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MECHANICAL PROPERTIES OF OPEN CELL FOAMS: SIMULATIONS BY LAGUERRE TESSELATION PROCEDURE

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Abstract. The Laguerre tessellation procedure is used for simulation of microstructures of open-cell foams. In contrast with the conventional Voronoii tessellation, the Laguerre one permits to simulate the foam microstructures with a given law of distribution of cell diameters. An original finite element method is developed for calculating the elastic properties: the ligaments are modelled as Timoshenko beams and each ligament is treated as one finite element. The size of the representative volume element for reliable calculations of the effective elastic properties is evaluated by computational experiments. Dependence of the properties on the cell size distributions and ligament shapes are analyzed.

Keywords: open-cell foams, representative volume element, random space tessellation, homogenization, effective elastic properties

1. Introduction. The microstructure of open-cell foams consists of a set of ligaments (random beam-like elements of the hard phase of the foam) connected in a number of nodes. One of the main objectives is predicting dependencies of the mechanical and physical properties on details of the microstructure. For simulation of elastic properties and fracture processes, the finite element method (FEM) has been widely used (Zhu *et al.* (2000), Roberts and Garboczi (2002)). The first step in application of this approach is constructing the foam skeleton using statistical models of the microstructure. As a rule, the Voronoii tessellation procedure is used to produce polyhedron cells inside a chosen representative volume element (RVE). The polyhedron edges are taken as ligaments axes and then, after definition of the shapes of the ligaments, FEM is applied to calculating stresses and strains in the ligaments for given boundary conditions on the RVE boundary. The effective elastic constants are obtained by averaging detailed strain and stress fields over the RVE. The detailed stress distribution in the ligaments provides an important information for simulation of the fracture processes.

An important problem in the framework of FEM is the proper choice of the RVE size. Usually, the number of cells inside RVE is restricted by the capacities of programs and computers. Standard FEM packages permit to consider RVE's containing about a hundred of cells. However, analyses (see, e.g., Kadashevich and Stoyan (2005)) show that the number of cells should be over a thousand.

Yet another problem is the simulation of foam microstructures with the given cell size distributions. It cannot be solved by Voronoii tessellation procedure. (It is impossible to define an initial set of seed points that produces Voronoi polyhedrons with prescribed cell size distribution.) Note that the effective properties of the foams, as well as fracture processes in, essentially depend on the said distribution. The present work focuses on the mentioned problems.

2. The Laguerre tessellation procedure. To construct foam skeletons with the given distribution of cell diameters, the Laguerre tessellation procedure is adopted. Firstly, a set of balls of random diameters $d^{(i)}$ with the distribution law coinciding with the actual cell size distribution is generated. Then, the balls are closely packed within the RVE. (In our study, the RVE V is taken as a cube of $2\times2\times2$ size). Thus generated set of ball centres $x^{(i)}$ and ball diameters $d^{(i)}$ is used for the Laguerre tessellation of the RVE into a set of polyhedrons. The Laguerre polyhedron corresponding to i-th ball consists of the points of this ball and points x of the RVE for which parameter $t=\left[|x^{(i)}-x|^2-(d^{(i)}/2)^2\right]^{1/2}$ is smaller than for any other ball center $x^{(j)}$ (Aurenhammer and Klein, 2000).

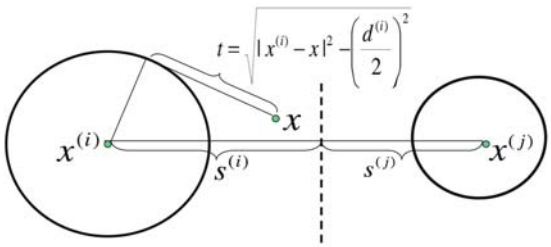

Figure 1. The border between two polyhedrons by the Laguerre tessellation procedure.

The common border of the Laguerre polyhedrons that correspond to two neighbouring balls i and j centred at points $x^{(i)}$ and $x^{(j)}$, is orthogonal to the interval (i,j) connecting the ball centres, and the border plane intersects this interval in proportion $s^{(i)}/s^{(j)}$ (see Fig.1),

$$\frac{s^{(i)}}{s^{(j)}}=\frac{4|x^{(i)}-x^{(j)}|^2+(d^{(i)})^2-(d^{(j)})^2}{4|x^{(i)}-x^{(j)}|^2+(d^{(j)})^2-(d^{(i)})^2}\,. \tag{1}$$

The dashed line in Fig.1 is the Laguerre polyhedron border that passes between the i-th and j-th neighbour balls. (In the Voronoi tessellation, this border passes at midpoint of interval (i,j).) It was shown, by Aurenhammer and Klein (2000) that all Laguerre polyhedrons are convex and span 3D-space. Finally, the law of cell

diameter distribution turns out to be close to the distribution of the initial ball diameters.

