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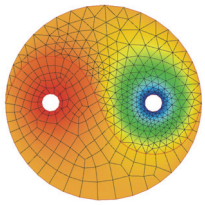

MODELING STRUCTURES OF CELLULAR MATERIALS FOR APPLICATION AT VARIOUS LENGTH-SCALES

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Abstract

The paper presents the spectrum of methods and results for design of structures, which are frequently applied in numerical simulations of properties and processes taking place in cellular materials. The methods described here are universal for many applications at various length-scales. They can be efficiently applied for complex cellular structures such as polycrystals or foams, where the elements (grains or pores) are distributed and shaped in a controlled way. The digital material representations created by these methods can be used for a number of numerical techniques such as: Molecular dynamics (MD), Monte Carlo (MC), Cellular Automaton (CA), Finite Element Method (FEM) or Finite Volume Method (FVM). The examples of structures consisting of atoms, fields or finite elements are presented in this paper. The applications of such structures are demonstrated by the properties and processes relevant to the specific length scales.

Key words: nanomaterials, multiscale modeling, interface, polycrystals, digital material representation

1. INTRODUCTION

Most engineering materials have a polycrystalline structure. The design and manufacture of such materials can be successfully facilitated through novel numerical simulation techniques.

Properties of materials, strictly related to their structure, can be generally shaped by modification of two features: chemical composition and structure. Some of the properties are mostly related with chemical composition (i.e., density, Young modulus) and some can be successfully improved by modification of the structure (i.e., yield stress) (Bazarnik et al., 2012; Lewandowska & Kurzydlowski, 2008). Additionally, for some applications the chemical composition is generally defined and the only change can be realized by modifying the structure. This is especially true for light-weight materials where the relative strength (strength/density) is of key importance (Chrominski et al., 2013; Lewandowska & Kurzydlowski, 2009).

Properties of materials are very often related with the processes induced in the structure by external forces (i.e., plasticity or thermal stability) (Dobosz et al., 2009; Lewandowska et al., 2008). Whereas some properties and processes can be identified and described at the atomic level (Zhang et al., 2005; Bachurin & Gumbsch, 2010), others require micro or macro-scale approaches (Wejrzanowski & Kurzydlowski, 2005; Mazdziarz et al., 2010).

All simulations focused on cellular materials require an initial structure with features that can be defined and controlled. Polycrystalline materials are characterized by the size and shape distribution of

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grains (Wejrzanowski et al., 2010). Since grain boundaries play an important role in polycrystalline materials (especially nanomaterials) (Sauvage et al., 2012), distribution of grain orientation which results in distribution of grain boundary misorientation should be defined. Another feature is the spatial arrangement of grains in space defining the level of anisotropy or inhomogeneity.

Several methods for the creation of cellular structures have been proposed in the literature. These methods can be divided into three groups. The first group is based on the geometrical construction of structure (Lautensack & Sych, 2006; Redenbach, 2009; Wejrzanowski et al., 2013). The second involves simulation of real processes such as nucleation and growth (Cybulka et al., 2007; Madej et al., 2013; Sieradzki & Madej, 2013). The last one is devoted to numerical reconstruction of cellular structure by image processing methods (Ludwiga et al., 2009; Bhandari et al., 2007; Saadatfar et al., 2004).

Since the key issue for all of the structural models is to represent the geometry of real material, the manner of creation is less important than the final result. In this paper we propose methods for designing cellular structures with defined distribution of size and orientation of grains/cells.

The example structures present the applicability of the proposed method to the modeling of isotropic and homogenous polycrystals at various scales.

2. METHODS

The algorithm for modeling polycrystalline structures to be employed in simulations with different methods relevant to the given scale is presented in figure 1.

In the first step of the proposed algorithm the set of spheres is generated. Each sphere is defined by its position in 3d space and its radius. They are placed in a relatively big box with a condition of no overlapping (see figure 2a). Each direction of the box can be defined as periodic or non-periodic.

In the computations various distributions of sphere sizes can be adopted. The log-normal distribution of volume with the pre-selected average value, E(V) and the variation coefficient, CV(V), was used for example structures presented here (see figure 2b).

