Mechanical properties of polymer foams : influence of the internal architecture on the stiffness

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Résumé :

Nous avons développé une méthode permettant d'obtenir le tenseur de rigidité complet de matériaux poreux par simulation par éléments finis. Cette méthode a été appliquée sur différentes microstructures périodiques inspirées de structures cristallines. Les tenseurs de rigidité complets permettent d'accéder á l'anisotropie du comportement élastique et ainsi d'étudier les effets de l'organisation. Une méthode similaire a aussi été développée pour étudier les effets de la microstructure sur les limites du comportement élastique.

Abstract

We developed a finite element simulation method to obtain the total stiffness tensor of cellular materials. It was used on several periodic microstructures inspired by crystal structures. With complete stiffness tensors, we can access the anisotropy of the elastic behavior and from there the effect of the microstructures can be studied. A relatively close method was developed to study the effects of the architecture on the limits of the elastic behavior.

Keywords : Polymer foam, elasticity, mechanical properties, stiffness tensor, microstructure

1 Introduction

Closed cell foams consist of a set of gas bubbles separated by thin membranes of a solid phase more or less rigid. These structures confer special properties that make them widely used for applications in sealing, noise and/or thermal insulation and for lightweight structure purpose.

Foam microstructures are complex, and very often, due to the manufacturing process, they present anisotropic behavior. Currently available literatures show that the mechanical response of polymer foams is dependent on the density, size and shape of the cells and of the nature of the material. Therefore it is crucial to be able to quantify and measure these parameters to work towards an understanding of the mechanical properties and set models to link the macroscopic behavior of the cellular material to an "equivalent" bulk material. In the present study, the mechanical behavior of polymers foams was analyzed in their domains of elasticity in relationship to their internal voids organization and in order to interpret the anisotropic behavior only to the structure.

A finite element simulation method was developed and allows to determine the full stiffness tensor of any foam microstructure, regardless its complexity and its randomness. For periodic microstructures inspired from the crystalline systems (CS, CC, CFC, HCP), the obtained results, in comparison to those from the literature , showed precision up to 10^{-1} on the values of the elastic constants of the tensor. For a given porosity, the simple cubic structure presents both the higher and the lower Young modulus regarding the loading directions and compared to other distributions. Following a numerical experience, nonlinearities induced by the geometry (or topology) from those induced by the material of the wall are analyzed.

The numerical analysis developed in the context of this study, shows that periodic structures present a significant anisotropy which is not experimentally detectable in case of real foam with intrinsically more random structures. Beyond this aspect, a more fundamental issue could be rise up by tackling the level of disorder in the cell organization necessary to give an isotropic behavior.

2 Stiffness tensor

The objective was to develop a finite elements simulation process to modelize the elastic behavior of an heterogeneous foam as an equivalent homogeneous material. The method used was first proposed by Heitkam et al. [1].

2.1 Concept

The linear elastic behavior is described by Hooke's law (1) , linking the stress σ, the strain ε and the stiffness tensor $\mathbf{C}$. The inverse of $\mathbf{C}$ is the compliance tensor $\mathbf{D}$. Adopting Voigt's notation, strain and stress vector contain 6 elements. Stiffness and compliance tensor are symmetrical and so consist of 21 independent elements.

$$\sigma = \mathbf{C}\varepsilon \tag{1}$$

The elastic strain energy U per volume V for an homogeneous material is a function of stress and strain (2), which mean it can be expressed as a function of $\mathbf{C}$ or $\mathbf{D}$ as follow :

$$\frac{U}{V} = \frac{1}{2}\varepsilon^T\sigma = \frac{1}{2}\varepsilon^T\mathbf{C}\varepsilon = \frac{1}{2}\sigma^T\mathbf{D}\sigma \tag{2}$$

