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EFFECTIVE CHARACTERISTICS OF POROUS MEDIA AS A FUNCTION OF POROSITY LEVEL

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Abstract:

A combined approach is worked out, based on the two-scale asymptotic analysis and periodic boundary integral equation method, allowing us to analyze homogenized effective characteristics of porous media containing closed dispersed pores displaced at nodes of the regular spatial lattices. The presented numerical results are concerned with an initially isotropic medium containing spherical pores displaced at nodes of the FCC lattice.

1 Introduction

In the present paper an approach developed in [1-3] is modified in such a way, that it can be suitable for analyzing porous media containing uniformly distributed closed pores from zero to high porosity levels. Generally, such a medium has random distribution of pores. However, for modeling purposes we will use a deterministic approach based on choosing one or several interfering spatial lattices, nodes of which contain pores of different size, shape, and orientation; see Fig.1, where a medium containing two different lattices is presented.

Fig. 1.

Presumably, the best suited for modeling dispersed composites or porous media with the uniform distribution of inclusions or voids, is the Face Centered Cubic (FCC) lattice; see Fig.2. This lattice is not only the closest packed, but it also leads to the minimum induced anisotropy comparing with the Simple Cubic (SC) and Body Centered Cubic arrays; see [4 - 6] for discussions.

Fig. 2.

In deriving basic equations it is assumed that the medium is elastic and anisotropic, and that no restrictions on the specific kind of anisotropy is imposed. However, numerical computations are implemented for an isotropic medium with spherical pores. The other assumption concerns the displacement field, which is supposed to be infinitesimal, so equations of the linear theory of elasticity can be applied.

The main problem for a porous medium with uniformly distributed pores is in its effective characteristic determination; in the case of elasticity it means determination of the effective (or averaged) components for the elasticity tensor. Along with this main problem several others can be solved in parallel, namely determination of level of microstructural stresses in a matrix material, these are highly oscillating stresses, which may have high magnitude and can initiate volume fracture. The other problem is determination of scattering cross sections by pores, this is related to the ratio of the energy scattered by inclusions or pores to the incident wave energy. The latter problem is interesting due its direct connection to non-destructive testing of porous materials.

The closest solutions in mechanics of heterogeneous media, including porous media can be obtained by applying the two-scale asymptotic analysis [7 - 11]. In this method it is assumed that two fields exist: (i) the global field, which is described by “slow” variables; and, (ii) a local field, having high oscillations, which is described by “fast” variables. Application of the two-scale asymptotic analysis to the problem stated above will be considered in a more detail later on.

In the two-scale asymptotic method the effective elasticity tensor related to the porous medium can be represented by the following expression

$$\mathbf{C}_0 = f\,\mathbf{C} + \mathbf{K}, \tag{1.1}$$

where $\mathbf{C}_0$ is the effective (homogenized) elasticity tensor, f is the volume fraction of the pores, $\mathbf{C}$ is the elasticity tensor of the material without pores (matrix), and $\mathbf{K}$ is a correcting tensor, or “corrector”. It is clear from Eq. (1.1), that the main difficulty in determination of the effective elasticity tensor is in finding the corrector.

Determination of the corrector in the two-scale asymptotic method demands the solution of the cell problem, which in turn consists of (i) setting up a boundary-value problem on the internal boundaries between pore(s) and the matrix material in a cell; and, (ii) formulating a periodic boundary-value problem on the outer boundary of a cell. The latter one is of the non-classical type in the sense that it is formulated on the boundary, which due to periodicity must have angular points and edges.

Along with FEM and finite differences methods, the following other methods for obtaining the solution to the cell problem are known. In [12 - 14], methods based on the Eshelby’s transformation strain were applied to analyses of isotropic media with ellipsoidal inclusions. The advantage of these methods resides in their principle possibility to analyze media with anisotropic components, while from the computational point of view these methods are not very convenient since they lead to the three-dimensional integral equations with weakly singular kernels, and the problem reduces to the solution of the ill-posed problem for the integral equations of the first order.

