ATOMISTIC MODELS OF POLYCRYSTALLINE AND POROUS STRUCTURES

T. Burczyński[1], A. Mrozek[2]

[1]Institute of Fundamental Technological Research, Polish Academy of Sciences
Pawinskiego 5B, 02-106, Warsaw, Poland

[2]AGH University of Science and Technology, al. Mickiewicza, 30-059 Kraków, Poland

1. Introduction

The main purpose of this contribution is to present and discuss the features of the Molecular Dynamics (MD) methods [6] of building polycrystals with randomly orientated grains of given size and porous structures of adjustable density. Such atomic models can serve as initial solutions for the further MD simulations e.g. investigation of the behaviour of the nanodefects or determination of the mechanical characteristics where models built of ideal, regular lattices, which reveal anisotropic properties are not suitable. Although computationally expensive, MD-based methods have one main advantage compared to the artificial-geometrical ones: they produce stable, equilibrated structures, in almost all cases ready to the further use [3].

2. Methods of creation of molecular models

The following approaches are presented in this presentation: controlled cooling, compression of the nanoparticles and controlled range of interatomic interactions [3, 5]. All described approaches are illustrated with the appropriate numerical examples. Due to limited space of this abstract, only a few results of the simulations are shown. Two nanocrystalline structures, obtained using the third of mentioned methods are presented in Fig. 1.

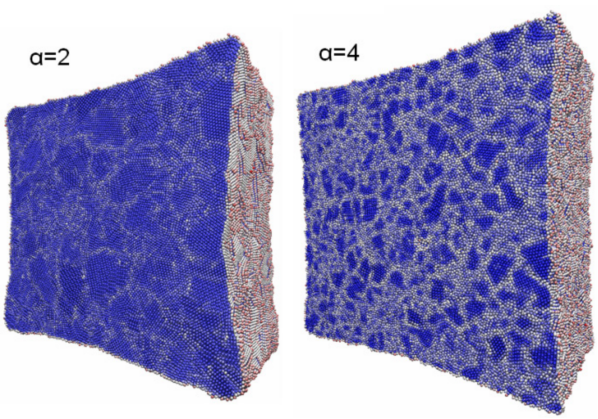

Fig. 1. Polycrystalline structures.

Both structures were obtained in the same conditions, during cooling a 32 nm ideal FCC cube (c.a. 2 mln of atoms) from 3000 K to 300 K in constant time of 2 ns. Only the scaling parameter α [4] which defined the curvature (thus interaction range) of the Morse potential was changed from 2 $Å^{-1}$ to 4 $Å^{-1}$. The influence of this parameter on the average size of the grains is clearly visible.

Creation of the atomistic models with different, adjustable porosity is presented in Fig. 2. All the assumptions remain unchanged, but initial solution was prepared by random deleting certain number of atoms from regular FCC lattice. The EAM potential [2], dedicated to modelling metallic materials, was applied in this case.

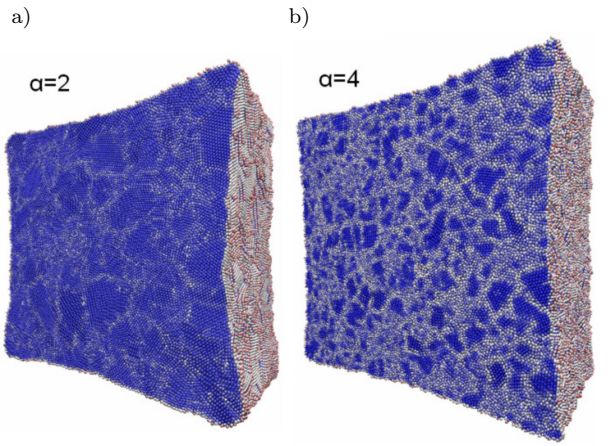

Fig. 2. Structures with: a) 15% and b) 30% porosity (respect to the ideal FCC lattice).

3. Estimation of the mechanical parameters

The methods of the estimation of the effective macroscopic mechanical properties, based on the nano-level tensile and shearing tests and so-called Non-Equilibrium Molecular Dynamics [7] will be performed, and computed for the various types of obtained atomistic structures. Obtained results, such as strain-stress relations, Young's and Kirchoff's moduli will be presented and compared with the results available in scientific literature and discussed during presentation.

I addition to potential applications of such atomistic models mentioned in the first paragraph, created structures can be also used in the methods of numerical homogenization or multiscale modelling e.g. in the author's developed versions of the multiscale modeling algorithms [1].

References

1. T. Burczyński, A. Mrozek, R. Górski, W. Kuś (2010). The molecular statics coupled with the subregion boundary element method in multiscale analysis, *Int. J. Multi. Comp. Eng.*, **8**, 319–330.
2. M.S. Daw, S.M. Foiles, M.I. Baskes (1993). The embedded-atom method: a review of theory and applications, *Mat. Sci. Rep.*, **9**, 7-8, 251–310.
3. A.M. Krivtsov (2003). Molecular dynamics simulation of impact fracture in polycrystalline materials, *Meccanica*, **38**, 61–70.
4. P.M. Morse (1929). Diatomic molecules according to the wave mechanics. II. Vibrational levels, *Phys. Rev.*, **34**, 57–64.
5. A. Mrozek, T. Burczyński (2012). Computational models of nanocrystalline materials, *Applied Sciences and Engineering* (ECCOMAS 2012) J. Eberhardsteiner *et al.* (eds.).
6. D. Rapaport (2005). *The Art of Molecular Dynamics Simulation*, Cambridge University Press.
7. M.E. Tuckerman, Ch.J. Mundy, S. Balasubramanian, M.L. Klein (1997). Modified nonequilibrium molecular dynamics for fluid flows with energy conservation, *J. Chem. Phys.*, **106**, 13, 5615–5621.