The equivalent homogeneous material have to store the same amount of energy than the heterogeneous one. Therefore, the 21 elements of $\mathbf{C}$ can be computed by applying 21 specific deformation to the heterogeneous material and calculating the corresponding strain energy. First, applying 6 sets of strain consisting of one non-zero element $\varepsilon_l \neq 0$ lead to the elastics energy U_l and diagonal terms C_{ll} can then be determined (equation 3). Then, applying 15 sets of strain with two non-zero elements $\varepsilon_k \neq 0$ and $\varepsilon_l \neq 0$ give the U_{kl} terms. The non-diagonal terms C_{kl} can then be determined according to equation 4. The same method can be used with stress sets instead of strain to obtain the compliance matrix.

$$C_{ll} = 2\frac{U_l}{\varepsilon_l^2 V} \tag{3}$$

$$C_{kl} = \frac{U_{kl} - U_l - U_k}{\varepsilon_l \varepsilon_k V} \tag{4}$$

It can be applied for two dimensional models : a plane strain hypothesis is equivalent to a zero term on the non planar direction and allow the calculation of the stiffness tensor while a plane stress hypothesis

leads to the compliance tensor. Only six terms have to be determined in case of 2D problem.

The complete compliance tensor, obtained either directly or as the inverse of the stiffness tensor, can be used to compute Young's modulus E_{kk} (5), Poison ratios ν_{kl} (6) and shear modulus G_{kl} (7) in its chosen basis. It can also be rotated [2] to get those values in any direction. The rotation is reduced at the directions contained in the 2D plane when 2D models are considered.

$$E_{kk} = \frac{1}{D_{kk}} \tag{5}$$

$$\nu_{kl} = -\frac{D_{lk}}{D_{ll}} \tag{6}$$

$$G_{23} = \frac{1}{D_{44}} \qquad G_{13} = \frac{1}{D_{55}} \qquad G_{12} = \frac{1}{D_{66}} \tag{7}$$

Since numerical simulation allow to compute the strain energy, it is probably the easiest method to calculate the whole elastics properties.

2.2 Finite elements method

In order to apply the required loads, an hypothesis about the deformation was made. The first possibility was to consider that the deformation is identical to that of an homogeneous material.But due to the high heterogeneity of the considered foam, this hypothesis lead to relatively inaccurate results however it can be used on any microstructure. Another possibility is to consider the foam as periodic. This restrained the possible structure to either completely organized or randomized with periodic conditions but with a better accuracy.

Even if an extension to non-periodic structures is under consideration, all results shown here were obtained by using periodic boundary conditions in order to apply all the required strains. This require the studied microstructure to be represented by a periodic cuboid. Due to the periodic conditions, the amount of cells required for an organized structure is low, generally equal to the number of cells contained in the unit cell. For a randomized structure, the quantity of cells required for representativeness of the structure is higher.

For accuracy of the stiffness tensor, small strains should be used, at least for the material to remain linear. Since those limits are not always known, strains of 1% or less were used. For numerical simulation, small strains are not an issue.

The method was first tested on a bulk material with totally anisotropic properties. For such a case, every terms of the stiffness tensor were computed with a relative accuracy of 10^{-6}.

The main focus of this method was to characterize the variation of the elastic modulus as a function of the direction. In order to test both tensor rotation algorithm and the method self coherence, two simulations were conducted on the same structure oriented in two different basis. The resulting stiffness tensor were then rotated in order to be compared. The resulting tensors were anisotropic but had a relative accuracy of 10^{-4}.

Several works have already calculated the elastic properties of some particular microstructure trough mathematical approximations [3][4]. Those results provide a way to compare results obtained with the numerical simulation method. Table 1 summarize the results regarding cubic microstructure with spherical voids.

ϕ	Num	IW	dif(%)
0,05	0,901	0,894	0,76
0,10	0,810	0,802	0,99
0,15	0,729	0,722	1,00
0,20	0,656	0,650	0,96
0,25	0,590	0,586	0,62
0,30	0,528	0,527	0,10
0,40	0,412	0,423	2,58
0,50	0,301	0,331	8,94

TABLE 1 – Comparison of the relative elastic moduli obtained by numerical simulation or by Iwakuma's numerical approximation for different porosity ϕ

A decent accuracy is obtained for medium porosity. Two sources of inaccuracy can be detected : first, the author stated that the mathematical model used show increasing error for porosity of 0.25 or less. Then, the porosity of a finite element model is not totally exact because of discretization of the boundary during the meshing : for example, the real porosity of the model is not 0.1 but 0.0978. This represent an relative error of 2.2%. This have to be taken into consideration and further results consider the true porosity of the finite element models.

