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# A computational continuum-discrete model of materials

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**Abstract.** The paper contains a description of a multiscale algorithm based on the boundary element method (BEM) coupled with a discrete atomistic 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. The continuum domain is modelled by using BEM. The application of BEM reduces the total number of degrees of freedom in the multiscale model. Some numerical results of simulations at the nanoscale are shown to examine the presented algorithm.

**Key words:** continuum-discrete model, multiscale modelling, boundary element method, static analysis.

## 1. Introduction

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

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.

Most of the multi-scale models considered two neighbouring length scales, while some other examines bridged more than two length scales. Coupling of a discrete model such as an atomic model and continuum model was undertaken in [1]. A recent survey on multi-scale modelling was provided in [2]. It summarized and compared various coupling techniques between the atomic model and a continuum model. In all papers [2,3] the continuum model is considered in the framework of the finite element method (FEM). The coupling molecular dynamics (MD) and FEM is presented in [3].

This paper deals with a multiscale 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 [4,5]. 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. The discrete scale is modelled using Lennard-Jones potential. This potential is sufficient for benchmark problems, but for more realistic computations potentials like Embedded-Atom-Method EAM [6] should be used. Examples of analysis using one-scale MD and Morse potential can be found in [7]. The presented multiscale algorithm can be used for different types of interatomic potentials. The potentials in the atomic scale are prepared using results from *ab initio* computations.

## 2. The continuum model

Consider a continuum model of material on the microscale level as an elastic medium which occupies a domain $\Omega$ bounded by a boundary $\Gamma$. The field of displacement $\mathbf{u}(\mathbf{z}), \mathbf{z} \in \Omega$, is described by Navier-Lame equation:

$$(\lambda + \mu) grad\ div \mathbf{u} + \mu \nabla^2 \mathbf{u} + \mathbf{b}(\mathbf{z}) = 0, \quad \mathbf{z} \in \Omega \tag{1}$$

where $\lambda$ and $\mu$ are the Lame parameters characterizing the material medium.

Equation (1) should be completed by boundary conditions:

$$\begin{aligned} \mathbf{u}(\mathbf{x}) &= \mathbf{u}_o(\mathbf{x}), \quad \mathbf{x} \in \Gamma_u \\ \mathbf{t}(\mathbf{x}) &= \sigma \mathbf{n} = \mathbf{t}_o(\mathbf{x}), \quad \mathbf{x} \in \Gamma_t \end{aligned} \tag{2}$$

where $\sigma = (\sigma_{ij})$ is a stress tensor, $\mathbf{n}$ is a unit normal vector outward to the boundary $\Gamma$, $\Gamma_u \cup \Gamma_t = \Gamma$ and $\Gamma_u \cap \Gamma_t = \emptyset$.

To solve the boundary-value (1) and (2) the boundary element method is used [8]. The problem is transformed to the following vector boundary integral equation:

$$\begin{aligned} &\mathbf{c}(\mathbf{x})\mathbf{u}(\mathbf{x}) + \int_\Gamma \mathbf{T}(\mathbf{x},\mathbf{y})\mathbf{u}(\mathbf{y}) d\Gamma(\mathbf{y}) \\ &= \int_\Gamma \mathbf{U}(\mathbf{x},\mathbf{y})\mathbf{t}(\mathbf{y}) d\Gamma(\mathbf{y}) + \int_\Omega \mathbf{U}(\mathbf{x},\mathbf{z})\mathbf{b}(\mathbf{z}) d\Omega(\mathbf{z}) \end{aligned} \tag{3}$$

where: $\mathbf{U}(\mathbf{x},\mathbf{y})$ and $\mathbf{T}(\mathbf{x},\mathbf{y})$ are the fundamental solutions of electrostatics, $\mathbf{u}$ and $\mathbf{t}$ are the vectors of displacements

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and tractions, respectively, $\mathbf{b}(\mathbf{z})$, $\mathbf{z} \in \mathbf{\Omega}$, denotes a vector of body forces, $\mathbf{c}$ is a free term coefficient which depends on the boundary geometry.

