# MOLECULAR MODELS OF POLYCRYSTALLINE AND POROUS MATERIALS

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**Abstract**

Creation of the metallic polycrystalline and porous structures based on the molecular dynamics (MD) simulations are presented in this paper. The simple Morse potential, as well as, the more sophisticated Embedded Atom Method (EAM) are engaged to model atomic interactions. The presented methods of creation of the polycrystalline and porous molecular models are discussed and illustrated with proper numerical examples. The series of tensile tests and comparison of the mechanical properties between obtained polycrystalline structures is included, along with the description of the algorithm of the computation of the mechanical properties and the stress-strain relations. Additional tests are carried out with ideal Morse and EAM monocrystals in order to validate our molecular models and results. The simulations of creation polycrystalline and porous models are performed using the massively-parallel MD solver with NVT ensemble and tensile tests utilize so-called Non-Equilibrium Molecular Dynamics (NEMD).

**Key words**: nanomechanics, polycrystals, porous materials, molecular dynamics, digital material representation, mechanical properties

## 1. INTRODUCTION

All simulations based on the molecular dynamics (MD) method need initial solution – sets of atom's coordinates and velocities. Depending on the type and aim of the simulation, the initial positions of atoms can be generated randomly or arranged into unique spatial structure called digital representation of the material.

In the simplest models, atoms are placed in the nodes of the regular crystal lattice built from infinitely replicated unit cells such as: the simple cubic (SC), the body centered (BCC), the face centered (FCC) and the hexagonal close packed (HCP) cells (Chatterjee, 2008).

These models have anisotropic mechanical properties, characteristic for monocrystals. The preparation of a proper nanoscale material representation which properly mimics features well known from the macroscopic world is a real challenge, because in addition to the right type of the atomic interactions, the spatial configuration of atoms and number of nanodefects is crucial and incorporate to the overall macroscopic properties.

The purpose of this article is to present and discuss the features of the MD-based methods of building polycrystals with randomly orientated grains of various size and porous structures of adjustable density. All described approaches are illustrated with the appropriate numerical examples. The effective macroscopic mechanical properties are computed for the various types of obtained atomistic structures. Such molecular models can play a role of the initial solutions for further molecular dynamics simulations e.g. investigation of the behaviour of the nanodefects, where models built of ideal, regular lattices are not suitable.

## 2. ATOMIC POTENTIALS

The models of interatomic interactions, used in the MD to describe the potential energy and atomic forces, determine the reality, efficiency and precision of performed simulations. It is clear that the right type of the atomic potential should be chosen before starting the non-quantum molecular simulation.

Generally the most popular the atomic potentials can be generally divided in to two main classes: the first – consists of the simple two- or three-body (e.g. Morse, Lennard-Jones and Stillinger-Weber) interaction models, given in the parametric analytical form. The second group are the more sophisticated many-body and *ab-initio* based approaches, like the Embedded Atom Method (EAM) and the Bond-Order potentials. The EAM model become popular last years and is widely used in the modelling of metallic materials. The values of the potential's parameters can be obtained experimentally or - in the case of EAM – on the base of the *ab-initio* computations. The simple pair-wise models are commonly use in a large-scale molecular simulations especially due to low cost of the computations. The most popular in mechanical engineering computations pair-wise and many-body approaches will be discussed here in the detail.

### 2.1. Morse Potential

One of the most popular and commonly used pair-wise potentials is the interaction model introduced by Morse (1929). This potential has the following form:

$$V^{Morse}\left(r_{ij}\right) = D_e\left[e^{-2\alpha\left(r_{ij}-r_0\right)} - 2e^{-\alpha\left(r_{ij}-r_0\right)}\right], \quad (1)$$

and three fitting parameters. Dissociation energy $D_e$ refers to the minimum value of the potential energy at the equilibrium distance between two atoms denoted by $r_0$ (figure 1). The equilibrium distance is strictly correlated with the lattice constant since two particles attract each other when the distance between them is greater than $r_0$ and repulse on smaller distances to avoid possible collision.