An example of the Laguerre tessellation of a cubic region containing two hundred cells is shown in Fig.2. For carrying out the tessellation, the algorithm of Tenemura *et al* (1983) was adopted. The histograms of cell diameter distributions for the tessellation shown in Fig.2 (left) are presented on the right in Fig.2.

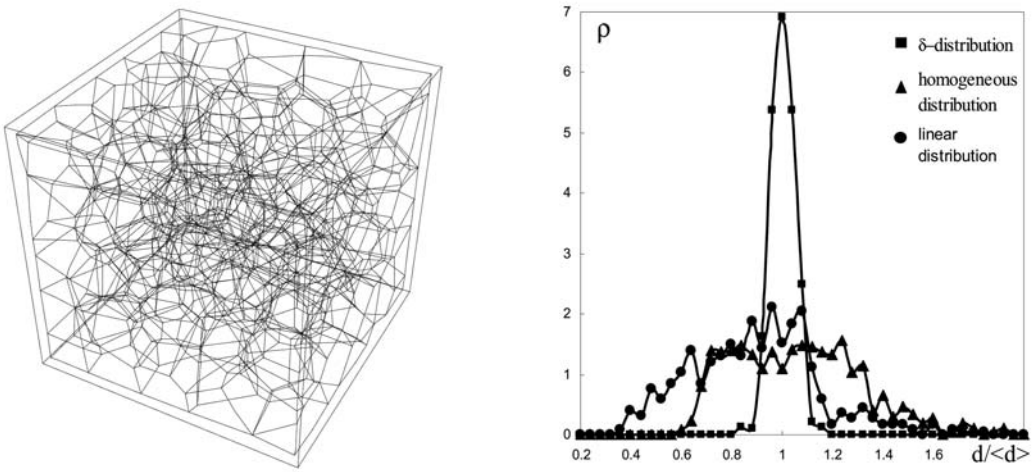

Figure 2. Laguerre tessellation of the cube (left) and some distributions of cell diameters after the tessellation (right)

Diameter d of a cell is calculated from equation $d = 2\sqrt[3]{3v/(4\pi)}$ where v is the volume of the cell. The line with black squares corresponds to the set of balls of approximately the same diameters, the line with triangles corresponds to homogeneous distribution of the diameters in interval $(0.5\langle d\rangle,\ 1.5\langle d\rangle)$, the line with circles – to linear distribution of the ball diameters in the interval $(0.3\langle d\rangle,\ 1.2\langle d\rangle)$. Here $\langle d\rangle$ is the mean value of the ball diameters.

2. Ligament form approximation and FEM. A cross-section of a typical ligament in open cell foams has a quasi-triangular form. We assume here that a ligament is a straight beam with cross sectional area described by the equations

$$\begin{aligned} y(x,\varphi) &= R(x)\left(\cos(\varphi) + a_1^{-1}\cos(2\varphi)\right), \\ z(x,\varphi) &= R(x)\left(-\sin(\varphi) + a_1^{-1}\sin(2\varphi)\right), \\ R(x) &= R(\xi(x)) = a_2\left(1 + a_3\xi(1-\xi)\right), \quad \xi = x/l. \end{aligned} \tag{2}$$

Here φ is angle parameter, $0 \leq \varphi < 2\pi$, (y, z) are Cartesian coordinates in the plane of the ligament cross-section, coordinate x is along the ligament axis. If parameter a_1 ($2 \leq a_1 < \infty$) is large, the ligament section is almost circular. For $a_1 = 2$ this section is a curved thriangle with the casp-like angles. Function $R(x)$ defines the axial form of the ligament that is thinner in the middle region than in the regions near the ends. Parameters a_1, a_2, a_3, and l define the overall shape of the ligament. The proposed approximation allows calculating the basic geometrical characteristics (section area, volume, moments of inertia) of the ligament in closed forms.

Simulation of the foam microstructure inside the RVE gives us the skeleton of the foam microstructure: the coordinates of the nodes and connections between them. The parameters of the ligaments are the other part of information necessary for performance of the FEM calculations. The version of the FEM developed in this work for calculation of elastic fields in the ligaments is based on a Timoshenko beam element. The material of the beams is isotropic with Young module E and Poisson ratio ν. Because the total elastic energy of the ligament described by Eqs.(2) is calculated in a close analytical form, every ligament is considered as a super element in this method. As a result, the FEM algorithm turns out to be very efficient and allows us to consider the RVE with several thousand of cells inside it.