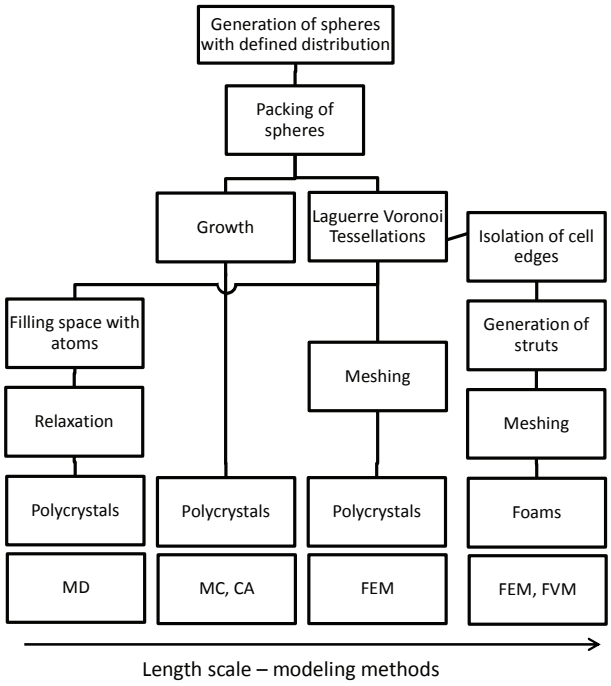
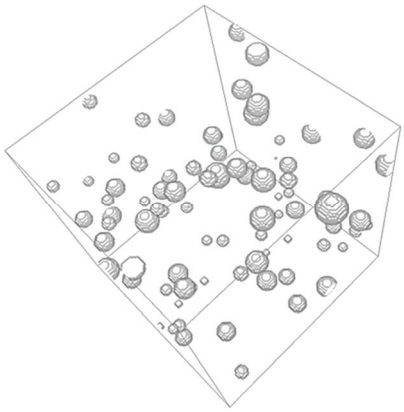
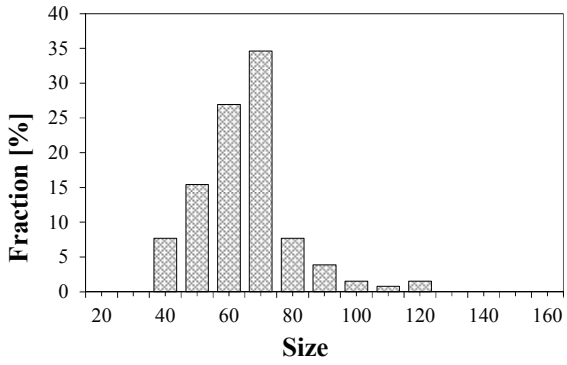


Fig. 1. *Schematic illustration of procedures for modeling polycrystalline and foam structures.*



a)



b)

Fig. 2. *Initial spatial distribution of spheres a) and sphere diameter distribution b).*

The second step is devoted to the packing of spheres generated in step 1. During the packing process box size is reduced via random motions of spheres to increase their density (Al-Raoush & Al-

saleh, 2007). This step in the procedures terminates when box size is reduced to the minimum possible dimensions (see figure 3).

Those two steps are the same for all of the structure types.

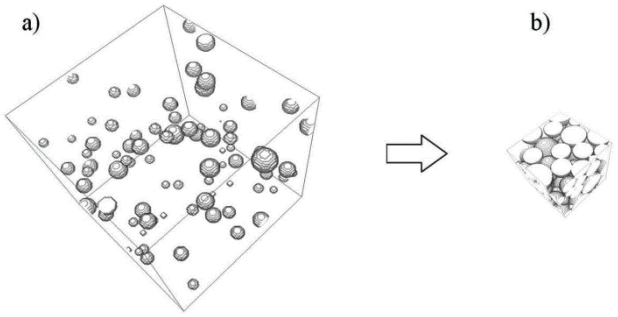


Fig. 3. *Spheres before a) and after packing b).*

2.1. Structures for Atomic-scale Molecular Dynamics Applications

In order to obtain the atomic structure of a polycrystal, additional steps are required. After sphere packing, the Laguerre-Voronoi tessellations (Fan et al., 2004) are applied to obtain cellular structures.

