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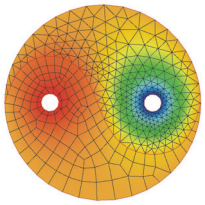
AKAPIT

**COMPUTER METHODS IN MATERIALS SCIENCE**

Informatyka w Technologii Materiałów

**Vol. 7, 2007, No. 2**



# APPLICATION OF THE COUPLED BOUNDARY ELEMENT METHOD WITH ATOMIC MODEL IN THE STATIC ANALYSIS

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**Abstract**

The multiscale algorithm based on the boundary element method (BEM) coupled with a discrete atomistic model is presented in this paper. The application of BEM reduces the total number of degrees of freedom in the multiscale model. The atomic model uses empirical pair-wise potentials to describe interactions between atoms. The Newton-Raphson method is applied to solve a nanoscale model. Some results of the numerical simulations are shown to examine the elaborated algorithm.

**Key words**: multiscale modelling, boundary element method, atomic model, static analysis

## 1. INTRODUCTION

The strength and stiffness of engineering materials are effected by the characteristics at various length scales. Atomic defects such as vacancies and dislocations play a role at the atomic scale, while characteristics of grain boundaries at the micro- or meso-scales contribute to the material strength. In order to understand and predict mechanical behaviours of engineering materials it is necessary to incorporate all those characteristics in different length scales.

Recently, multiple-scale models of engineering materials have been developed to address the coupling of different length scales for various applications.

Most of the multi-scale models consider two neighbouring length scales, while some other examine bridged more than two length scales. Shenoy et al. (1999) undertook coupling of a discrete model such as an atomic model and continuum model. Liu et al. (2004) provided a recent survey on multi-scale modelling. They summarized and compared various coupling techniques between the atomic model and a continuum model. In all papers the continuum model is considered in the framework of the finite element method.

This paper deals with a multi-scale algorithm based on the boundary element method (BEM) coupled with a discrete atomistic model. It is a developed version of the own approach presented in (Mrozek & Burczynski, 2006). In this approach, the material behaviour at the atomic level can be simulated 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 does not need discretization of the continuum's domain.

## 2. THE ATOMIC MODEL

The discrete atomic model is applied to simulate deformations of the atomistic lattice under loads.

 ISSN 1641-8581

This model is based on the equilibrium equations of atomic interaction forces (Kwon, 2003). The equilibrium state of the lattice corresponds to the minimal value of the total potential energy of the atomic structure. To describe the potential energy and interactions between two atoms the empirical Lennard-Jones and Morse potentials (figure 1), repectively, are used:

$$\Phi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1}$$

$$\Phi(r) = \varepsilon\left[e^{2\alpha(r_0 - r)} - 2e^{\alpha(r_0 - r)}\right] \tag{2}$$

where $\Phi$ denotes the potential energy, $r_0$ is equilibrium bond length, $\sigma$ - the collision diameter and $\varepsilon$ is the dissociation energy.

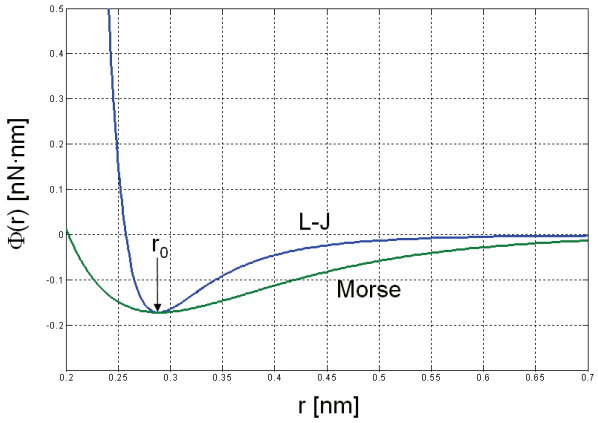


***Fig. 1.*** *Interatomic pair potentials.*

The interaction forces (figure 2) between each pair of atoms in the lattice are computed as the derivative of interatomic potential respect to the distance between two atoms (3):

