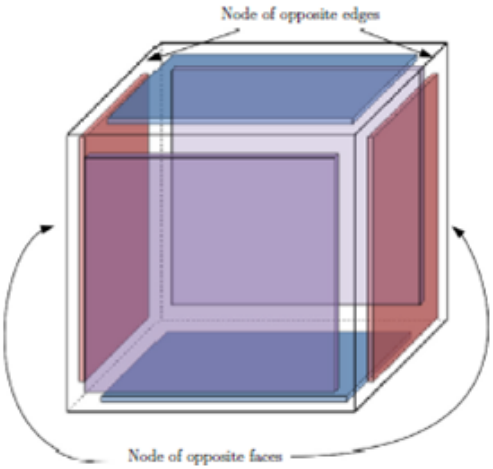


Fig 6 : Periodic boundary conditions periodicity of opposite faces and edges

3.Variance and integral range A

A good way to have a convenient measurement of RVEsizeof a stationary and ergodic random structure is the notion of A,Cailletaud et al. (1994). This notion has already been introduced byKanit et al.[1] for microstructures with Voronoi mosaics and used by ElMoumen [7]. Thiswork is an extension for other type of microstructures, in order touse this parameter for establish a relationship between two different microstructures. In mathematical morphology, for a largevolume V, the variance is expressed in terms of A by:

$$D_Z^2(V) = f(1-f)(Z_1 - Z_2)^2 \left[\frac{A}{V}\right] \qquad (6)$$

where$D_Z^2(V)$ is the variance obtained by set different n realizationsof each volume size V and A is the **integral range**of the random function Z.

The variance $D_Z^2(V)$ is an indication of the accuracy of the estimation. Theoretically, if volume V is a RVE the variance will be vanished. However, in practice the size of the RVE is determined for a desired error.

The absolute error on the mean value M of the homogenized properties defined with n independent realizations is deduced from the interval of confidence by:

$$\varepsilon_{abs} = \frac{2D_Z(V)}{\sqrt{n}} \qquad (7)$$

The relative error is defined as: $\varepsilon_{rel} = \frac{\varepsilon_{abs}}{M} = \frac{2D_Z(V)}{M\sqrt{n}}$ (8)

Using Eq. (8), one is able to define the required number of realizations of volume V to estimate the mean property M with a given relative error :

$$n = \frac{4D^2{}_Z(V)}{M^2\varepsilon_{rel}^2} \qquad (9)$$

In addition, the minimal RVE size for a given number of realizations and a given relative error can be by :

$$V^{RVE} = \left(\frac{4D^2{}_Z}{nM^2\varepsilon_{rel}^2}\right) A \qquad (10)$$

As it can be seen, the RVE size determination requires the variance $D_Z^2(V)$ and the mean value M to be calculated accurately. In practice, for n realizations of the volume V these quantities can be estimated by:

$$M = \frac{1}{n}\sum_{i=1}^{n} \bar{Z}(V)_i \qquad (12)$$

$$D_Z^2(V) = \frac{1}{n-1}\sum_{i=1}^{n}(\bar{Z}(V)_i - M)^2 \qquad (13)$$

It is obvious that the estimation accuracy of these quantities strongly depends on the number of realizations. Hence, n is chosen in order that variations of the variance and the mean value M become negligible.

IV. Result And Discussion

1.Computation of elastic properties tensor

The elastic constants are calculated using the homogenization approach. Determination of all elastic constants requires six different load cases, three pure axial and three pure shear, to be imposed on a RVE.Containing elongated and nearly unidirectional pores, porous materials (lotus-type) exhibit transverse isotropy. In the case of transversely isotropic materials, the number of independent elastic constants reduces to five, then we have : $c_{11}=c_{22}$, $c_{13}=c_{23}$, $c_{44}=c_{55}$ and $c_{66}=(c_{11}-c_{12})/2$.

If a finite volume V of a transversely isotropic material is considered, then the response of only one realization of the volume V will not be transversely isotropic. On the contrary, the transversely isotropic behavior can be better estimated by averaging over a number of realizations of the volume V. The more the number of realizations, the more accurate the estimation. The apparent elastic constants for each volume size are calculated using the finite element simulations results in conjunction with the homogenization approach. The Fig 5, 6 and 7 illustrate the mean value and the variance of elastic constants.