The main difference between typical Poisson-Voronoi tessellations and the Laguerre-Voronoi type is the placement of the tessellation plane (Hardenacke & Hohe, 2010). In the typical variant the plane is located between the sphere centers and in the Laguerre-Voronoi algorithm the plane is placed between sphere surfaces. A schematic explanation of the difference between those two algorithms is given in figure 4.

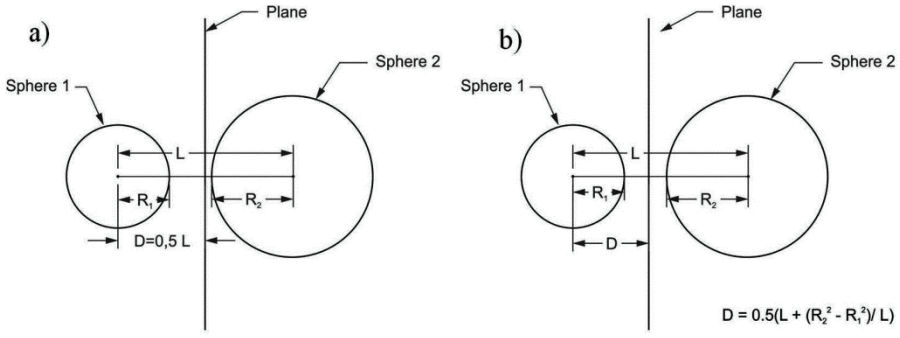


Fig. 4. *Schematic illustration of Poisson-Voronoi a) and Laguerre-Voronoi b) tessellations.*

After tessellations each cell/grain is then filled by a lattice of atoms with a defined type of atoms, lattice and orientation. Lattice type can be chosen from a list of space groups (Hahn, 2002) and the orientation of each grain is defined by three Euler angles (Arfken, 1985).

After that procedure the positions of atoms at the grain boundaries are not in their equilibrium state. That is why the relaxation step is required before any further calculations. The relaxation is usually performed in NPT (isothermal-isobaric ensemble) mode enabling to apply relatively low temperature and pressure. Under such conditions structural transformations are prevented and the volume of the system is slightly reduced by increasing the density of atoms at grain boundaries.

An example of the structure of polycrystalline iron with random grain orientation, before and after relaxation, is presented in figure 5.

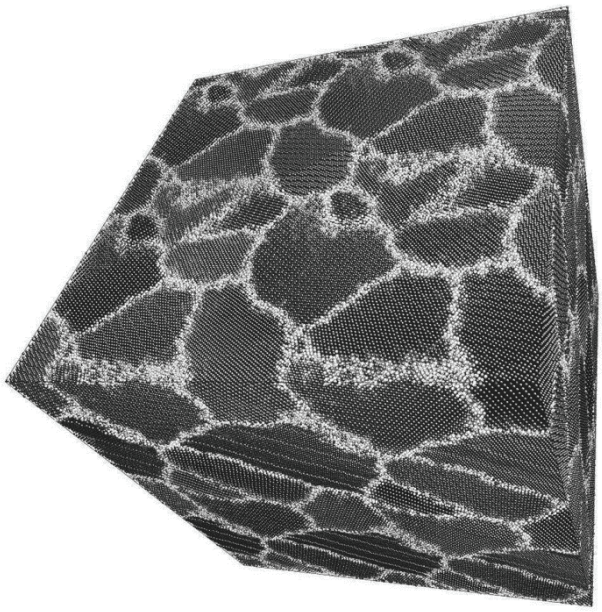


Fig. 5. *Example structure of polycrystalline iron with the average equivalent grain diameter of 10 nm. The structure is multiplied by 2 in all directions to better present periodic boundary conditions.*

The structure shown in figure 5 contains more than 2 million atoms and was relaxed in NVT mode by application of EAM (Embedded Atom Method) potential (Daw & Baskes, 1984; Daw & Foiles, 1993). Since the orientation of grains in this structure was random, low and high angle grain boundaries can be identified (see figure 6).