To solve Eq. (3) the boundary $\Gamma$ of the continuum domain $\mathbf{\Omega}$ is discretized using three node quadratic boundary elements $\Gamma^e$, $\Gamma = \bigcup_{e=1}^{E} \Gamma^e$. The boundary fields of displacements and tractions are approximated by means of nodal values and shape functions:

$$\begin{aligned} \mathbf{u} &= \mathbf{N}\mathbf{u}^n \\ \mathbf{t} &= \mathbf{N}\mathbf{t}^n. \end{aligned} \tag{4}$$

The boundary element method [8] is applied to solve approximately the Eq. (3). Second order shape functions are used to approximate boundary tractions and displacements. Algebraic counterpart of Eq. (3) is given in matrix form:

$$[\mathbf{H}]\{\mathbf{u}\} = [\mathbf{G}]\{\mathbf{t}\} + \{\mathbf{B}\} \tag{5}$$

where the matrix $[\mathbf{H}]$ depends on boundary integrals of the fundamental solution $\mathbf{T}$, the matrix $[\mathbf{G}]$ on boundary integrals of the fundamental solution $\mathbf{U}$ and the matrix $\mathbf{c}$, $\mathbf{B}$ depends on body forces and column matrices $\mathbf{u}$ and $\mathbf{t}$ contain nodal values of boundary displacements and tractions, respectively.

Taking into account boundary conditions (2) Eq. (4) is transformed to system of linear algebraic equations:

$$[\mathbf{A}]\{\mathbf{X}\} = \{\mathbf{Y}\} \tag{6}$$

where the matrix $[\mathbf{A}]$ is built from matrices $[\mathbf{H}]$ and $[\mathbf{G}]$, the column matrix $\mathbf{X}$ contains unknown nodal values of displacements and tractions and the matrix $\mathbf{Y}$ depends on boundary conditions.

A part of the boundary $\Gamma$ of the continuum domain $\Omega$ is contacted in the interface with embedded atoms. Since the BEM model uses tractions instead of nodal forces, the transformation of the interatomic forces to the tractions is needed. It can be done by comparing the work of the nodal forces $\mathbf{F}$ (left side) and the work of the tractions $\mathbf{t}$ (right side):

$$\mathbf{u}^{nT}\mathbf{F} = \int_{\Gamma^e} \mathbf{u}^T \mathbf{t} d\Gamma^e \tag{7}$$

After substitution (4) to (7), finally one can be obtained:

$$\mathbf{t}^n = \left[ \int_{\Gamma^e} \mathbf{N}^T \mathbf{N} \mathbf{J} d\Gamma^e \right]^{-1} \cdot \mathbf{F} \tag{8}$$

were J is the Jacobian, defined:

$$J = \frac{d\Gamma}{d\xi} = \sqrt{\left(\frac{dx_1(\xi)}{d\xi}\right)^2 + \left(\frac{dx_2(\xi)}{d\xi}\right)^2} \tag{9}$$

$x$ and $\xi$ are respectively global and local coordinates.

## 3. The discrete model

The discrete atomic model is applied to simulate deformations of the atomistic lattice under loads. This model is based on the equilibrium equations of atomic interaction forces [9]. The equilibrium state of the lattice corresponds to the minimal value of the total potential energy of the atomic structure. The potential energy is described using different equations depending on distance between each 2, 3 or many atoms. The parameters of the equations are computed to provide best fit to various properties of a material (equilibrium lattice constant, elastic constants, etc.). The parameters of the potentials equations are prepared on the base of *ab initio* calculations. The best results can be obtained performing whole computations using *ab initio* approach, but the computer cost of such approach would be very large. To describe the potential energy and interactions between atoms the empirical potentials can be used:

– the Lennard-Jones 2-body potential:

$$\Phi(\mathbf{r}_{ij}) = 4\varepsilon \left[ \left( \frac{\sigma}{\mathbf{r}_{ij}} \right)^{12} - \left( \frac{\sigma}{\mathbf{r}_{ij}} \right)^{6} \right] \tag{10}$$