The last parameter - $\alpha$ defines the curvature and the range of atomic interactions. This feature is clearly illustrated in figure 1, along with interpretation of the rest of Morse potential parameters.
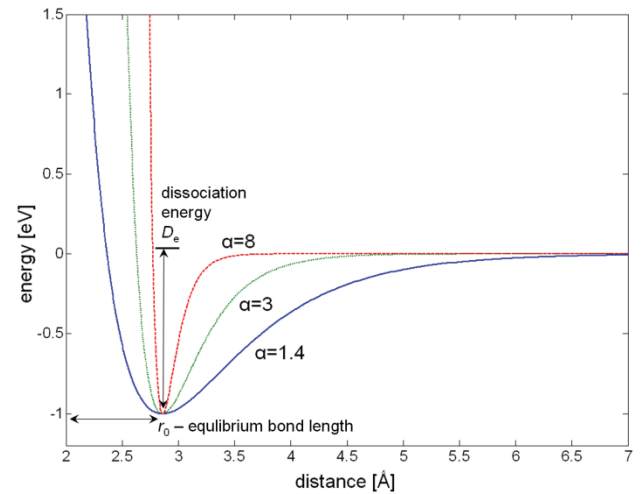
***Fig. 1.*** *Curvatures of the Morse potential function, for different values of α parameter.*

The values of Morse potential's parameters, fitted to the properties of the monoatomic metals are provided e.g. by Girifalco and Weizer (1959).

### 2.2. Embedded Atom Method

Different, more accurate approach of modelling metallic materials (Daw & Baskes, 1984; Daw et al., 1993; Foiles et al., 1986). The information about surrounding environment is provided by an additional term, which describes amount of the energy necessary to embed atom in the background electron density of the neighbouring atoms. In the EAM, the total energy of the monoatomic system is typically represented as:

$$V^{EAM} = \frac{1}{2}\sum_{i,j>i} V_2\left(r_{ij}\right) + \sum_i F^{embed}\left(\overline{\rho}_i\right) \quad (2)$$

where $V_2$ is the standard two-body potential, and $F^{embed}$ denotes the embedding energy of the *i*-th atom in the surrounding with the spherically averaged electron density:

$$\overline{\rho}_i = \sum_{j\neq i} \rho(r_{ij}) \quad (3)$$

developed by the electrons of all other atoms in the considered system.

The values of $V_2$, $F^{embed}$ and $\rho$, as the functions of appropriate variables, are usually obtained form *ab-initio* calculations. Thus they are usually given in a discrete, tabularized form. Deep study of the developing EAM potentials for aluminium and nickel atoms is presented by Mishin et al (1999).

The EAM, and its relatives, is one of the most popular approaches and plays important role in the modelling metallic materials at the molecular level.

The main drawbacks of this model are the higher computational cost compared to the potentials given in the direct analytic formulas and preclusion of the directional bonding due to the spherically averaged electron density. To overcome the bonding limitations, so-called modified embedded atom method (MEAM) was introduced and applied in the molecular dynamics packages (Baskes, 1992; Baskes & Johnson, 1994).

## 3. METHODS

Several methods of creation polycrystalline and porous structures have been recently developed. Such techniques are usually based on the three different approaches:
- geometrical constructions,
- digital image processing,
- molecular dynamics (MD) simulations.

The geometrical methods (e.g. Voronoi tessalation) divide simulation domain into to set of polyhedra (de Berg et al., 2000). In each polyhedron, the regular atomic lattice is generated with random crystallographic orientation. Algorithms of this kind are fast and usually do not require huge computational powers. The main drawbacks of these methods are problems with obtaining natural, realistic shape with proper random distribution of the artificially generated polycrystals. Additionally, molecular models created in this way need extra MD runs due to equilibration of the whole structure, especially at the grain's boundaries. Another group of geometrical methods are approaches based on the Cellular Automata and Monte-Carlo methods (Sieradzki & Madej, 2013) and grain growth algorithms (Madej et al., 2011; Sitko & Madej, 2013). In the mesoscale, the models based on the fast multipole boundary elements method can be successfully applied (Ptaszny & Fedelinski, 2011).

The fundamentals of the MD method have been explained in many thematic books e.g. (Griebel et al., 2007; Rapaport, 2004). Unlike the pure geometrical approaches, in the MD simulations the polycrystalline structure is created as a result of the atom's motion according to Newton's equations of motion under specified thermodynamic conditions and atomic interaction model. This fact obviously imply higher computational cost, however algorithms are simpler and more intuitive than ones used in geometrical constructions or and result with the stable, equilibrated models of materials created on the physical basis. This means that atomistic structures obtained in this way are ready to use in the further simulations because usually utilize the same atomic potentials and final temperatures.

The most common, MD approaches of creation of the polycrystalline structures are controlled cooling (Holian et al., 1991; Krivtsov, 2003), compression of the nanoparticles (Krivtsov & Wiercigroch, 2001) and controlled range of interatomic interactions. All these methods were also used by authors of this work to create molecular models of polycrystallines and gave good results (Mrozek & Burczyński 2012; 2013). The first two approaches are only briefly described in this paper. The third one, based on the influence of the potential shape and range of atomic interactions is extended to the porous materials and illustrated with two- and three-dimensional examples. Presented method can be treated as an alternative to the so-called condensation techniques, described by Krivtsov (2003).