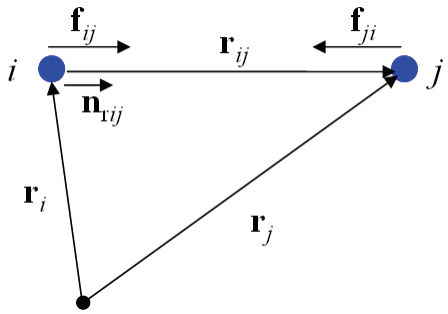


***Fig. 2.*** *Forces acting between i-th and j-th atom.*

$$\mathbf{f}_{ij} = -\frac{\partial\Phi(r_{ij})}{\partial r_{ij}}\mathbf{n}_{r_{ij}} \qquad \mathbf{f}_{ji} = -\mathbf{f}_{ij} \tag{3}$$

where: $\mathbf{n}_{rji}$ is the unit position vector between atoms *i* and *j*.

Figure 3 shows the initial positions of the two atoms (labelled $\mathbf{X}_i$, $\mathbf{X}_j$) and the initial distance vector $\mathbf{R}_{ij}$.

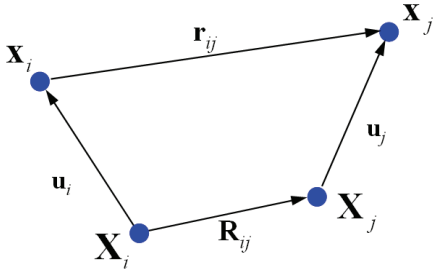


***Fig. 3.*** *Initial and displaced positions of the two atoms.*

The displacements $\mathbf{u}_i$ and $\mathbf{u}_j$ are applied to these atoms, respectively, and the resultant distance vector $\mathbf{r}_{ij}$ can be obtained:

$$\mathbf{r}_{ij} = \mathbf{R}_{ij} + \Delta\mathbf{u}_{ij} \tag{4}$$

where:

$$\Delta\mathbf{u}_{ij} = \mathbf{u}_j - \mathbf{u}_i$$

The distance vectors $\mathbf{r}_{ij}$ can be also obtained using the Cauchy-Born rule and information about the local deformation gradient (Sunyk & Steinmann, 2002).

Since the interaction force between atoms in displaced position can be written as:

$$\mathbf{f}_{ij}(r_{ij}) = f_{ij}(r_{ij})\mathbf{n}_{rij} \tag{5}$$

where:

$$\mathbf{n}_{rij} = \frac{\mathbf{R}_{ij} + \Delta\mathbf{u}_{ij}}{\mathbf{r}_{ij}}$$

Now equation (5) yields:

$$\mathbf{f}_{ij}(r_{ij}) = f_{ij}(r_{ij})\frac{\Delta\mathbf{u}_{ij}}{r_{ij}} + f_{ij}(r_{ij})\frac{\mathbf{R}_{ij}}{r_{ij}} \tag{6}$$

and the following equilibrium equation can be formulated:

$$f_{ij}(r_{ij})\frac{\Delta\mathbf{u}_{ij}}{r_{ij}} + f_{ij}(r_{ij})\frac{\mathbf{R}_{ij}}{r_{ij}} = 0 \tag{7}$$

Equilibrium equation (7) can be written in the matrix form (for two dimensional case):

$$\begin{bmatrix} k & 0 & -k & 0 \\ 0 & k & 0 & -k \\ -k & 0 & k & 0 \\ 0 & -k & 0 & k \end{bmatrix}\begin{pmatrix} u_{ix} \\ u_{iy} \\ u_{jx} \\ u_{jy} \end{pmatrix} - \begin{pmatrix} k(x_i - x_j) \\ k(y_i - y_j) \\ k(x_j - x_i) \\ k(y_j - y_i) \end{pmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{8}$$

or



$$\mathbf{P}(\mathbf{u}) = \begin{Bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \end{Bmatrix} \equiv k \begin{Bmatrix} (u_{ix} - u_{jx}) - (x_i - x_j) \\ (u_{iy} - u_{jy}) - (y_i - y_j) \\ (u_{jx} - u_{ix}) - (x_j - x_i) \\ (u_{jy} - u_{iy}) - (y_j - y_i) \end{Bmatrix} = \mathbf{0} \quad (9)$$

where: $k:=f_{ij}(r_{ij})/r_{ij}$ ; $x_n$, $y_n$ are initial coordinates of the $n$-th atom, $u_{nm}$ is the component of displacement of atom $n$ in the $m$-th direction.