– the Morse [10] 2-body potential:

$$\Phi(\mathbf{r}_{ij}) = \varepsilon \left[ e^{2\alpha(\mathbf{r}_0 - \mathbf{r}_{ij})} - 2e^{\alpha(\mathbf{r}_0 - \mathbf{r}_{ij})} \right] \tag{11}$$

– the Stillinger-Weber [11] 3-body potential:

$$\Phi\left(\mathbf{r}_{ij}, \mathbf{r}_{ik}, \mathbf{r}_{jk}\right) = v_2(\mathbf{r}_{ij}) + v_3\left(\mathbf{r}_{ij}, \mathbf{r}_{ik}, \mathbf{r}_{jk}\right) \tag{12}$$

– the EAM [6] potential (many-body potential):

$$\Phi\left[\mathbf{r}_{ij}, \bar{\rho}(\mathbf{r})\right] = ED\left[\bar{\rho}(\mathbf{r})\right] + V(\mathbf{r}_{ij}) \tag{13}$$

where: $\Phi$ denotes the potential energy, $\mathbf{r}$ – vector containing distance between atoms, $\mathbf{r}_0$ is equilibrium bond length, $\sigma$ – the collision diameter and $\varepsilon$ is the dissociation energy, $v_2(\mathbf{r}_{ij})$ – pair potential, $v_3\left(\mathbf{r}_{ij}, \mathbf{r}_{ik}, \mathbf{r}_{jk}\right)$ – triplet potential, $V(\mathbf{r}_{ij})$ – is a potential energy for core to core repulsion between atoms, $\bar{\rho}(\mathbf{r})$ – describes the electron density and depends on the atom density (and distances of all atom surrounding considered one), $ED\left[\bar{\rho}(\mathbf{r})\right]$ – is the embedding function depending only on electron density value $\bar{\rho}(\mathbf{r})$. The Lennard-Jones and Morse for material used in numerical examples functions are shown in Fig. 1.

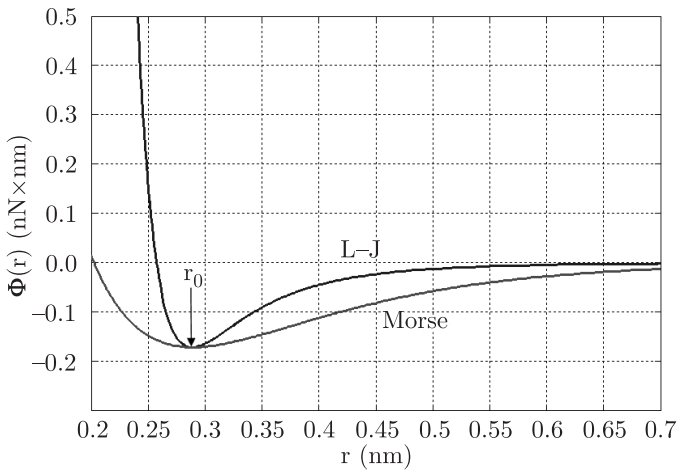


Fig. 1. Interatomic pair potentials

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

$$\mathbf{f}_{ij} = -\frac{\partial \Phi(r_{ij})}{\partial r_{ij}} \mathbf{n}_{r_{ij}}; \qquad \mathbf{f}_{ji} = -\mathbf{f}_{ij}. \tag{14}$$

Consider homogeneous deformations of an infinite representative crystallite (Fig. 3). The kinematic relation is given by the 1st order Cauchy-Born rule:

$$\mathbf{r}_{ij} = \mathbf{K} \times \mathbf{R}_{ij} \tag{15}$$

$\mathbf{K}$ is the 1st order deformation gradient which defines a linear tangent map which is given by the tensor:

$$\mathbf{K} = \nabla \varphi \tag{16}$$

where $\varphi(\mathbf{X})$ is deformation map which relates the placement X in the material configuration to the placement $\mathbf{x} = \varphi(\mathbf{X})$ in the spatial configuration (Fig. 3).