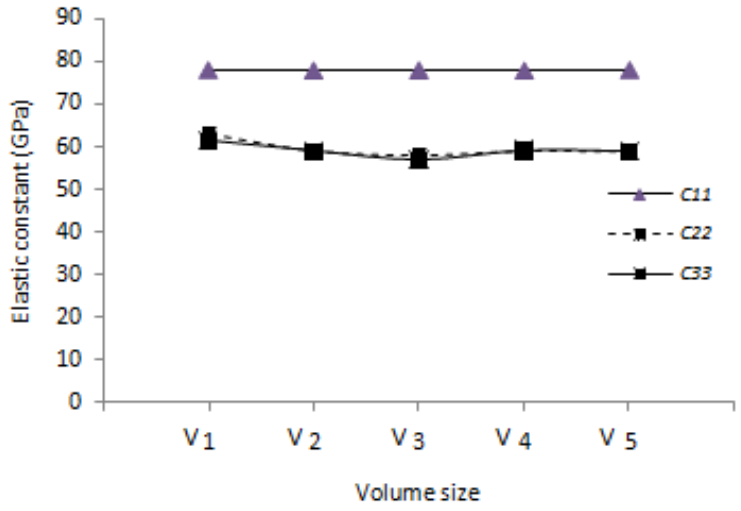


Fig 7. The mean value and variance for the apparent elastic constants c_{11}, c_{22} and c_{33}

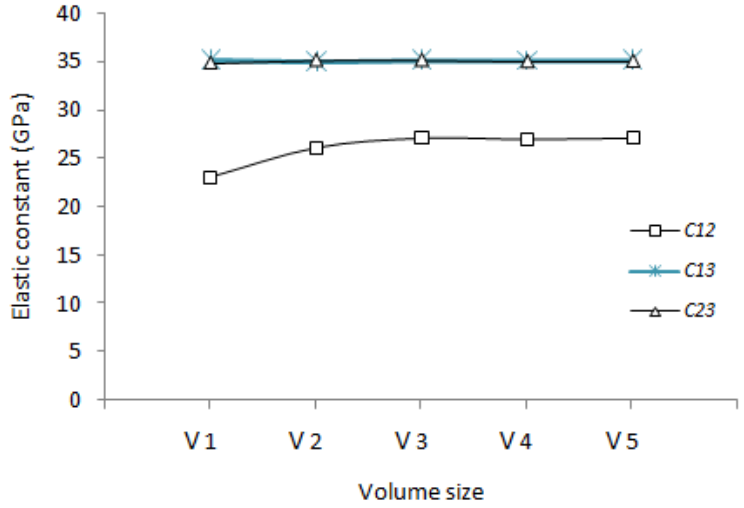


Fig 8. The mean value and variance for the apparent elastic constants c_{12}, c_{13} and c_{23}

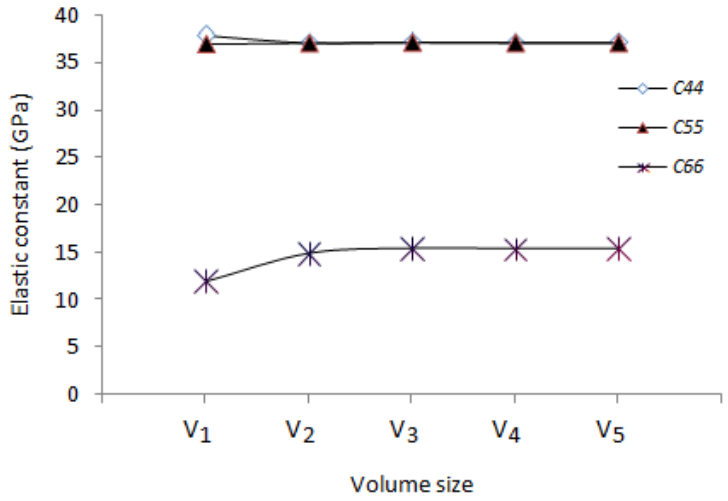


Fig9 . The mean value and variance for the apparent elastic constants c_{44}, c_{55} and c_{66}

Fig. 7, 8 and 9 show that the mean values of the apparent elastic constants are almost constant for volume sizes equal and greater than V_3 which therefore can be considered as good estimations for the effective elastic constants. Besides, the results indicate that volume element smaller than V_3 cannot accurately estimate the effective properties at all.