In [15, 16], media with isotropic components were studied by applying a method based on the periodic fundamental solution for an elastic medium, which originally was constructed in [17]. Because of multipolar expansions used for solving the inner boundary value problem this method is confined to inclusions of spherical form. A similar approach was also used for analyzing dispersed composites with isotropic components, but it was based on the Galerkin technique for solution of the inner boundary value problem [18].

Periodic fundamental solutions for media with arbitrary anisotropy were developed in [2]. In combination with the boundary integral equation method (BIEM) these fundamental solutions were applied to solution of the cell problem for composites with anisotropic inhomogeneities and porous media in [1, 3], analysis of microstructural stresses in the matrix material was considered in [20]. Problems of wave scattering by pores were studied in [21] by application of the same method. Some of obvious advantages of this method are due to potential possibility to reduce the solution of the inner boundary-value problem to summation of the rapidly convergent series, while periodic boundary conditions on the outer boundary are satisfied automatically due to periodicity of the fundamental solution.

The following analysis is targeted to obtaining homogenized values for both Lamé constants of a porous medium, containing spherical pores displaced at the nodes of the FCC spatial lattice. The analysis is carried out for all admissible porous ratios $f \in [0; f_{\lim})$, where $f_{\lim} \approx 0.74$ is the highest porosity for spherical pores displaced at the nodes of the FCC-lattice.

2 Basic notations

The equations of equilibrium for a homogeneous anisotropic medium can be written in the form:

$$\mathbf{A}(\partial_x)\mathbf{u} = -\operatorname{div}_x \mathbf{C} \cdot\cdot \nabla_x \mathbf{u} = 0, \tag{2.1}$$

where $\mathbf{u}$ is a displacement field. It is assumed that the elasticity tensor $\mathbf{C}$ satisfies the following condition of positive definiteness:

$$\mathbf{S}\cdot\cdot\mathbf{C}\cdot\cdot\mathbf{S} > 0, \qquad \underset{\mathbf{S}\in R^3\otimes R^3,\ \mathbf{S}\neq 0}{\forall \mathbf{S}}, \tag{2.2}$$

which is generally adopted for problems of mechanics of inhomogeneous media.

Let $\mathbf{E}$ denotes the fundamental solution of Eq. (2.1). The fundamental solution must satisfy the following equation:

$$\mathbf{A}(\partial_x)\cdot\mathbf{E}(\mathbf{x}-\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y})\mathbf{I}, \tag{2.3}$$

where $\mathbf{I}$ stands for the identity matrix.

Applying the Fourier transform to Eq. (2.1), gives the symbol of the operator $\mathbf{A}$:

$$\mathbf{A}^{\wedge}(\xi) = (2\pi)^2\,\xi\cdot\mathbf{C}\cdot\xi, \qquad \xi\in R^3. \tag{2.4}$$

Similarly, applying the Fourier transform to Eq. (2.3) yields

$$\mathbf{A}^{\wedge}(\xi)\cdot\mathbf{E}^{\wedge}(\xi) = \mathbf{I}, \qquad \xi\in R^3. \tag{2.5}$$

Combining Eqs. (2.4) and (2.5) we obtain:

$$\mathbf{E}^{\wedge}(\xi) = \mathbf{A}^{\wedge}(\xi)^{-1}. \tag{2.6}$$

Proposition 2.1. a) Symbol $\mathbf{A}^{\wedge}(\xi)$ is positive definite at any $\xi\neq 0$; b) Symbol $\mathbf{E}^{\wedge}(\xi)$ is positive definite at any $\xi\neq 0$; c) Symbol $\mathbf{A}^{\wedge}(\xi)$ is positive homogeneous of degree 2 with respect to ξ; d) Symbol $\mathbf{E}^{\wedge}(\xi)$ is positive homogeneous of degree –2 with respect to ξ.