2.3 Results

In order to study the effects of cells shape and organization a number of simulations have been conducted on different microstructures inspired by crystal systems : spherical cells in standard organizations : primitive cubic (PC), body centered cubic (BCC), face centered cubic (FCC) and hexagonal close packed (HCP) . For cells shape, a kelvin cell model (non spherical cells in a BCC pattern) was considered. None of the resulting stiffness tensor were isotropic (fig 1). However, they showed symmetries equivalent to those of the corresponding microstructures : with the exception of HCP, all those structures present a cubic symmetry, which means that three orthogonal axis are always equivalent. The results for HCP structure show a cylindrical symmetry, which was also expected.

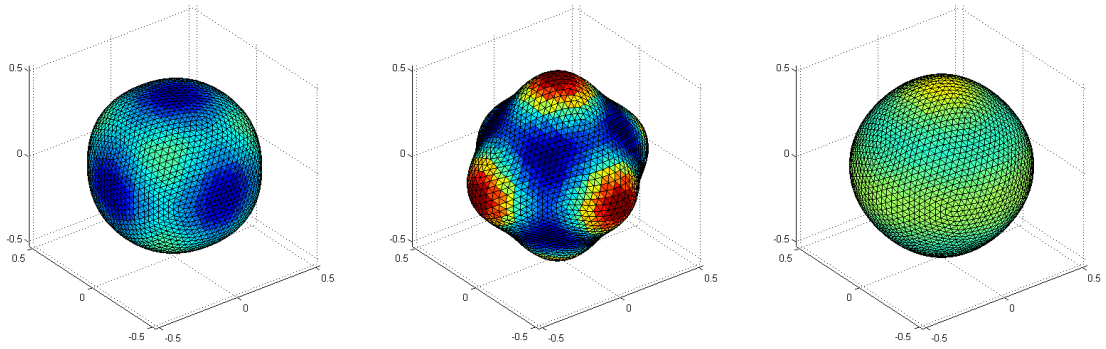

FIGURE 1 – Representation of relative Young modulus depending of the direction for three organized microstructure with a porosity of 0.4 : kelvin cells, PC and HCP spheres

Simple geometrics criteria can explain these anisotropies : for PC , which present the most important one, the presences of "struts" parallel to the mains axis explain the improved performance. However,