The structure described in figure 5 was periodic in all directions. Thus it represents the unit of bulk material. Simple modification of boundary conditions enables one to create polycrystalline thin films (see figure 7) or fibers.

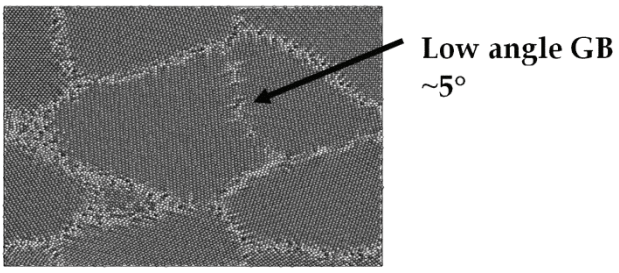


Fig. 6. *The region of the structure from figure 5 presenting low and high grain boundaries.*

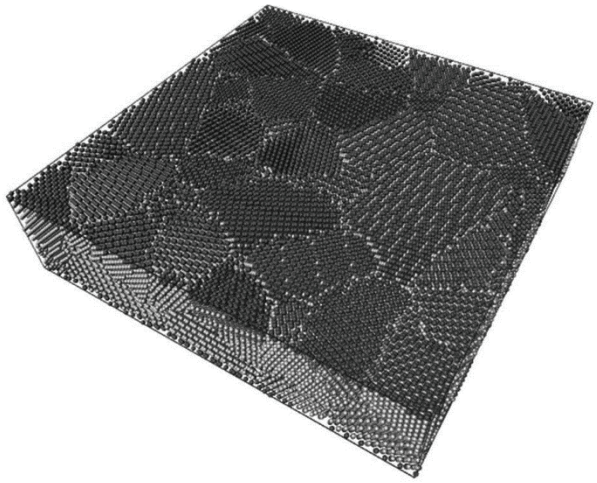


Fig. 7. *Atomic model representing the structure of iron thin film. The thickness is 4nm; the average equivalent diameter of grains is 4 nm.*

2.2. Structures for Meso-scale Monte Carlo and Cellular Automaton

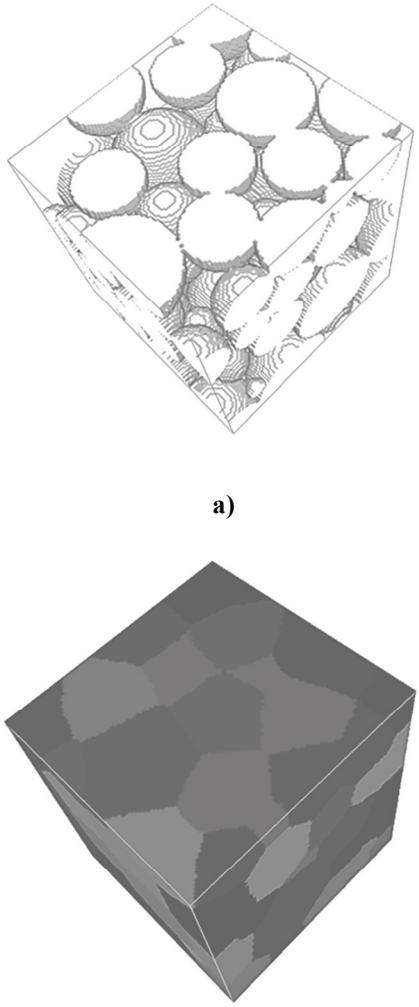
Meso-scale models realized by the Monte Carlo or Cellular Automaton approaches require a significantly different form of structure representation than atomic models. These methods operate on fields (voxels), which implicitly contain many atoms. The position of fields is usually discretized and defined by vectors with integer numbers. Various kinds of discretization are possible, but most of the models are created with a cubic one, which makes it compatible with 3d images.

Sphere generation is very similar here, but the position of the spheres and their radius are defined in the integer space.

Similarly, packing of spheres is done using the same algorithm as described earlier.