Proof. a) Flows out from positive definiteness condition (2.2) for the elasticity tensor. Indeed, taking $\mathbf{S} = \mathrm{sym}(\mathbf{a}\otimes\xi)$, $\mathbf{a}\in R^3$, $\mathbf{a}\neq 0$ in (2.2) and taking into consideration (2.4), we arrive at the desired positive definiteness of the symbol $\mathbf{A}^{\wedge}(\xi)$. Proof b) relies on symmetry and positive definiteness of the symbol $\mathbf{A}^{\wedge}(\xi)$, that gives

$$\mathbf{a}\cdot\mathbf{A}^{\wedge 1/2}\cdot\mathbf{E}^{\wedge}\cdot\mathbf{A}^{\wedge 1/2}\cdot\mathbf{a}=|\mathbf{a}|^2>0, \qquad \underset{\mathbf{a}\in R^3,\ \mathbf{a}\neq 0}{\forall\mathbf{a}}, \tag{2.7}$$

and since $\mathbf{a}\cdot\mathbf{A}^{\wedge 1/2}$ spans the whole R^3 space, inequality (2.6) completes the proof. Proofs of conditions c) and d) are obvious.

Corollary. Symbol $\mathbf{E}^{\wedge}$ is real analytical everywhere in $R^3\setminus 0$.

Remark 2.1. While symbol of the fundamental solution is defined by a simple analytical expression (2.6), its Fourier inverse in a closed form is known only for some specific kinds of elastic anisotropy; see [22] for discussing methods of constructing fundamental solutions for media with arbitrary anisotropy. As will be shown in the next section, constructing the spatially periodic fundamental solution does not need constructing non-periodic fundamental solution.

3 Constructing spatially periodic fundamental solutions

Consider a homogeneous anisotropic medium, loaded by the periodically distributed force singularities, located in nodes $\mathbf{m}$ of a spatial lattice Λ.

Let $\mathbf{a}_i$, $(i=1,2,3)$ be linearly independent vectors of the main periods of the lattice, so that each of the nodes in R^3 can be represented in the form:

$$\mathbf{m}=\sum_i m_i\mathbf{a}_i\,, \tag{3.1}$$

where $m_i\in Z$ are the integer-valued coordinates of the node m in the basis $(\mathbf{a}_i)$.

Remark 3.1. Not all of the spatial lattices can be represented in the form (3.1). An example of the hexagonal lattice in R^2 (Fig. 3), shows that representation (3.1) is not sufficient for describing all the nodes. In such cases, two or more different lattices admitting representation (3.1), should be considered. For the considered plane hexagonal lattice four embedded rectangular lattices should be introduced.

Fig. 3. Plane hexagonal lattice

The adjoint basis $(\mathbf{a}_i{*})$ is introduced in such a manner that $\mathbf{a}_i{*}\cdot\mathbf{m} = m_i$. Thus, vectors of the adjoint basis are orthogonal to the corresponding vectors of the initial basis $(\mathbf{a}_i)$. The lattice corresponding to the adjoint basis will be denoted by $\Lambda *$.

Now, the periodic delta-function corresponding to the singularities located at the nodes of the lattice Λ can be represented the form:

$$\delta_p(\mathbf{x}) = V_Q^{-1} \sum_{\mathbf{m}^* \in \Lambda^*} \exp(-2\pi i \mathbf{x} \cdot \mathbf{m}^*)\,, \tag{3.2}$$

where V_Q is the volume of the fundamental region (cell) Q. Formula (3.2) defines the periodic delta-function uniquely.

Remark 3.2. Formula (3.2) is the generalization to the 3-dimensional case of the well-known decomposition of the one-dimensional periodic δ-function, into Fourier series; see [23].

Substitution of the periodic fundamental solution $\mathbf{E}_p$ into Eq. (2.1) must yield

$$\mathbf{A}(\partial_{\mathbf{x}})\mathbf{E}_p(\mathbf{x}) = \delta_p(\mathbf{x})\mathbf{I}\,, \tag{3.3}$$

where $\mathbf{I}$ is the identity matrix. Looking for $\mathbf{E}_p$ also in the form of harmonic series, taking into account representation (3.2), and comparing coefficients at the exponential terms in (3.3) from both left and right, we arrive at

$$\mathbf{E}_p(\mathbf{x}) = V_Q^{-1} \sum_{\mathbf{m}^* \in \Lambda_0^*} \mathbf{E}^\wedge(\mathbf{m}^*) \exp(-2\pi i \mathbf{x} \cdot \mathbf{m}^*), \tag{3.4}$$

where $\Lambda_0{}^*$ is the adjoint lattice without the zero node. It should be noted that Eq. (3.4) defines the periodic fundamental solution up to an additive (tensorial) constant, that is because any constant tensorial value vanishes at substituting into initial Eq. (2.1).