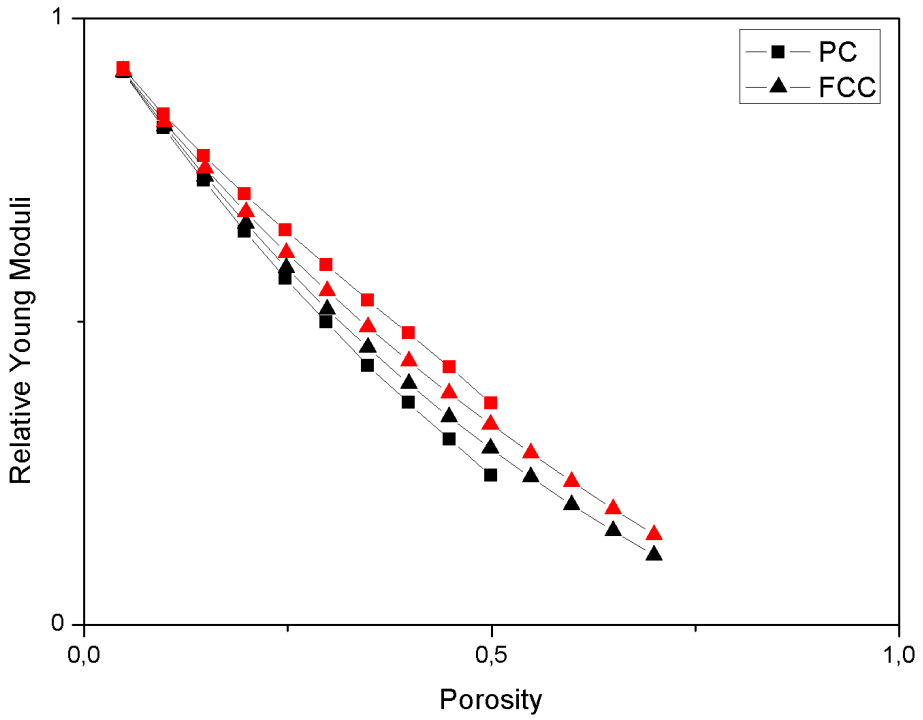

FIGURE 2 – Minimum and maximum Young modulus (direction-Dependant) for different microstructures depending of the porosity

for a loading in the direction [111], those struts will undergo a bending loading and be less relevant, explaining the weakening.

Figure 2 shows the variation of the Young modulus for two microstructures, both made of spherical voids. The variations of the modulus depend on the structure and the porosity. While the porosity still remain the main factor for those modulus, the load direction can also be relevant : for a porosity of 0.5, the ratio between maximum and minimum modulus reach 1.48 for a PC structure.

The average modulus for those microstructures are almost equivalent, but their dependency to direction is not. As such, the most anisotropic (PC) display both highest and lowest modulus for a given porosity : the direction of the load is an important factor to take into account to predict the elastic behavior of organized foam.It should also be noted that the variations of the shear modulus are linked to those of the Young modulus so their amplitude will be similar.

Equation 8 is a standard way to characterize the dependence of the relative Young modulus E_r of a foam on relative density ϕ. However, there is not much about anisotropic modulus. A try to fit both minimum and maximum modulus according to this equation showed clearly that anisotropy can not be described that way.

$$E_r = \rho_r^a \tag{8}$$

Real foams often present anisotropic microstructure, generally because of the processes used for their

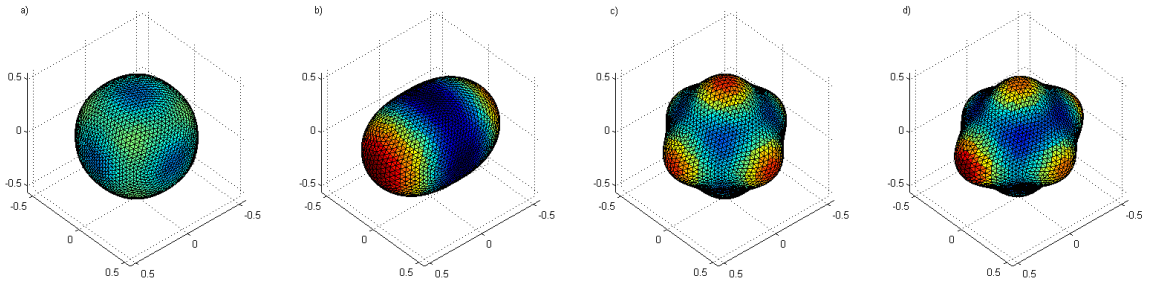

FIGURE 3 – Comparaison of the direction dependence of the Young modulus for two microstructures with the introduction of anisotropy : Kelvin cells (a,b) and PC (c,d) for a porosity of 0.4