### 3.1. Controlled cooling

This method mimics thermal processing of the real metallic materials. During the process of melting of the regular atomic lattice, the temperature, thus the kinetic energy of the thermostated system, increases. Atoms start to move with high velocities like in real boiling metallic liquid and in the certain time step take random positions with proper interatomic distances determined by features of the applied potential. This is an important thing, because in the case of randomly generated coordinates, distances between the atoms much shorter than equilibrium bond length result with high potential energies and may cause MD simulation unstable. From the other hand, too long distances may isolate atoms form interaction with others in the considered system.

Subsequent decreasement of the temperature reduces kinetic energy of atoms, which start to solidify, forming polycrystalline structure. The melting temperature and the speed of the cooling are critical and determine the size and shape of the created, randomly orientated, polycrystalline grains. Values of these parameters depend on type (mass) of atoms, potential model (pair-wise, many-body) and size of the molecular system and should be tuned experimentally for given type of atomic potential. This method can be used with any common type of boundary conditions (i.e. periodic or so-called reflecting walls) in two or three dimensional simulations.

In order to decrease cost of computations, the melting part may be replaced with specially prepared initial solution (Krivtsov, 2003; Mrozek & Burczyński 2012). An unstable, inappropriate (for given type of atomic potential) atomic lattice forces spontaneous rearrangement of atoms, which forms another stable spatial configuration with a nanocrystalline structure. E.g. in the molecular modelling of FCC metals like nickel or aluminium the unstable initial solution can be build of regular SC or BCC lattice, generated with appropriate (for given atom's type) lattice constant. An example of polycrystal, created using this method during author's previous research (Mrozek & Burczyński, 2013) is shown in figure 3b.

This process can be also boosted by high kinetic energy of the particles (i.e. high starting temperature). It can be noted that skipping the melting part reduces the total number of integration steps, thus imply the lower cost of the MD computations.

### 3.4. Compression of the nanoparticles

The set of small, separated molecular structures of arbitrary shape and size is being squeezed in the controllable way and form a large polycrystalline structure. This process, in contrast to previous methods, can be carried out at low temperatures, even near absolute zero. This method can be also used to create models of the polycrystalline materials with predefined size and crystallographic orientation of the grains (Mrozek & Burczyński 2013), as well as to generate molecular structures with controllable porosity like rocks or concrete (Krivtsov & Wiercigroch, 2001). The effects of the compression of the nanoparticles are presented on the 2D and 3D models, with various initial configurations.

### 3.5. Controlled range of atomic interactions

This approach combines energetically unstable initial configuration, cooling and the features of different shapes of the atomic potential functions. This algorithm is similar to the previously described one, however, the cooling process is performed at constant speed and the size of the grains and the type of structure is controlled by changing the effective interaction range of the potential. The long-range interactions results with structures with bigger grains and vice-versa. After equilibrating at desired, final temperature, the potential function can be replaced with another one.

The Morse potential can be easily applied in this method, due to very convenient mathematical formulation: the range of the atomic interactions depends directly on the scaling parameter $\alpha$ (see figure 2).

Slightly different method can be used to obtain structures with desired density and porosity. Preparation of porous models starts from artificially generated ideal, regular closed-packed lattice with imposed periodic boundary conditions. Atomic lattice should completely fill the simulation's domain. In the second step, certain number of atoms, corresponds to the desired density, is removed from randomly chosen nodes of the lattice.

In such prepared initial solutions, the neighbours of deleted atoms have high potential energy, far form the equilibrium state. The energy minimization routine can be performed using conjugated gradient algorithm (e.g. Polak-Ribiere scheme) or molecular statics Newton-Raphson solver (Burczyński et al., 2010). The first method is applied in this work. Such a treatment ensures that whole atomic structure will be sufficiently equilibrated at the zero temperature. and prepared for the further investigations. In the subsequent step the molecular model is carefully heated form 0 to 300 K with a constant rate of 0.1 K/ps and stabilized at 300 K.

An alternative approach of creation of porous molecular models of concrete-like materials – so called condensation technique is described and illustrated with examples by Krivtsov (2003). That method utilizes the Mie and the Lennard-Jones potentials, instead of the Morse forumula.