Lemma 1. The series on the right side of Eq. (3.4) is convergent in the L^1-topology, defining the fundamental solution of the class $\overline{L}^1(Q,\ R^3 \otimes R^3)$, where $\overline{L}^1$ is a class of integrable in Q functions with the zero-mean value.

Proof of the lemma can be found in [2].

4 Effective elasticity tensor

For clarity and simplicity it will be assumed that the considered medium has the only one kind of uniformly distributed voids placed in the nodes of spatial lattice Λ. A region occupied by an individual void in a cell Q will be denoted by Ω.

The two-scale asymptotic analyses being applied to such a medium produces the following expression for the corrector [3]:

$$\mathbf{K} = -V_Q^{-1} \int_{\partial\Omega} \mathbf{C} \cdot\cdot (\nu_{\mathbf{Y}} \otimes \mathbf{H}(\mathbf{Y})) dY, \tag{4.1}$$

where Y are the “fast” variables, $\mathbf{H}$ is the third-order tensor field. This tensor field is the solution of the following boundary value problem:

$$\begin{aligned} &\mathbf{A}(\partial_Y)\mathbf{H}(\mathbf{Y}) = 0,\ \mathbf{Y} \in Q \setminus \Omega \\ &\mathbf{T}(\nu_Y, \partial_Y)\mathbf{H}(\mathbf{Y})\ \big|_{\partial\Omega} = -\nu_Y \cdot \mathbf{C} \end{aligned} \cdot \tag{4.2}$$

In Eqs. (4.1) and (4.2) ν_Y represents field of the external unit normal to the boundary $\partial\Omega$, and the elasticity tensor $\mathbf{C}$ is referred to the matrix material.

Lemma 2. Boundary-value problem (4.2) admits the unique solution.

Proof of the lemma can be found in [3].

Remark. Supposition that the tensor $\mathbf{C}$ in Eq. (4.2) is not strong elliptic, violates proof of Lemma 2.

Now, the solution of the boundary value problem (4.2) for the third-order tensor traction field $-\nu_Y \cdot \mathbf{C}$ can be constructed by applying the boundary integral equation method, giving the following representation for the desired solution [3]:

$$\left(\tfrac{1}{2}\mathbf{I} + \mathbf{S}\right)\mathbf{H}(\mathbf{Y}') = \mathbf{H}_c \ \ \mathbf{Y}' \in \partial\Omega, \tag{4.3}$$

where $\mathbf{H}_c$ is a constant tensor, and $\mathbf{S}$ is the singular integral operator resulting from a restriction of the double-layer potential on the surface $\partial\Omega$. Some of the relevant properties of operator $\mathbf{S}$ are discussed in [22].

Substituting Eq. (3.4) for the periodic fundamental solution into expression for the operator $\mathbf{S}$ allows us to obtain a lower (on energy) bound for the corrector; i.e.

$$\mathbf{K} = -8\pi^2 V_Q^{-2} \sum_{\mathbf{m}^* \in \Lambda_0^*} \left(\chi\,\hat{}_\Omega\,(\mathbf{m}^*)\right)^2 \mathbf{C} \cdot\cdot\, \mathbf{m}^* \otimes \mathbf{E}\,\hat{}\,(\mathbf{m}^*) \otimes \mathbf{m}^* \cdot\cdot\, \mathbf{C} \tag{4.4}$$

where $\chi\,\hat{}_\Omega$ is the Fourier image of the characteristic function of the region Ω. An expression for the upper bound can be obtained similarly [3].

Theorem. The series appearing on the right side of Eq. (4.4) is absolutely convergent, provided Ω is a proper open region in Q.

