8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

MULTISCALE MODELLING USING FINITE AND BOUNDARY ELEMENT METHODS COUPLED WITH DISCRETE ATOMIC MODEL

***Tadeusz Burczyński[1], Waclaw Kuś[2] and Adam Mrozek[3]**

[1] Silesian University of Technology, Department for Strength of Materials and Computational Mechanics Konarskiego 18a, 44-100 Gliwice, Poland e-mail: tb@polsl.pl

[2] Silesian University of Technology, Department for Strength of Materials and Computational Mechanics Konarskiego 18a, 44-100 Gliwice, Poland e-mail: waclaw.kus@polsl.pl

[3] Silesian University of Technology, Department for Strength of Materials and Computational Mechanics Konarskiego 18a, 44-100 Gliwice, Poland e-mail: adam.mrozek @polsl.pl

Key Words: *Multiscale modelling, molecular statics, finite and boundary element methods (FEM, BEM)*

ABSTRACT

The multiscale models of engineering materials have been developed for the coupling of different length scales for various applications. Most of the multi-scale models consider two neighbouring length scales and are based on the coupling of a discrete model such as an atomic model and continuum model. The continuum model is usually considered in the framework of the finite element method [4].

This paper presents numerical algorithm, which uses boundary and finite element methods coupled with a discrete atomistic model. The application of BEM [1] and atomic model in multiscale simulations is a developed version of the own approach [2]. In this technique, the material behaviour at the atomic level can be modelled and the total number of degrees of freedom is reduced, because in most cases only a small part of the multi-scale model contains atoms and BEM doesn't need any discretization of the continuum's interior. The construction of the proposed multiscale model is following: the discrete atomic model occupies only rather small area of the model, where the simulation at the nanoscale should be performed (Fig. 1c). The rest of the structure is modelled by FEM or BEM (Fig. 1a and 1b, respectively). The coupling between two domains is realized by interface region, which contains so-called embedded atoms which coordinates are equal to the corresponding nodes of boundary elements or internal points. The boundary conditions are applied on the continuum model.

Discrete model of the molecular lattice makes use of the equilibrium equations of molecular interaction forces. The Lennard-Jones potential [5] is applied to benchmark examples and the embedded atom method [3] (EAM) is used for more accurate description of atomic interactions in the metalic material. The Newton-Raphson scheme is engaged to solve this non-linear problem.

Some benchmarks and numerical simulations are performed using described technique.

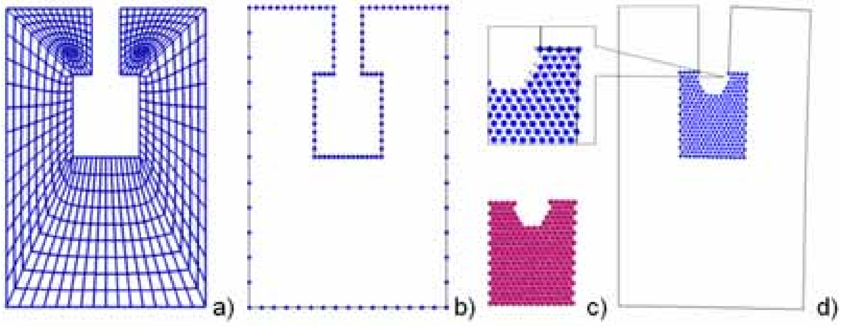

Figure 1. Construction of the multiscale model: a) FEM mesh, b) BEM mesh, c) atomic lattice, d) numercal results – equilibrium state of the deformed plate.

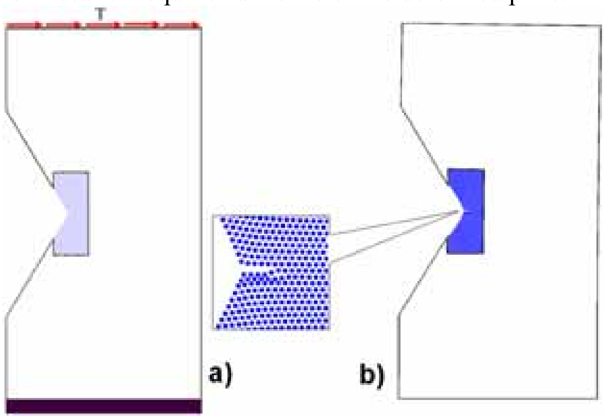

Figure 2. Shearing plate with V- notch: a) model b) results of the simlation – equilibrium state under the shearing load

The aluminium plate with V-notch is taken under consideration (Fig. 2a). The bottom of the plate is constrained and the shear load on the opposite side is applied. The discrete hexagonal lattice contains 2033 atoms with randomly added imperfections. The deformed plate is presented in the figure 2b. Opening of the crack at the centre of the notch can be observed. The middle layers of atoms moved in opposite directions and the new equilibrium state is achieved.

Acknowledgment
The research is partially financed from the Polish science budget resources as a research project (2007-2008) and the Foundation for Polish Science.

REFERENCES

[1] T. Burczyński, The Boundary Element Method in Mechanics, WNT, Warsaw (in Polish), 1995

[2] T. Burczynski, A. Mrozek, W. Kuś, A computational continuum-discrete model of materials, Bulletin of the Polish Academy of Sciences, 50, 1,pp. 85-89, 2007

[3] M. S. Daw, M. I. Basket, Semiempirical, Quantum Mechanical Calculation of Hydrogen Embrittlement In Metals, Phys. Rev. Lett. 50, 1285-1288, 1983

[4] W. K. Liu, E.G. Karpov, S. Zhang, H.S. Park, An introduction to computational nanomechanics and materials, Computer Methods in Applied Mechanics and Engineering, pp. 1529-1578, 2004

[5] R. Sunyk, P. Steinmann, On higher gradients in continuum-atomistic modelling, International Journal of Solids and Structures ,40, pp. 6877-6896, 2002