After the packing stage, the spheres are filled with voxels with values creating an array of properties relevant for the particular application. These can be grain number, chemical composition, orientation, temperature, etc.

Most discrete meso-scale-models instead of tessellations use the growth method to divide space into grains (Madej et al., 2013; Sieradzki & Madej, 2013). Growth is realized by subsequent dilation of spheres and stops when voxels from different grains meet each other. The result of this operation is presented in figure 8.



a)

b)

Fig. 8. *Spheres packed in box a) and polycrystal obtained by sphere growth b).*

The use of different distributions of sphere diameter enables one to generate polycrystals with various dispersion of grain size usually described by the variation coefficient of grain volume, CV(V), or equivalent diameter, CV(D).

An example of a polycrystalline structure with the same average grain diameter and different variation coefficient is presented in figure 9.

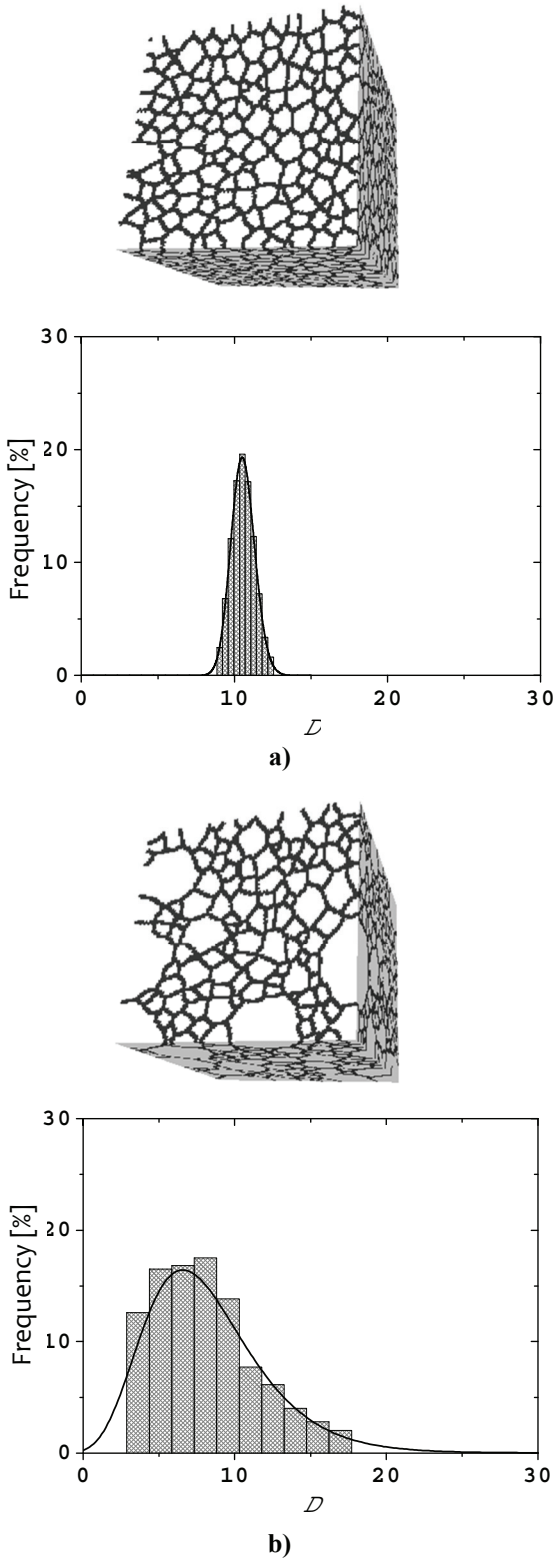


Fig. 9. Meso-scale model of polycrystal with homogenous, CV(D) = 0.1, a) and non-homogenous, CV(D)=0.75, b) grain equivalent diameter distribution.