Proof of the theorem can be found in [3]

5 Effective characteristics for porous medium with isotropic matrix and spherical pores displaced at the nodes of the *FCC*-lattice

The elasticity tensor for an isotropic matrix material has the following components (in Voigt's six-dimensional matrix notation):

$$\begin{aligned} &c^{11} = c^{22} = c^{33} = \lambda + 2\mu \\ &c^{12} = c^{23} = c^{31} = \lambda \\ &c^{44} = c^{55} = c^{66} = \mu \end{aligned} \quad , \tag{5.1}$$

where λ and μ are Lamé constants, satisfying the following condition, which ensures positive definiteness of the elasticity tensor

$$3\lambda + 2\mu > 0, \quad \mu > 0 \tag{5.2}$$

Substituting elasticity tensor (5.1) into expression (4.4), and taking into account that for the unit ball $\Omega \subset R^3$, the Fourier image of the corresponding characteristic function χ_Ω has the form

$$\chi_\Omega^\wedge(\xi) = \frac{1}{\pi|\xi|^2}\left(\frac{\sin(2\pi|\xi|)}{2\pi|\xi|} - \cos(2\pi|\xi|)\right), \tag{5.3}$$

we arrive at the expression (4.4) for the lower bound for the corrector, where for an isotropic medium the symbol of the fundamental solution takes the form [2, 3]:

$$\mathbf{E}^\wedge(\xi) = \frac{1}{\left(2\pi|\xi|\right)^2 \mu}\left(\mathbf{I} - \frac{\lambda+\mu}{\lambda+2\mu}\frac{\xi\otimes\xi}{|\xi|^2}\right). \tag{5.4}$$

Performing summation in the right-hand side of (4.4), and using expression (1.1) for the homogenized elasticity tensor, we get homogenized (non-dimensional) Lamé's constants for the porous medium.

In Fig. 4 the dependence of the homogenized Poisson's ratio on number of the retained nodes at summation in (4.4), is presented. Actually, the number of nodes in Fig. 4 corresponds to n^3. The plotted curves are obtained for the zero value of Poisson's ratio of the matrix material and $E=1$, where E stands for Young's modulus.

Fig. 4. Dependence of the homogenized Poisson's ratio on number (n^3) of nodes and the porosity level *f*.

The plots for variation of both Lamé's constants are presented in Fig. 5. The curves in these plots correspond to the porous media with different values for Poisson's ratio ν of the matrix material, and $E=1$.

Fig. 5. Dependence of Lamé's constants on the porosity level: a) λ; b) μ;
1) ν = -0.8; 2) ν = -0.6; 3) ν = -0.4; 4) ν = -0.2; 5) ν = 0; 6) ν = 0.2; 7) ν = 0.4;

As these graphs show, despite the initial Poisson's ratio of the matrix material, there is a tendency to vanish for both Lamé's constants at the high porosity level.

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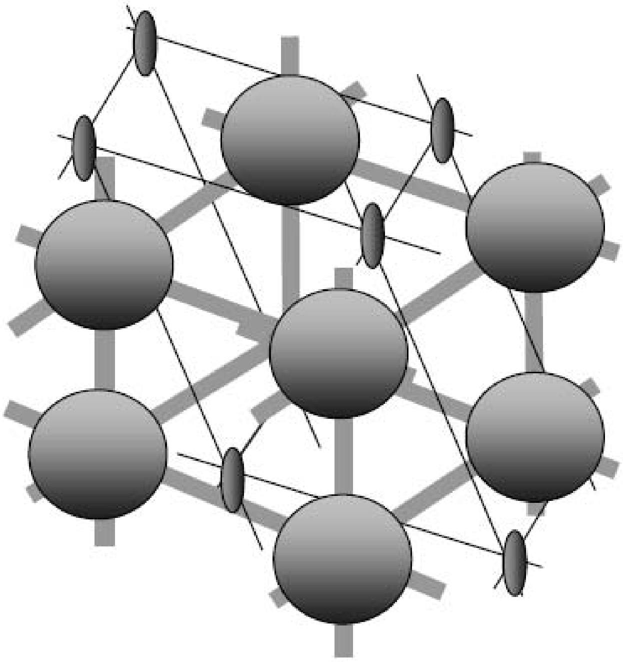