For the FEM calculations, the boundary conditions on the surface Ω of the cubic RVE are taken in the following form. Let us define the components of displacement vector $u_i^{(k)}$ in all surface nodes $x^{(k)}$ ($x^{(k)} \subset \Omega$) by the equation

$$u_i^{(k)} = \varepsilon_{ij} x_j^{(k)}, \tag{3}$$

where ε_{ij} is a fixed symmetric tensor. All angles of rotation at the surface nodes are assumed to be equal to zero. These conditions are sufficient to obtain a unique solution of the elasticity problem and calculate stresses and strains in all the ligaments.

The effective elastic module tensor C_* of the foam material connects the mean values of the stress $\langle \sigma_{ij} \rangle$ and strain $\langle \varepsilon_{ij} \rangle$ tensors over the RVE

$$\left\langle \sigma_{ij} \right\rangle = C_{*ijkl} \left\langle \varepsilon_{kl} \right\rangle, \quad \left\langle \sigma_{ij} \right\rangle = \frac{1}{V} \int_V \sigma_{ij} dv, \quad \left\langle \varepsilon_{ij} \right\rangle = \frac{1}{V} \int_V \varepsilon_{ij} dv. \tag{4}$$

Let us consider a volume of the equivalent homogeneous material that coincides with the RVE and is loaded with forces $f_j(x)=n_k(x)\sigma_{kj}(x)$ on its surface Ω. Here n_k is the external normal to Ω. The volume integral (4) for $\langle\sigma_{ij}\rangle$ may be transformed into a surface integral using the Gauss theorem, and in the case of the beam structure, the mean stress tensor inside the cubic RVE may be calculated as follows

$$\left\langle \sigma_{ij} \right\rangle = \frac{1}{8} \sum_{x^{(k)} \in \Omega} F_j^{(k)} x_i^{(k)} , \tag{5}$$

where $F_j^{(k)}$ is the vector of the concentrated force acting in surface node $x^{(k)}$. It is taken into account that the volume of cube V is equal to 8. For the affine surface deformation (3), the mean strain tensor $\langle\varepsilon_{ij}\rangle$ defined in Eq.(4) coincides with tensor ε_{ij} in boundary conditions (3). Thus, using Eqs.(4) and (5) one can calculate the components of tensor C_{*ijkl} if forces $F_j^{(k)}$ in the surface nodes are obtained from the solution of the elasticity problem for the considered foam structure.

3. Numerical results. Let discuss the problem of appropriate size of RVE. In series of numerical experiments, the balls with a small scatter in diameters were packed inside the RVE, and the Laguerre tessellation was used to generate foam microstructures, as described in section 1. Circular cylindrical ligaments with parameters a_1=100, a_3=0 were considered. Parameter a_2 depends on the volume concentration of the hard phase. We increased the number of cells inside the RVE from one hundred to fifteen hundreds. For the calculation of the effective elastic modulus E_*, extensions of the RVE in three orthogonal directions were performed, and three independent shear deformations were applied to the RVE surface for calculation of μ_*. Anisotropy of the effective modules with respect to tension and shear deformations was evaluated by parameter α, and variation of the effective Young module by coefficient β:

$$\alpha = 2\mu_* E_*^{-1}(1+\nu_*), \quad \beta = E_*^{-1}\sqrt{\left\langle (E_* - \langle E_* \rangle)^2 \right\rangle} . \tag{6}$$

Here, effective moduli E_*, μ_* and ν_* are obtained from independent affine deformation of the RVE and coefficient α is equal to 1 if the foam structure is isotropic. The average in (6) is taken over three different directions and over realizations of random microstructures for a fixed number of cells inside the RVE.

In Fig.3, the dependencies of the reduced effective Young E_R and shear μ_R moduli on the number of cells (N) inside the RVE are presented. The reduced moduli are defined by the equations

$$E_R = E_* E^{-1} p^2, \quad \mu_R = \mu_* \mu^{-1} p^2, \quad p = \rho_* \rho^{-1}. \tag{7}$$

Here ρ is the density of the foam hard phase, ρ_* is the density of the foam, p is the volume concentration of the hard phase. The graphs in Fig.3 correspond to the volume concentration of the hard phase p=0.01.