The system of nonlinear equations (9), describing one atomic bonding, is solved iteratively, using the Newton-Raphson method:

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \left[\mathbf{J}^n\right]^{-1} \mathbf{P}^n \quad (10)$$

where:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial P_1}{\partial u_{ix}} & \frac{\partial P_1}{\partial u_{iy}} & \frac{\partial P_1}{\partial u_{jx}} & \frac{\partial P_1}{\partial u_{jy}} \\ \frac{\partial P_2}{\partial u_{ix}} & \frac{\partial P_2}{\partial u_{iy}} & \frac{\partial P_2}{\partial u_{jx}} & \frac{\partial P_2}{\partial u_{jy}} \\ \frac{\partial P_3}{\partial u_{ix}} & \frac{\partial P_3}{\partial u_{iy}} & \frac{\partial P_3}{\partial u_{jx}} & \frac{\partial P_3}{\partial u_{jy}} \\ \frac{\partial P_4}{\partial u_{ix}} & \frac{\partial P_4}{\partial u_{iy}} & \frac{\partial P_4}{\partial u_{jx}} & \frac{\partial P_4}{\partial u_{jy}} \end{bmatrix} \quad (11)$$

The Jacobian matrix [**J**] and the vector **P** are computed for all atoms, which interact with others in circular area. The cut-off radius is defined as a multiplicity of the lattice constant. After aggregation of [**J**] and **P**, the constraints are applied using the elimination method. The main concept is to assume some initial positions of molecules (e.g. undeformed lattice) and obtain final, stable equilibrium configuration of atoms with appropriate boundary conditions.

## 2. THE CONTINUUM MODEL

One assumes that continuum model of material on the microscale level is an elastic medium which occupies a domain Ω bounded by a boundary Γ.

The behaviour of the continuum model is described by the following vector boundary integral equation:

$$\mathbf{C}\mathbf{u} + \int_\Gamma \mathbf{T}\mathbf{u} d\Gamma = \int_\Gamma \mathbf{U}\mathbf{t} d\Gamma + \int_\Omega \mathbf{U}\mathbf{b} d\Omega \quad (12)$$

where: **U** and **T** are the fundamental solutions, **u** and **t** are the vectors of displacements and tractions, respectively, **b** denotes body forces, **C** is a free term coefficient and depends on the boundary shape.

The boundary element method (Burczynski, 1995) is applied to solve approximately the equation (12). The boundary Γ of the continuum domain is discretized using three node quadratic boundary elements. Second order shape functions are used to approximate boundary tractions and displacements. The application of BEM to the equation (12) results the following system of linear algebraic equations (13):

$$\mathbf{H}\mathbf{u} = \mathbf{G}\mathbf{t} + \mathbf{B} \quad (13)$$

Matrices **H** and **G** depend on the fundamental solutions **T** and **U**, respectively. **B** depends on body forces.

Since BEM uses tractions instead of nodal forces, the transformation of the interatomic forces to the tractions is needed. The expression (14) shows the equality of the work of the nodal forces (left side) and the work of the tractions (right side):

$$\mathbf{u}^{nT}\mathbf{F} = \int_l \mathbf{u}^T \mathbf{t} dl \quad (14)$$

The vector $\mathbf{u}^n$ denotes the nodal displacements, **F** - of nodal forces, $l$ is the length of the boundary element. The boundary displacements and tractions can be expressed, respectively:

$$\mathbf{u} = \mathbf{N}\mathbf{u}^n \quad (15)$$

$$\mathbf{t} = \mathbf{N}\mathbf{t}^n \quad (16)$$

where **N** is the shape function matrix, $\mathbf{t}^n$ is the unknown vector of the traction's nodal values.

After substitution (15) and (16) to (14), finally one can be obtained:

$$\mathbf{t}_n = \left[\int_{-1}^{1} \mathbf{N}^T \mathbf{N} J(\xi) d\xi\right]^{-1} \cdot \mathbf{F} \quad (17)$$

where $J(\xi)$ is the Jacobian connected with transformation to local coordinate $\xi$.

## 3. THE MULTISCALE MODEL

The construction of the multiscale model is shown in figure 4.