## 4. MECHANICAL PROPERTIES

According to Roylance (2000), the Young's modulus of the molecular structure can be estimated by division of the second derivative of the potential energy at equilibrium state by equilibrium distance:

$$E = \frac{1}{r_0} \frac{d^2 V(r_{ij})}{dr_{ij}^2}\bigg|_{r_{ij} \to r_0} \quad (4)$$

However, such estimation refers to the averaged properties of the material at the zero temperature and the information of the spatial configuration of the atomic structure can by provided only by the type and parameters of the potential itself.

To overcome this problem, simulations of the tensile tests of molecular models of the polycrystalline and porous structures at finite temperature

should be performed. This can be done using classical MD or so-called Non-Equilibrium MD (NEMD).

The classical MD simulation of the tensile test at the finite, nonzero temperature is based on the four steps:

- equilibration of the undeformed investigated molecular model at desired temperature,
- application of the finite deformation/load to the atomic system,
- equilibration of the *deformed/loaded* structure (at desired temperature),
- computation of the necessary, *time-averaged* quantities (i.e. stresses, deformations etc.).

The three last steps are repeated in the loop until the desired final deformation is achieved. Note, that additional equilibration in each iteration of the above algorithm is time-consuming. An alternative way of performing simulations of the continuously strained atomic system is application of the Non-Equilibrium Molecular Dynamics, e.g. SLLOD algorithm, provided by Tuckerman et al. (1997).

In this method, considered molecular system is coupled to the Nose-Hoover thermostat (Nose, 1984; Hoover, 1985) and the motion of the particles is determined by the following set of Hamilton's equations:

$$\dot{\mathbf{q}}_i = \frac{\mathbf{p}_i}{m_i} + \mathbf{q}_i \cdot \nabla \mathbf{u},$$

$$\dot{\mathbf{p}}_i = \mathbf{f}_i - \mathbf{p}_i \cdot \nabla \mathbf{u} - \frac{p_\eta}{Q} \mathbf{p}_i,$$

$$\dot{\eta} = \frac{p_\eta}{Q}, \qquad (5)$$

$$\dot{p}_\eta = \sum_{i=1}^{N} \frac{p_i^2}{m_i} - dNk_BT.$$

The meaning of the used symbols is following: vectors $\mathbf{q}$ and $\mathbf{p}$ are the sets of atomic coordinates and momenta, respectively. The $\mathbf{f}_i$ denotes force, acting on the $i$-th particle with mass $m_i$, while $\nabla \mathbf{u}$ refers to the strain rate of the system under continuous deformation. The $d$ and $N$ refer to the dimension of the problem and number of degrees of freedom, respectively. Symbol $\eta$ is a time-dependant thermodynamic friction coefficient, $T$ is the desired temperature of the system and the $Q$ is the thermostat mass parameter defined as:

$$Q = dNk_BT\tau^2, \qquad (6)$$

where $\tau$ denotes relaxation time and $k_B$ is the Boltzman constant.

Since atomic system is deformed continuously with defined strain rate, such approach doesn't need time-consuming equilibration after each application of finite deformation.

The atomistic stresses can be calculated in different ways. Typical approach utilizes virial theorem (Shengping & Atluri, 2004; Tsai, 1979; Wen et al., 2008):

$$\boldsymbol{\sigma} = \frac{1}{\Omega} \sum_{i}^{N} \left[ -m_i \mathbf{v}_i \otimes \mathbf{v}_i + \frac{1}{2} \sum_{j \neq i}^{N} \mathbf{r}_{ij} \otimes \mathbf{f}_{ij} \right] \qquad (7)$$

where: $i$ and $j$ are the atom's indices, $\mathbf{v}_i$ is the velocity of the $i$-th particle, $\mathbf{f}_{ij}$ and $\mathbf{r}_{ij}$ are respectively: interaction force and distance between two particles. Summation is performed over all atoms occupying volume $\Omega$, in the presented applications - over all atoms in the simulation box. The virial stress theorem (7) has two parts: kinetic and potential ones and generally is not an equivalent of the Cauchy stress or any other macroscopic mechanical stress tensor. However, when the kinetic part of the virial equation is neglected and the values obtained in each integration step are averaged over the time and geometry, the atomistic stress may be reduced to the Cauchy stress with physical meaning (Zhou, 2003).

The other approaches of computation of the mechanical properties at the nano-level like spring and braced-truss models can be found in works by (Chiang et al., 2006; Scarpa et al., 2009).

The Young's modulus in the small deformation range can be easily determined computing the slope coefficient of the linear approximation of the stress-strain curve.

## 5. NUMERICAL EXAMPLES

Series of MD simulations are performed to show abilities of described methods and emphasize the advantages of the techniques based on changing the shape of the potential.