As measures of the departure from transverse isotropy the following deviationsare defined by :
$\delta_{12} = 2\frac{|c_{11}-c_{22}|}{c_{11}+c_{22}}$; $\delta_{123} = 2\frac{|c_{13}-c_{23}|}{c_{13}+c_{23}}$;$\delta_{45} = 2\frac{|c_{44}-c_{55}|}{c_{44}+c_{55}}$ and $\delta_{66} = 2\frac{|c_{11}-c_{12}-2c_{66}|}{c_{11}-c_{12}+2c_{66}}$

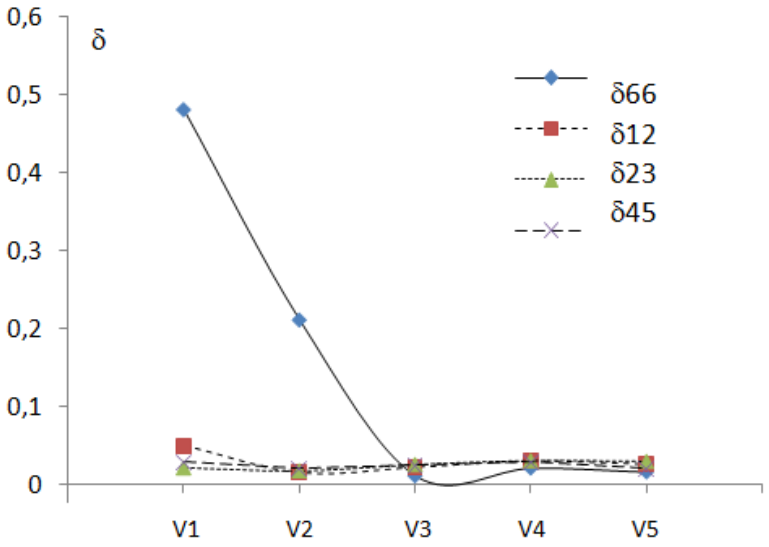


Fig10 . The variance of apparents elastic constant

Fig. 10 gives obtained deviations for each volume. Increasing the volume provides more accurate estimation of the transversely isotropic behavior. The deviations are negligible for all volume sizes, whereasδ_{66} is considerable for volume sizes smaller than V_3.The volume sizes smaller than V_3 can never guarantee transverse isotropy.It can be seen that c_{66} has the highest ratio of the mean value to the variance and consequently the greatest relative error. Therefore, RVE size is determined for this elastic constant.

2. Numerical and statistical homogenization

The first step is to calculate the constants **A** by fitting the Eq. (6) on the obtained results. For the lotus-type copper with the porosity p, the volume fraction of phase 1 (copper matrix) is and the volume fraction of phase 2 (pores) is p. Therefore, substituting of the non-porous copper for Z1 and zero forZ2 , Eq. (8) reduces to:

$$D^2_{C66} = p(1-p).c^2_{66}\ \left[\frac{A}{V}\right] \qquad (14)$$

After fitting the Eq. (6) on the obtained variance of for each RVE volume size : **A = 3250**

Fig. 11 shows a comparison between Eq. (6) and the obtained results. A very good agreement is observed showing the quality of the relation proposed by Kanit et al. [1] for determining lotus-type porous materials RVE size.

Knowing constants A, one is able to determine either number of realizations for a desired RVE size or RVE size for a desired number of realizations for a given precision. Such a large RVE cannot handle numerically, therefore smaller volume sizes should be tried. However, as the volume sizes smaller than V3 cannot guarantee both transversely isotropy and effective elastic properties, thus RVE size must be equal or greater than V_3.

Hence, volume size V_4 is chosen as RVE size, then 86 realizations are needed for relative error of 2%.