Figure 1. Different spatial lattices

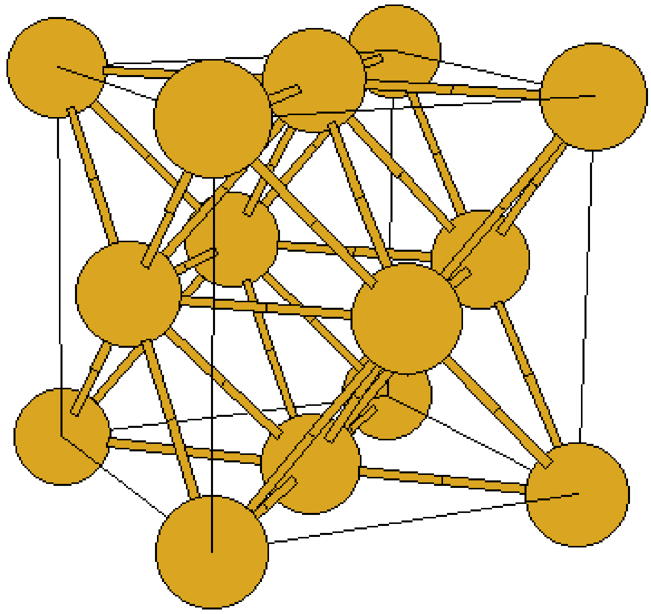

Figure 2. FCC lattice

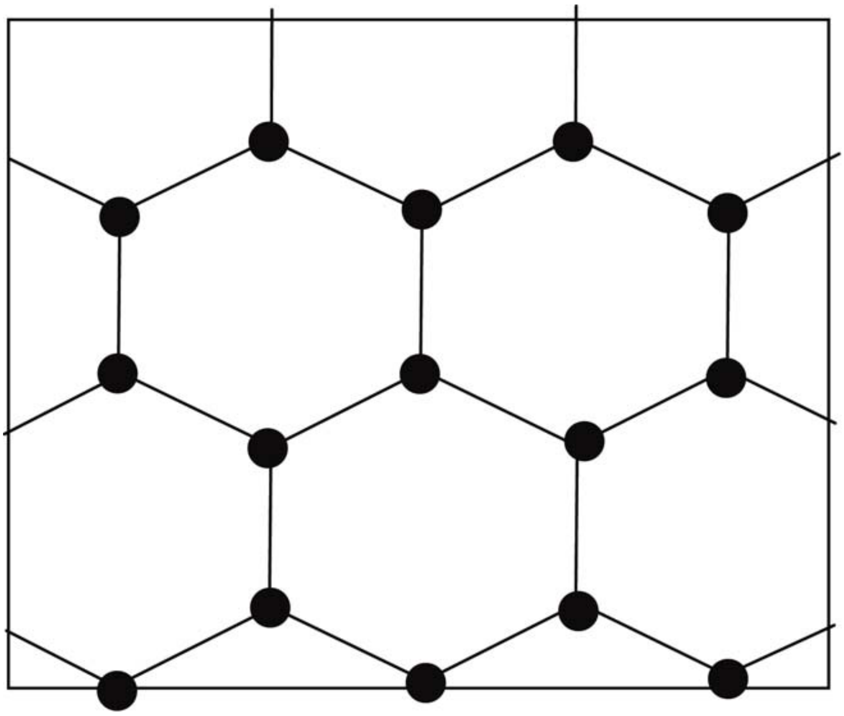

Figure 3. Plane hexagonal lattice

F

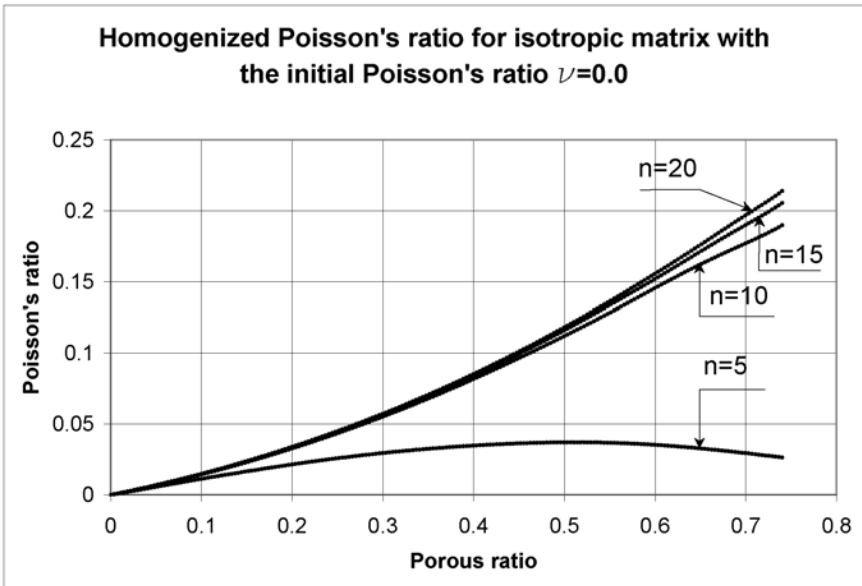

Figure 4. Dependence of the homogenized Poisson's ratio for FCC-lattice on number (n^3) of nodes and the porosity level f .

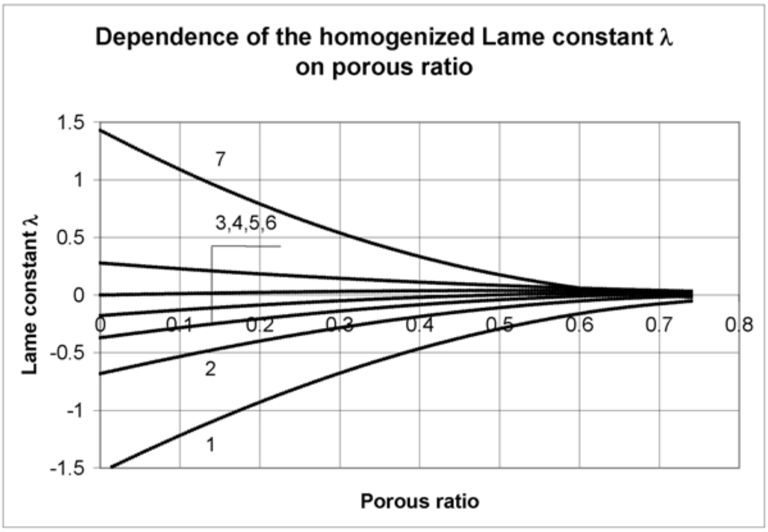