The following example shows large three-dimensional polycrystalline models obtained using this method. Initial solution contained c.a. 1.7 million of atoms formed into energetically unstable simple cubic lattice with lattice constant equal to 2.86 Å. The reflecting boundaries were imposed.
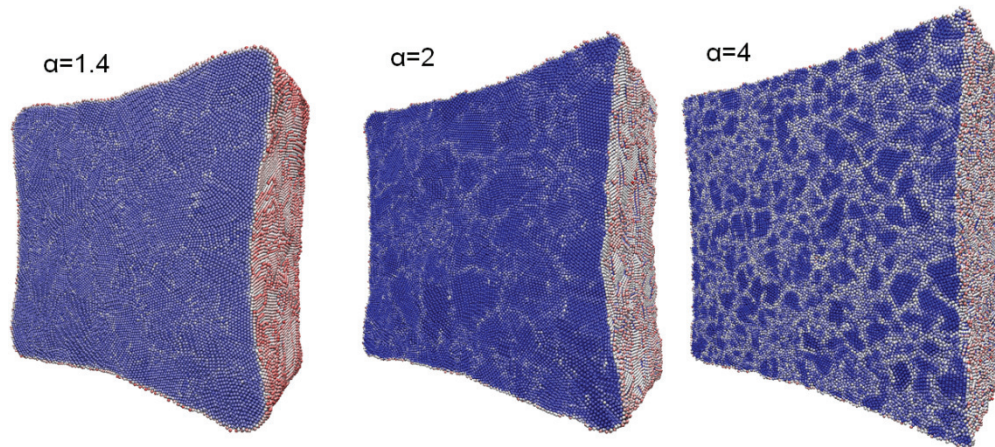
***Fig. 2.*** *3D nanocrystalline structures obtained for various ranges of interactions (α parameters).*

The set of randomly distributed initial velocities seeded to the temperature of 3000 K was generated and the Morse potential with $D_e = 1$ ev and $r_0 = 2.86$ was applied. Molecular system was cooled down to 300 K in the time of 2ns with integration step of 1fs.

Results of the simulation are presented in figure 2 for the values of the parameter $α$ equal to 1.4, 2 and 4 Å$^{-1}$, respectively, and shown that simulations with the narrowest potential functions, i.e. shortest interaction ranges produce structures with smallest grains. Created cube-like structures have approximate dimensions of 33×33×33 nm. Each structure was created after the same number of integration steps (i.e. constant cooling speed), however, this fact doesn't correspond to the constant time of the computation, since the longer interaction range needs defining of the longer cut-off radius and neighbour lists.

Creation of the molecular models with different, adjustable porosity is presented in the two subsequent examples.

Initial solution was prepared by random deleting certain number of atoms from 32×32×32 nm ideal FCC monocrystal, which contains over 2 millions of atoms. Periodic boundary conditions were imposed and the EAM potential for FCC aluminium (Jacobsen et al., 1987) was applied. The conjugated gradient based energy minimization was carried out and the molecular structure was heated and stabilized at the temperature of 300 K. The results, porous 3D models with various atomic densities are shown in figures 3 to 6. All the densities are given with respect to the density of regular FCC lattice. Additionally, previously obtained during "controlled cooling" process polycrystal model of the same size (Mrozek & Burczyński, 2013, as shown in figure 3b) is used for comparison of the mechanical properties.
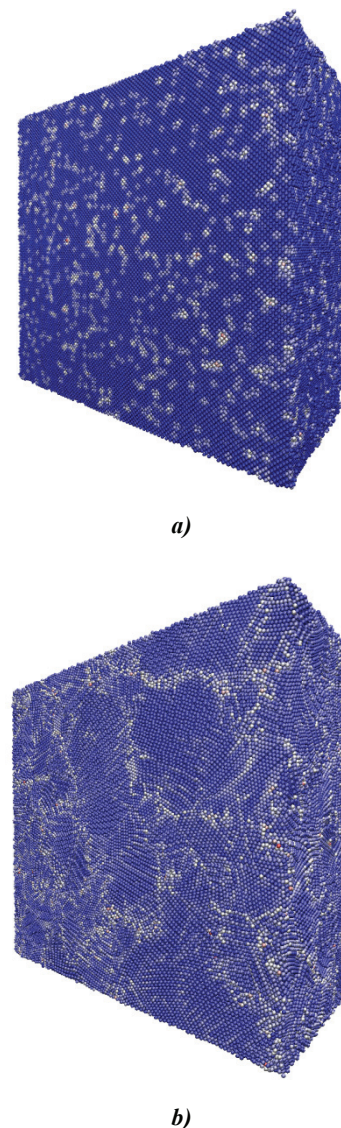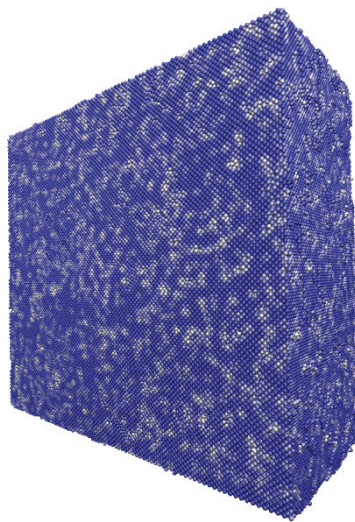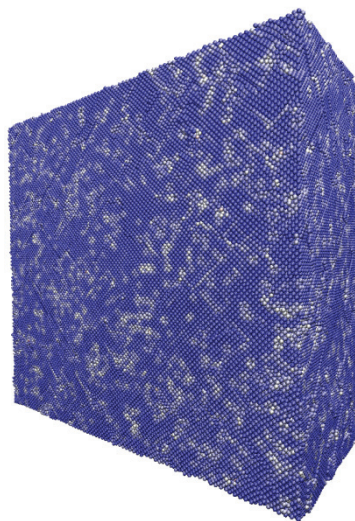