2.3. Structures for continuous-scale: Finite Element Method (FEM) and Finite Volume Method (FVM)

As mentioned, the first two stages, resulting in sphere packing, are the same in the generation of all types of structures (see figure 1). In the case of structures for FEM calculations, after sphere packing, the Laguerre-Voronoi tessellations are performed in order to divide the box into volumes (grains). In the last step each grain is meshed (see figure 10). Both tessellation and the meshing procedure can be performed by scripts written using FEM dedicated programs (i.e., ANSYS or ABAQUS).

An example polycrystalline structure, which can be used for FEM calculations, is presented in figure 10.

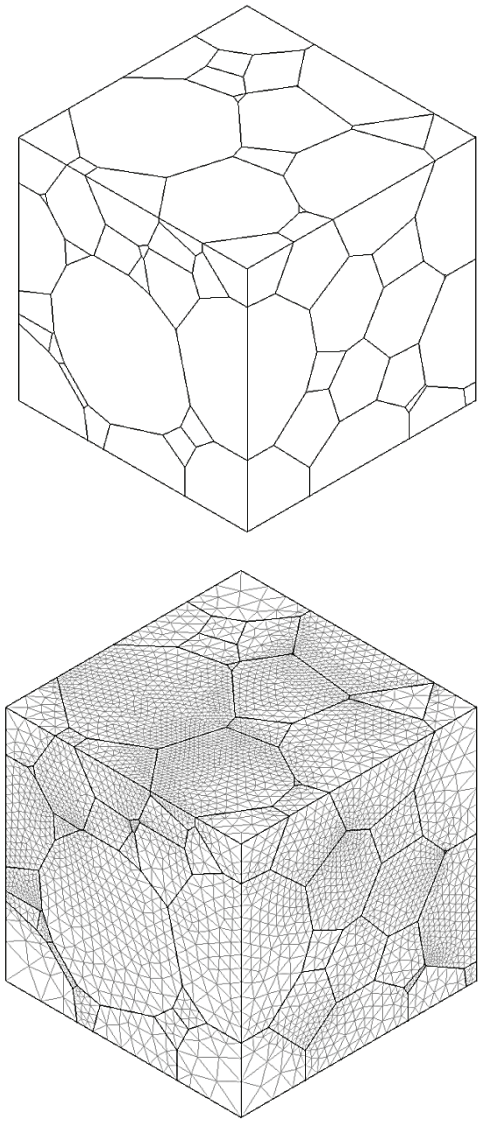
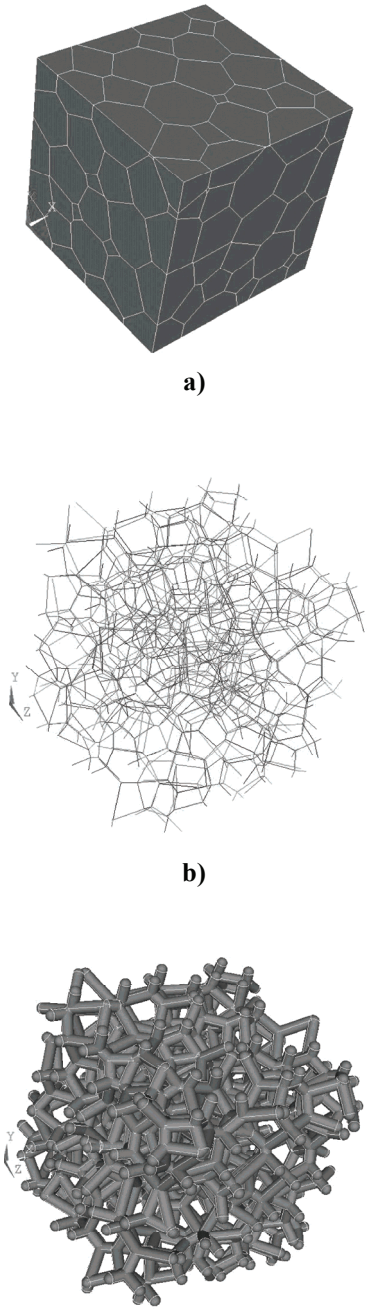


Fig. 10. Model of a polycrystal after the Laguerre-Voronoi tessellation procedure a) and meshing b). The structure contains 100 grains.