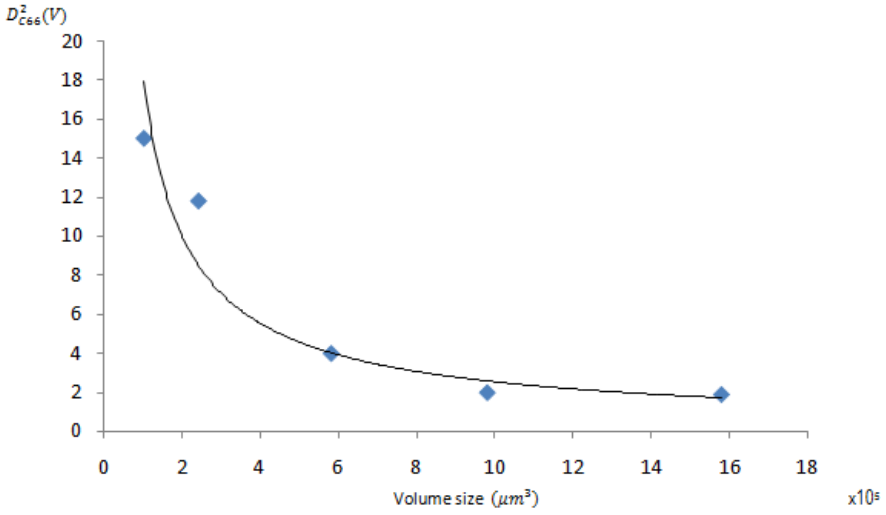


Fig 11. The variance of the apparent elastic constant c66

Finally, the effective elastic constants of porous materials are estimated with the following mean apparent elastic constants over 86 realizations.

$$C^{app} = \begin{bmatrix} 58.44 & 27.46 & 35.02 & 0 & 0 & -0.22 \\ 27.46 & 58.77 & 36.5 & 0 & 0 & 0.02 \\ 35.02 & 121 & 78.11 & 0 & 0 & -0.08 \\ 0 & 0 & 0 & 37.20 & 0 & 0 \\ 0 & 0 & 0 & 0 & 37.05 & 0 \\ -0.22 & 0.02 & -0.08 & 0 & 0 & 15.22 \end{bmatrix} \text{(GPa)}$$

Now, RVE size has been determined and effective elastic constants have been estimated for relative error of **2%.** In this section, the estimated effective elastic constants are compared with experimental results reported in Ichitsubo et al. [11] to find out whether the microscale geometry assumed to generate RVEs geometry is capable of capturing the real elastic behavior or not. The experimental results are given as the following tensor.

$$C_{Exp} = \begin{bmatrix} 60 & 28 & 37 & 0 & 0 & 0 \\ 28 & 60 & 37 & 0 & 0 & 0 \\ 37 & 37 & 78 & 0 & 0 & 0 \\ 0 & 0 & 0 & 35 & 0 & 0 \\ 0 & 0 & 0 & 0 & 35 & 0 \\ 0 & 0 & 0 & 0 & 0 & 16 \end{bmatrix} \text{(GPa)}$$

The small error indicates a very good agreement between the simulations and the experimental results. Therefore, the assumptions have been made to generate RVEs geometry are proved correct. Then, using this microscale geometry, one is able to accurately predict the elastic behavior of porous materials(lotus-type) with medium porosity.

V. Conclusion

The principal objective of this study is to order to predict the elastic behavior of lotus-type porous materials using a computational homogenization approach. This approaches are based on results of numerical simulations on the RVE, thus an attempt was made to properly define the RVE. Accordingly, the elastic behavior of a lotus –type copper with porosity of 31% was studied.

Several volumes, named realizations, are considered. These realizationsare used to determine some statistical parameters, such asvariance, and integral range of the microstructure. Theseparameters are used to quantify the effect of pores onthe elastic behavior of porous microstructures. The effectiveproperties and the size of the representative volumeelement (RVE) are related with all microstructure parameters.

The present study proved applicability of the numerical-statistical approach to elastic porous materials (lotus-type). The results indicated that using small RVEs can guarantee effective elastic properties and transversely isotropic behavior. However, it is important for RVE size not to be smaller than a specific volume size, causing departure form transverse isotropy and introducing great error in estimation of the effective properties. Comparing the obtained results with experimental ones, proved that the microscale geometry employed to generate RVE geometry can properly represent linear elastic lotus-type porous materials microstructure with medium porosity.

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