*a)*



*b)*

***Fig. 3.*** *Monocrystal with 2% porosity (a) and polycrystal (b), obtained using controlled cooling during previous research (Mrozek & Burczyński, 2013).*

conditions were imposed to the simulation box. All the measured quantities were averaged every each 500 timesteps. The kinetic term of the virial tensor (7) was neglected since the amount of kinetic energy is small, due to relative low temperature of the simulation.
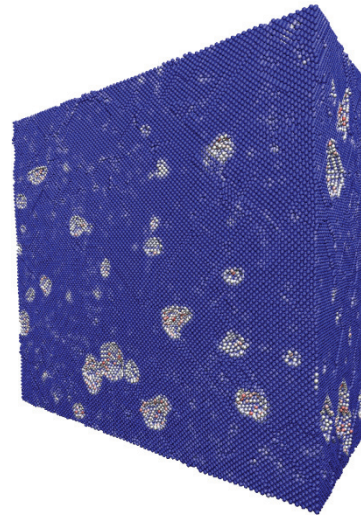

a)


b)

**Fig. 4.** *Structures with 5% (a) and 7.5% (b) porosity.*

It can be observed, that for the high densities (2-5% of porosity, respect to the regular FCC lattice) obtained models still have the monocrystalline structure with proportional number of vacanses (figure 3a and 4a). In the case of slightly higher porosities (removed approx. 7.5-10% of atoms) additional slips start to occur along the close-packed planes of the FCC lattice (figure 4b). Further decreasement of density results in formation of voids instead of vacanses (figures 5 and 6).
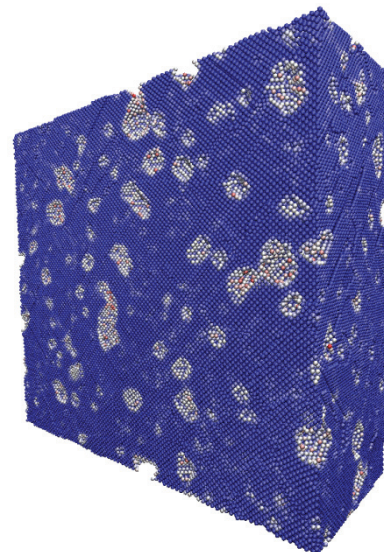
In order to validate obtained results, two tensile tests of the ideal FCC monocrystal with previously-cited Morse and EAM potentials fitted to the properties of the bulk aluminium are performed.

The investigated monocrystals had the same dimensions as obtained porous models and were continuously stretched with a constant strain rate corresponding to the velocity 10 m/s at the temperature of 10 K with time step equal to 1 fs. Periodic boundary


a)


b)