The structure of foams can be designed using similar procedures to the one used for the generation of polycrystals (Wejrzanowski et al., 2013). In that case, the face edges of grains/cells are extracted first. Then cylinders with a constant diameter are generated along the cell edges. Additionally, spheres that have diameters equal to those of the cylinders

are placed in the cell vertices to assure dimensional conformity along the edges.

The results of each step are presented in figure 11.



a)

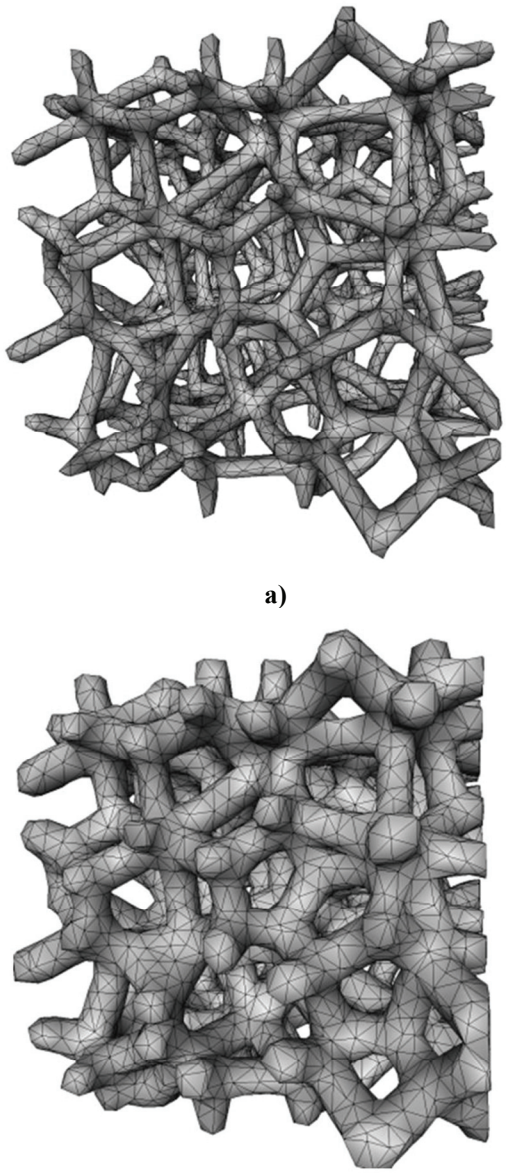
b)

c)

Fig. 11. *Procedure for modeling the structure of foams.*

In the last step meshing is performed using FEM dedicated programs (see figure 12).

Using this method it is possible to control cell size distribution of foam and strut diameter. An example of foams with the same initial cell size distribution and different strut diameter is shown in figure 12.

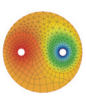


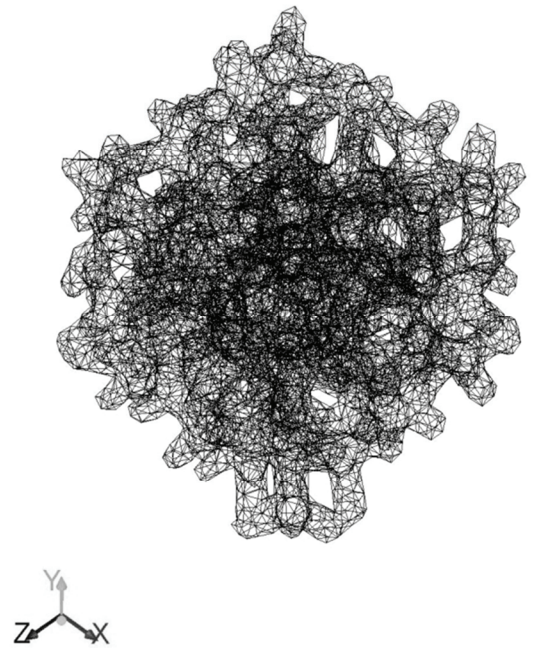
a)

b)