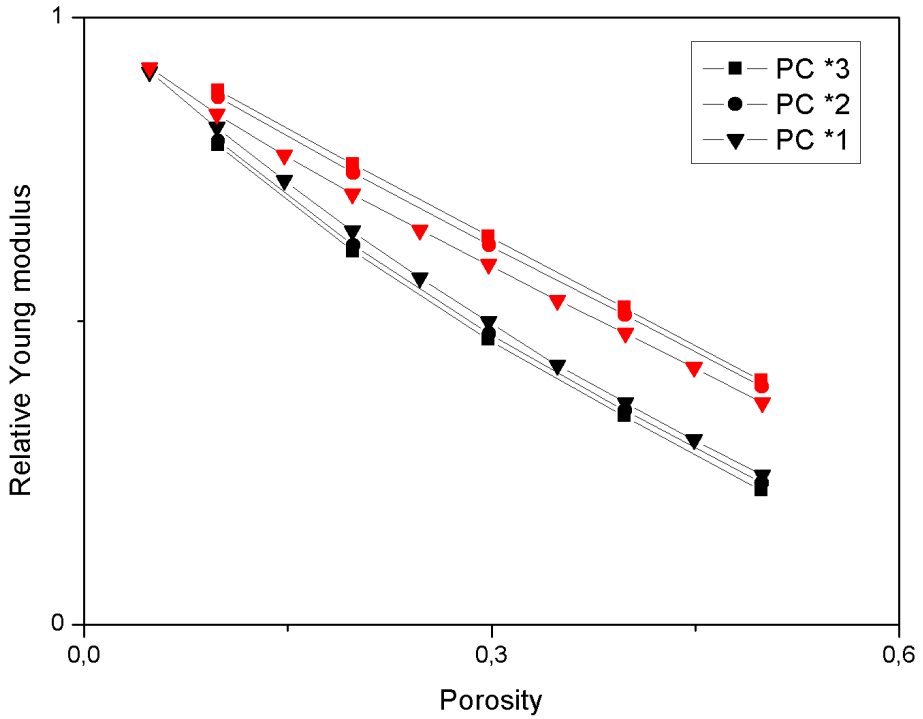

FIGURE 4 – Minimum and maximum Young modulus (direction-Dependant) for primitive cubic structures with different anisotropies

fabrication. A study of the effect of cell anisotropy on the elastic behavior has been conducted on the previously mentioned periodic structure : the same method was used with the introduction of an unidirectional shape coefficient by stretching the base microstructure accordingly. Those structural anisotropy clearly affected the elastic behavior of the models (fig 3) : the previously observed symmetries of both model and elastic behavior are not conserved : the equivalent material is strengthened in the anisotropic direction and weakened in the other. The introduced elastic anisotropy depend of both the original structure and the anisotropy coefficient used (fig 4).

The effect of cell anisotropy on the anisotropy of the cellular solid depends of the base microstructure :

for the ones studied, the microstructures showing a high base anisotropy are less affected. The base anisotropy direction can still be observed on the shaped microstructures.

Those results indicate that controlling cell anisotropy, at least for organized foam, may be useful for controlling their elastic behavior.

Previous studies, both experimental and theoretical, have shown that the elastics properties of foam are isotropic. Those studies were not about organized foam. The study of the effect of structural disorder on the anisotropy of the elastics properties, by introducing a controlled chaos in organized structure, is an interesting perspective.

3 Non linear behavior

Heterogeneous material can present two kind of linearity limits : the classical one due to material "plasticity", and a structural linearity limit due to geometrical parameter, like cell wall bending. Finite elements simulation allow to approach each limit separately.

3.1 Process

Detecting linearity limits is simple enough with the access to true strain and stress that finite element simulation allow. Any chosen stress set can be applied and the resulting linearity limit computed. Using enough distinct stress set allow for the construction of a yield surface.

Finite element simulation can output directly the point where any element in the studied material reach a non-linearity criteria, but this is not necessarily enough : due to the complex structure of the foam, this can happen in very localized points where it would have no effect on the global behavior of the material. What matter can also be the point where this non linearity begin to have an influence.

The standard protocol consist of first conducting the simulations with a purely elastic law, therefore computing the linearity due to the structure, before repeating with this time a more accurate law with a chosen non linearity criteria. The material of the studied foam had an hyperelastic behavior so and Ogden model is used, but the method can also be used with different criteria, like Von Mises for metallic foam.

A test on a full solid with a Mises plasticity criteria showed that this process can construct yield surface with a relative error of less than 10^{-7}.