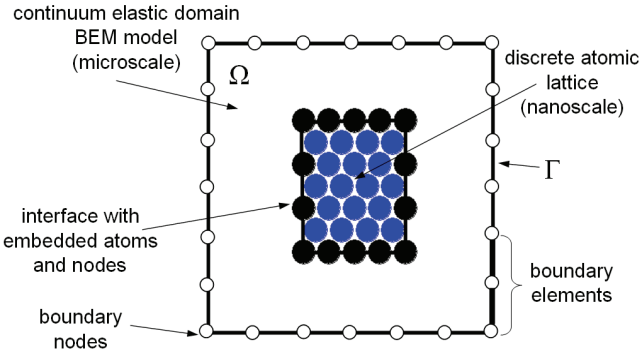


*Fig. 4. The coupled BEM-atomic multiscale model.*



The discrete atomic model occupies only rather small area of the model, where the simulation at the nanoscale should be performed. The rest of the structure is modelled by BEM. The interface domain contains so-called embedded atoms which coordinates are equal to the corresponding nodes of boundary elements. The boundary conditions are applied on the continuum model.

The algorithm of solving the coupled multiscale model is presented in the figure 5.

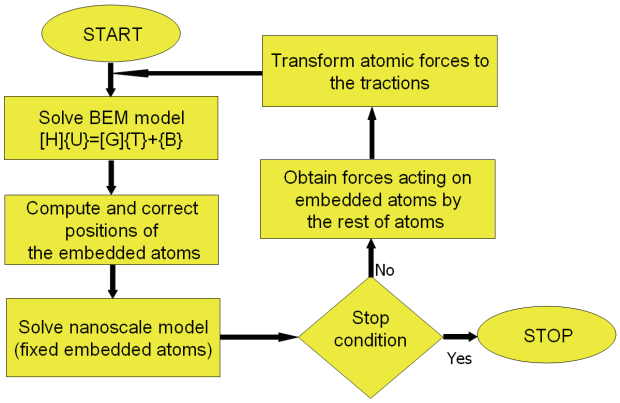


***Fig. 5.*** *The algorithm of solving coupled atomistic-BEM model.*

In the first step, the boundary conditions are applied and the BEM model is solved (figure 5). Displacements of the interface atoms are obtained and introduced as initial displacements of the outer boundary of the atomic lattice. In the next step, equilibrium positions of the atoms in the nanoscale model are computed, using the method described in the previous section. Finally, forces acting on interface atoms are computed and introduced as tractions nodal values to the BEM model. These computations are repeated iteratively until a stop condition is satisfied. The stop condition is executed when the difference between displacements of the embedded atoms during two iterations is less than an admissible value (error) $\varepsilon$.

## 4. NUMERICAL EXAMPLES

Some numerical simulations were performed using the technique described above sections. In the first example the plate witch the U-shape notch under the shear load is presented (figure 6a).

The left side of the plate is constrained and the shear load is applied on the opposite side. Some imperfections are introduced to the hexagonal atomic lattice. Dimensions of the plate are 18x12 [nm]. The continuum model contains 61 quadratic elements and 244 degrees of freedom. The atomic model contains 282 aluminium atoms, 546 degrees of freedom. The Lennard-Jones potential was used with the following parameters: $\sigma$ = 0.2575 nm, $\varepsilon$ = 0.1699 nN*nm, $r_0$ = 0.289 nm, values are taken from Sunyk & Steinmann, (2002).

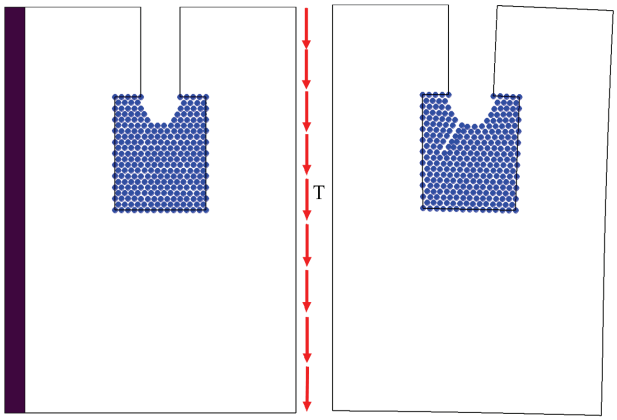


***Fig. 6.*** *The plate with the U-notch under the tensile load: a) initial equilibrium without any load, b) equilibrium state of the loaded plate.*

Figure 6b shows results of the numerical simulation. The atoms displaced to the new equilibrium positions under the loaded continuum model. It can be observed that a crack along the slip direction is arising.