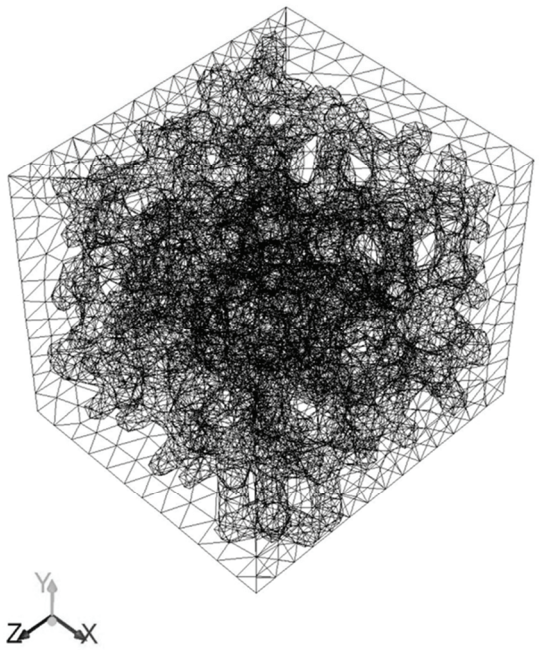
Fig. 12. *Foam geometry after meshing. Strut diameter is 10 times smaller than average cell diameter a). Strut diameter is 5 times smaller than average cell diameter b).*

The structures presented in figure 12 can be successfully applied to the calculation of mechanical and thermal properties of foams (Veyhl et al., 2011; Klett et al., 2004). In order to study flow phenomena through the foam pores, the volume constructed from struts must be subtracted from the box. The result of that operation can then be meshed and defined as gas or liquid field (see figure 13). This operation can be performed using FVM dedicated software.





a)



b)

Fig. 13. *An example of volume representing foam struts a) and volume representing pores b) after meshing.*

3. SUMMARY

A broad spectrum of cellular structures, relevant to particular scales and simulation methods, was presented in this paper. It has been shown that similar methods can be used to create polycrystalline structures to be applied in atomic, meso and continuum scales. The methods proposed here involved sphere packing and Laguerre-Voronoi tessellations, which allow one to directly control grain/cell size distribution, which is not possible with the commonly used Poisson-Voronoi tessellations.

The example structures presented in this paper can be successfully applied to the modeling of properties and processes at various scales such as: deformation, grain growth and melting among many others.

Numerical models of foams enable one to design and optimize the structure of materials for numerous applications, i.e., scaffolds or filters. Both deformation and flow of media through the foam structure can be simulated using structures presented in this paper.

This paper focused mainly on the generation of isotropic structures with spherical grain/cell shapes. However, further modification of these methods based on ellipsoid instead of sphere generation may facilitate the creation of structures of polycrystals and foams with morphological and crystallographic textures.

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MODELOWANIE KOMÓRKOWYCH STRUKTUR MATERIAŁÓW DLA ZASTOSOWAŃ W RÓŻNYCH SKALACH WYMIAROWYCH

Streszczenie

W artykule przedstawiono metody oraz wyniki projektowania struktur, które są stosowane do numerycznej symulacji własności i procesów występujących w materiałach komórkowych. Zaprezentowane metody mają charakter uniwersalny dla zastosowań w różnych skalach wymiarowych. Mogą być stosowane do takich materiałów jak polikryształy lub pianki, w których elementy (ziarna lub pustki) są rozłożone i ukształtowane w sposób kontrolowany. Cyfrowe reprezentacje materiału utworzone za pomocą zaproponowanych w pracy rozwiązań mogą stanowić podstawę dla takich numerycznych metod jak Dynamika Molekularna (ang. Molecular Dynamics - MD), Monte Carlo (MC), Automaty Komórkowe (ang. Cellular Automaton - CA), Metoda elementów Skończonych (ang. Finite Element Method - FEM) lub Metoda Objętości Skończonych (ang. Finite Volume Method - FVM). W artykule zaprezentowano przykłady struktur składających się z atomów, pól lub elementów skończonych. Przedstawiono również zastosowania tych struktur do opisu własności i procesów charakterystycznych dla różnych skal wymiarowych.

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