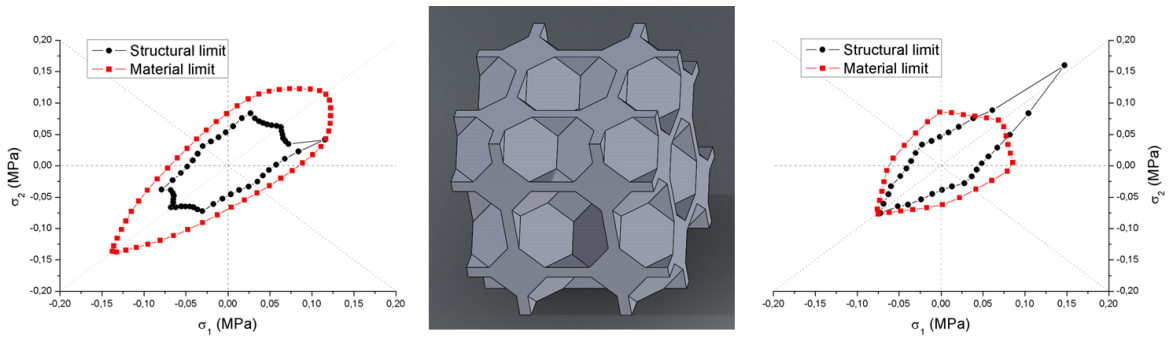

FIGURE 5 – yield surface for a Kelvin cells microstructure (center) under different load types : ϵ_3=0 (left) and σ_3=0 (right).

The finite element simulation realized here do not require a periodic microstructure. However, since the simulation is going out of linearity range, the quantity of cells required for the model to be representative

increase : previous study showed that for non linear behavior it can become large. The increase of both model size and simulation time means that computing power can become an issue and slow the use of this process.

Figure 5 was obtained for a Kelvin cells microstructure with porosity of 70% and considering walls material of 7 MPa as Young modulus and using a von Mises yield criterion of 1 MPa. Those results came from 3D simulation under two directional stresses (principal stresses proportionally applied). The third direction was either considered as free (figure 5 right) or blocked (figure 5 left). The linearity limits due to the structure and material nonlinearity have been computed for the two different conditions.

Since the microstructure has a cubic symmetry, equivalence between the axes was expected and found. The structure is totally geometrical and face thickness is constant. Non linearity due to the structure comes from the faces bending. Nonlinearities due to the material also depend on the structure because they first appear where stress concentrations can be found.

The differences between the two figures show that the nonlinearity due to the structure is dependent on hydrostatic pressure. Both material and structural limit behave differently in traction and compression and show a real weakness for mixed loading, especially when compressive load are added to tensile load.

Those results were obtained only for one specific microstructure and for specific direction due to high computation times, but construction of the whole yield surfaces are possible and nonlinear aspects for porous material can be understood in respect of the material used and the cell geometry. With this first example, it is particularly relevant that geometrical form of the cells is important in the determination of the yield limit.

4 Conclusion

A finite element method has been developed to determine complete stiffness tensor of polymer foam. Regarding typical crystallographic arrangement of voids, the PC structure presents the higher and the lower resistance depending on the directions of solicitations. Considerations of the morphology gave the reasons for that observation. From studies about anisotropic effect on the resultant stiffness, it appeared that elastic properties of foam can be well improved using elongated or stretched structures. A mean to reinforced mechanical properties in the elastic domain can thus be envisaged playing on the geometry of cells. At last, the nonlinear behavior of foams has been study, and further studies have been developed to determine whether the non-linearity aspect is due to the internal topology of the foam or because the wall's material has reached its yield limit.

Références

[1] S. Heitkam, W. Drenckhan, T. Titscher, D Weaire, D.C. Kreuter, D. Hajnal, Elastic properties of solid material with various arrangements of spherical voids, European Journal of Mechanics - A/Solids, 59 (2016), 252-264

[2] S. C. Cowin, M.M. Mehrabadi, Identification of the elastic symmetry of bone and other materials, Journal of Biomechanics, 22 (1989) 6/7, 503-515

[3] T. Iwakuma, S. Nemat-Nasser, Composite with periodic microstructure, Computers & Structures, 16 (1883), 13-19

[4] I. Cohen, Simple algebraic approximations for the effective elastic moduli of cubic arrays of spheres, Journal of the Mechanics and Physics of Solids, 52 (2004), 2167-2183

[5] L. J. Gibson, M. F. Ashby, Cellular solids structure and properties, Cambridge univ. press, 1997