The next example shows a plate with the V-shape notch (figure7a).

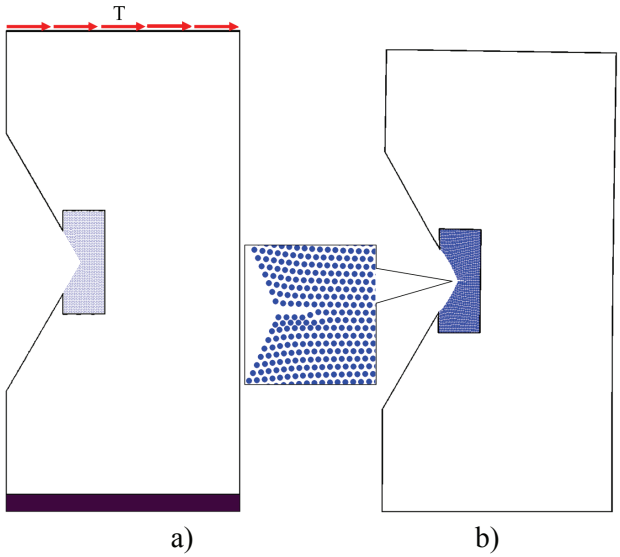


***Fig. 7.*** *The plate with V-notch under the tensile load: a) initial equilibrium without load, b) equilibrium state under shear load.*

The bottom of the plate is constrained and the shear load is applied on the top. Dimensions of the plate are 90x45 [nm]. Continuum model contains 176 quadratic elements and 704 degrees of freedom. The atomic model contains 2033 aluminium atoms. The parameters and material properties are the same as previous.



Results of the numerical simulations are presented in the figure 7b. The atoms moved to find a new equilibrium state. The opening crack at the centre of the notch is arising.

## 3. FINAL REMARKS

The presented method of analysis gives possibility of simulation, e.g. slips, crack behaviour and fracture at the atomic level and also may be used in modelling some technological processes in material science. The convergence of the Newton-Raphson method and the total number of iterations strongly depend on the initial positions of the atoms and their displacements taken form BEM. However, for small deformations of the atomic structure, the Newton-Raphson method is efficient. The process of minimization of the potential energy can be also done by using the evolutionary algorithm by Mrozek et al. (2005). The applications of these algorithms in prediction of atoms distribution give a great probability of finding the global optimal solutions, but this approach is very time consuming.

In the presented approach the first-order Cauchy-Born rule requires sufficiently homogeneous deformations of the continuum BEM model of material. This model is no more valid if the deformation becomes inhomogeneous because size effects cannot be taken into account. The extended Cauchy-Born rule can be considered by introducing the second-order deformation gradient (Sunyk & Steinmann, 2002). In this case the continuum BEM model will be describing by the application of the second order gradient stress theory (Habarta & Burczyński, 2006).

**Acknowledgement.** The research is financed by the Foundation for Polish Science (2005-2008).

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## ZASTOSOWANIE METODY ELEMENTÓW BRZEGOWYCH POŁĄCZONEJ Z DYSKRETNYM MODELEM MOLEKULARNYM W ANALIZIE STATYCZNEJ UKŁADÓW MECHANICZNYCH

Streszczenie

Artykuł przedstawia algorytm mający zastosowanie w analizie wieloskalowej materiałów. Dyskretny model molekularny sprzęgnięty został z kontynualnym modelem układu w skali mikro, rozwiązywanym za pomocą metody elementów brzegowych. Do opisu oddziaływań międzyatomowych wykorzystano potencjał Lennarda-Jonesa, natomiast końcowy układ równań nieliniowych rozwiązywany jest metodą Newtona-Raphsona. W artykule przedstawiono również przykłady testowe, pokazujące skuteczność prezentowanej metody.

*Submitted: September 25, 2006*
*Submitted in a revised form: November 13, 2006*
*Accepted: December 13, 2006*