**Fig. 5.** *Structures with 12.5% (a) and 15% (b) porosity.*

Obtained stress-strain curves during tensile and shearing tests are shown in the figure 7. Determined values of the Young's moduli using linear approximation in the small strains area (0-2%) are equal to 105.5 GPa and 103.9 GPa, respectively for the EAM and Morse potential. The value of the Young's modulus, predicted by Chiang et al. (2006) using Single Spring Single Lattice exceeds 110 GPa, while experimental values for the bulk aluminium are of order 80-90 GPa. The different behavior in the large strain area is caused by different handling of the long range interactions between these two potentials.
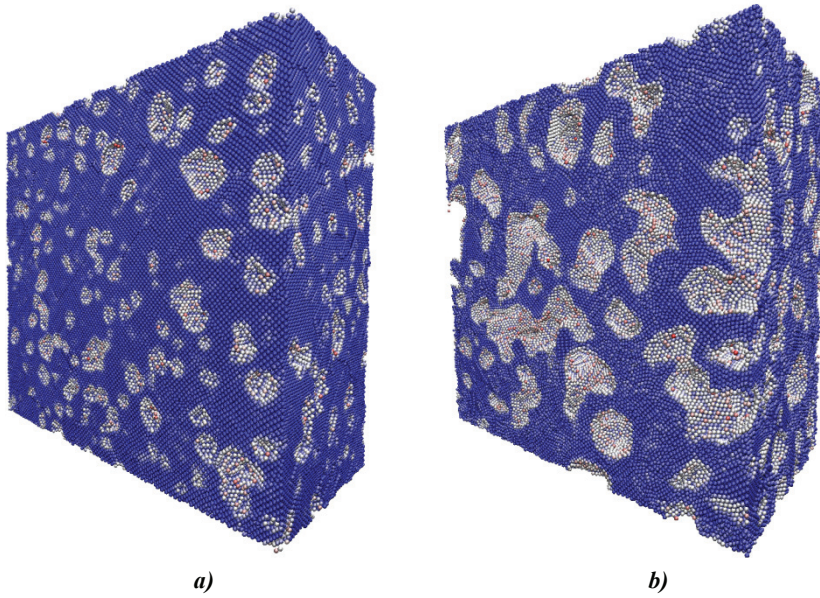
*a)* *b)*

**Fig. 6.** *Structures with 20% (a) and 30% (b) porosity.*

In the analogical way, the mechanical properties of the porous structures are investigated. Stress-strain curves, obtained for previously described models are shown in the figure 8. Additional characteristics an dproperties for EAM ideal moncrystal and polycrystal, taken form (Mrozek & Burczyński, 2013), are presented for comparison purposes (figure 3b). Dramatic decreasement of stiffness can be observed when molecular model changes its structure from monocrystalline with vacanses (removed approx. 2-7.5% of atoms, respect to the ideal FCC lattice) to the polycrystalline with
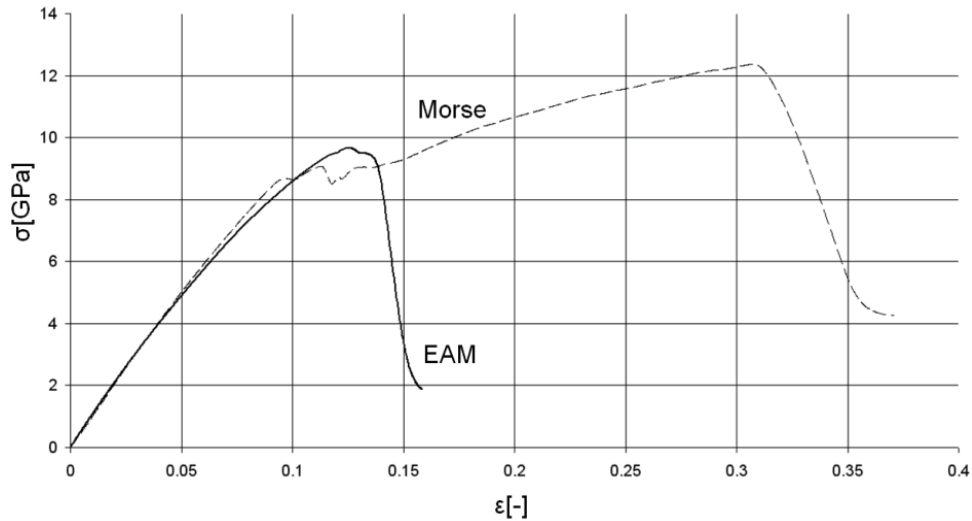