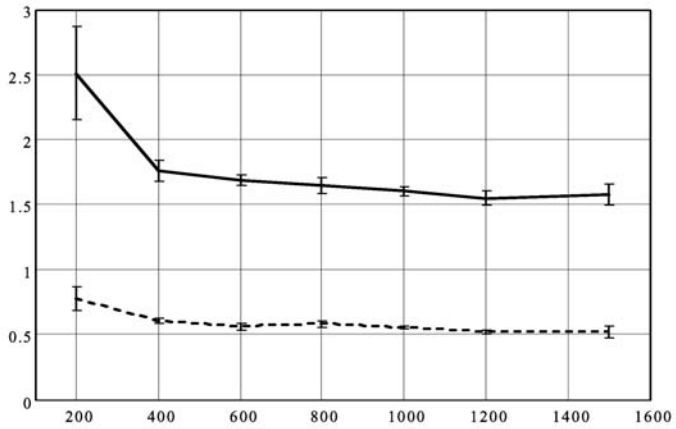

Figure 3. The dependencies of reduced Young E_R and shear μ_R moduli on number N of cells in the RVE for the volume concentration of the hard phase p=0.01.

Dependencies of anisotropy coefficient α and dispersion coefficient β on number N of cells in the RVE are shown in Fig.4 for p=0.01. Vertical bars show the dispersion among realizations of the microstructures with fixed values of cell number N. For every value of N, 5-7 realizations of the random structures were taken.

The main conclusion is that RVE should contain about 900-1000 cells in order to obtain reliable values of the effective elastic properties. If the number of cells inside the RVE is smaller, the dispersion of the effective elastic constants for different realizations of the foam microstructures increases (Fig.4). We emphasize that the mean value of these constants over the realizations does not coincide with the mean values of the constants for the RVE with sufficiently large number of the cells. Similar observation was made by Kanit *et al*. (2002), where the problem of the size of the RVE for random polycrystalline materials was considered.

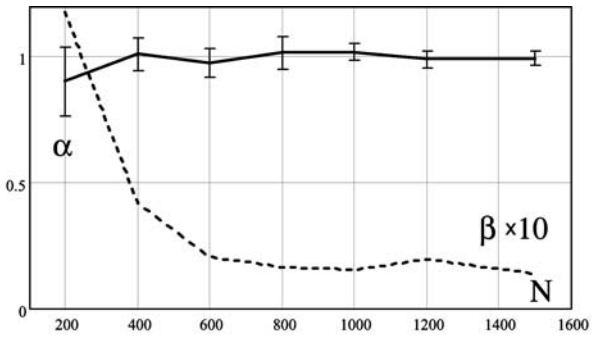

Figure 4. The dependence of parameters α and β of isotropy on number of cells in the RVE, p=0.01.

Dependencies of the normalized modulus E_*/E on the distribution of cell diameters in RVE and volume fraction p of the hard phase are shown in Fig.5

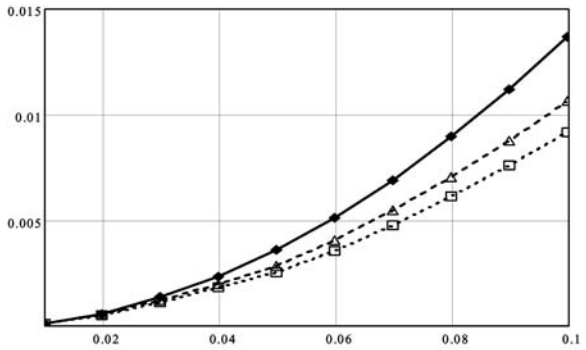

Figure 5. The dependences of relative effective Young module (E_*/E) on the law of distribution of the cell diameters and volume concentration p of the hard phase for the foams with circular cylindrical ligaments.

In this figure, the line with black rhombs corresponds to foams with almost equal diameters of the cells (the distribution function of the cell diameters is presented in Fig.2 by a line with black rhombs as well), the line with triangles corresponds to the homogeneous distribution of cell diameters in the interval ($0.5\langle d\rangle$,$1.5\langle d\rangle$) and the line with squares correspond to the linear distribution of cell diameters in the interval ($0.3\langle d\rangle$,$1.2\langle d\rangle$) (the corresponding distribution functions are shown in Fig.2). It is seen that the foams with a wide distribution of cell diameters have lower elastic moduli than foams with approximately identical diameters.

4. Conclusions. The size of the RVE is a key problem for numerical simulations. We estimated that the minimal number N of cells inside the RVE that ensures reliable values of the effective elastic constants depends on volume fraction p of the hard phase. At small volume fractions (p=0.01), the number is about 900-1000 and decreases as p increases, to 800 for p=0.05 and 400 for p=0.1. The Laguerre tessellation allows simulations for any prescribed cell size distribution law. But this procedure is more complex than the Voronoii tessellation.

We note the effect of the cell diameter distributions on the overall elastic properties. For foams with wide distribution of diameters, Young's modulus is smaller, as compared with the case of approximately equal cell sizes and the difference grows with volume fraction p of the hard phase. Also, foams with the linear distribution of cell diameters have lower Young's moduli that foams with homogeneous cell diameters distribution, at the same volume fraction p.

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