Dependence of the homogenized Lame constant λ
on porous ratio
Lame constant λ
Porous ratio
1.5
1
0.5
0
-0.5
-1
-1.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
7
3,4,5,6
2
1

Figure 5. a

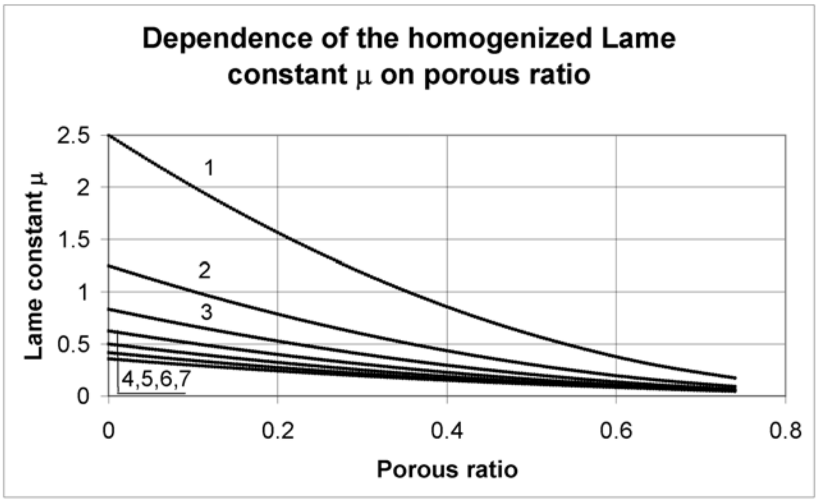

Figure 5 b

Dependence of Lamé's constants on the porosity level: a) λ; b) μ;
1) $\nu = -0.8$; 2) $\nu = -0.6$; 3) $\nu = -0.4$; 4) $\nu = -0.2$; 5) $\nu = 0$; 6) $\nu = 0.2$; 7) $\nu = 0.4$;