**Fig. 7.** *Stress-strain relations of the FCC monocrystals with different atomic potentials.*
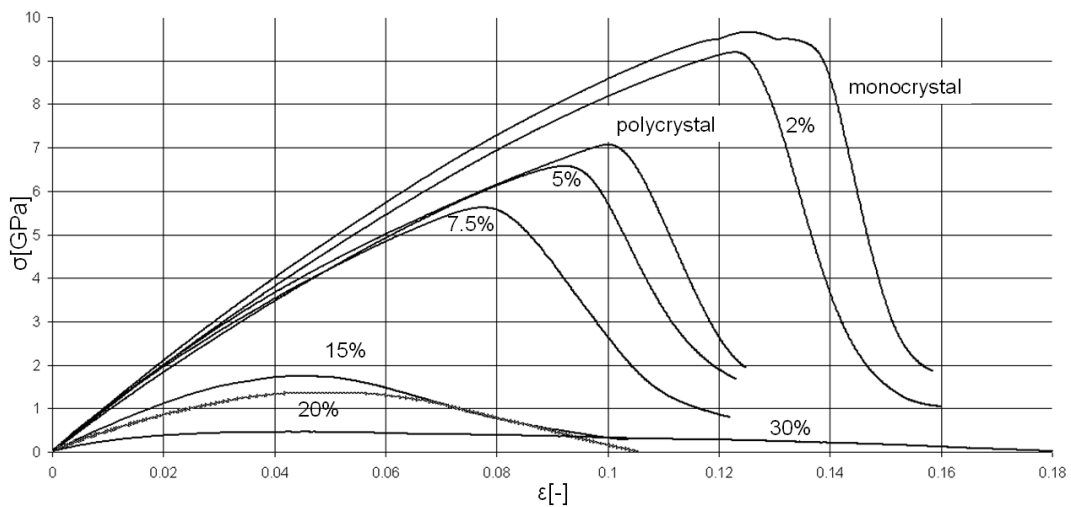


**Fig. 8.** *Stress-strain relations of the molecular models with various porosity (compared with mono- and polycrystal, see text for details).*

sphere-like voids (removed over 15% of atoms). Computed Young's moduli for each type of structure are summarized in table 1.

*Table 1. Properties of investigated molecular models*

| Model Al cube 32×32×32 nm EAM potential | Young's modulus [GPa] | Number of atoms |
|---|---|---|
| Monocrystal | 105.5 | 2048000 |
| Polycrystal | 98 | 2048000 |
| 2% porosity | 100 | 2007098 |
| 5% porosity | 91 | 1945922 |
| 7.5 porosity | 86 | 1791947 |
| 15% porosity | 54.7 | 1740509 |
| 20% porosity | 40.7 | 1638354 |
| 30% porosity | 17.1 | 1433587 |

## 6. CONCLUSIONS

Approaches of creation of the polycrystalline and porous molecular structures are presented and discussed in this paper. Both of them give possibility to control the average size of the grains and the porosity of the newly created structure.

The main drawback of all MD-based methods is high cost of the computations – much higher than the geometrical approaches. However, application of MD results with stable, equilibrated models of materials created on the physical basis (the behaviour of the atoms is determined by the specific interaction's model e.g. EAM in the case of metallic materials). This means that all the presented in this paper polycrystalline and porous models are ready to use and can serve as a base (i.e. initial solutions) for further MD simulations, e.g. investigation of the behaviour of the nanodefects or in the other cases, where models built of ideal, regular lattices are not suitable. Created structures can be used in the numerical homogenization in the author's developed versions of the multiscale modeling algorithms (Burczyński et al., 2010)

The main advantage of the approach based on the controlled range of atomic interactions is the constant number of iterations of MD algorithm, compared to the cooling method, where the size of the created grains depends directly of the cooling speed i.e. number of integration steps (Mrozek & Burczyński, 2013).

The obtained effective mechanical properties for the EAM aluminium mono- and polycrystals are in agreement with the macroscopic properties of the aluminium-based materials. Note, the values computed on the molecular level strongly depend on the applied molecular and interaction model, as well as methodology of investigation. A great juxtaposition of mechanical parameters of monoatomic metals is included in the paper by Chiang et al. (2006).

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## MOLEKULARNE MODELE MATERIAŁÓW POLIKRYSTALICZNYCH I POROWATYCH

Streszczenie

Tematyka pracy dotyczy metod tworzenia oraz badania własności mechanicznych atomowych modeli materiałów polikrystalicznych oraz porowatych przy wykorzystaniu Dynamiki Molekularnej. Przedstawionych zostało kilka różnych technik otrzymywania w/w struktur, m. in. kontrolowane schładzanie układu atomów oraz modyfikacja zasięgu oddziaływań międzyatomowych (funkcji potencjału atomowego). Każda metoda zilustrowana została przykładami, omówiony został również wpływ wybranych parametrów na wyniki symulacji numerycznej. W dalszej części artykułu opisano sposób wyznaczania własności mechanicznych modeli molekularnych: wyznaczania składowych tensora mikronaprężenia, krzywych naprężenie-odkształcenie i modułu Younga. Utworzone przedstawionymi metodami, zrównoważone i stabilne modele atomowe mogą posłużyć jako materiał wejściowy - rozwiązania początkowe – do dalszych symulacji wykorzystujących dynamikę lub statykę molekularną.