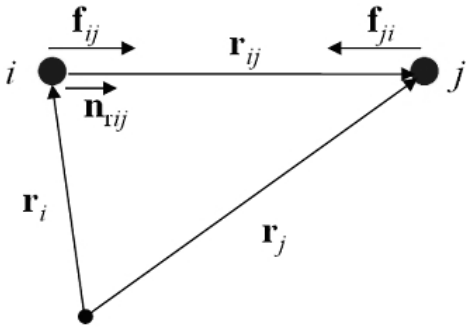


Fig. 2. Forces acting between $i$-th and $j$-th atom

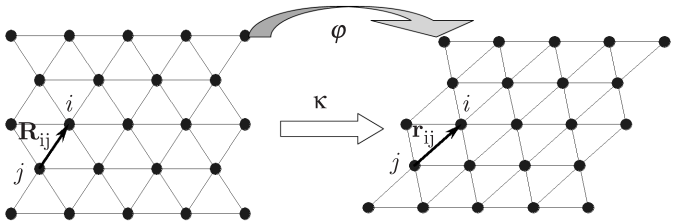


Fig. 3. The 1st order Cauchy-Born rule for homogeneous deformation

Since $\nabla\varphi$ can be expressed as:

$$\nabla \varphi = \mathbf{I} + \nabla \mathbf{u} \tag{17}$$

where:

$$\nabla \mathbf{u}_{ij} = \frac{\Delta \mathbf{u}_{ij}}{\mathbf{R}_{ij}} \tag{18}$$

after substitution (16) and (17) to (15), the following expression can be obtained:

$$\mathbf{r}_{ij} = \mathbf{R}_{ij} + \Delta \mathbf{u}_{ij} \quad \Delta \mathbf{u}_{ij} = \mathbf{u}_j - \mathbf{u}_i \tag{19}$$

Figure 4 shows the vector interpretation of (19): $\mathbf{X}_i$, $\mathbf{X}_j$ are the initial positions of the two atoms and the $\mathbf{R}_{ij}$ is the initial distance vector, $\mathbf{u}_i$ and $\mathbf{u}_j$ are displacements applied to these atoms, respectively and $\mathbf{r}_{ij}$ is the resultant distance vector.

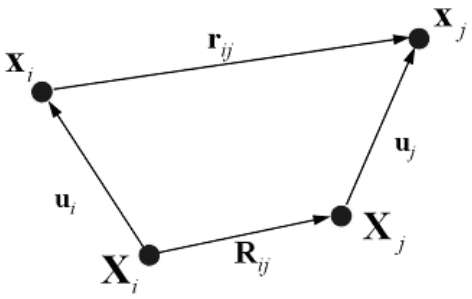


Fig. 4. Initial and displaced positions of the two atoms

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

$$\mathbf{f}_{ij}(r_{ij}) = f_{ij}(r_{ij}) \frac{\mathbf{r}_{ij}}{r_{ij}}. \tag{20}$$

After substitution (14) and (19) into above equation, the following expression can be formulated:

$$\mathbf{f}_{ij}(r_{ij}) = f_{ij}(r_{ij}) \frac{\Delta \mathbf{u}_{ij}}{r_{ij}} + f_{ij}(r_{ij}) \frac{\mathbf{R}_{ij}}{r_{ij}} \tag{21}$$

and the following equilibrium equation can be formulated:

$$f_{ij}(r_{ij}) \frac{\Delta \mathbf{u}_{ij}}{r_{ij}} - f_{ij}(r_{ij}) \frac{\mathbf{R}_{ij}}{r_{ij}} = 0 \tag{22}$$

or in the matrix form (for two-dimensional case):

$$\begin{bmatrix} k & 0 & -k & 0 \\ 0 & k & 0 & -k \\ -k & 0 & k & 0 \\ 0 & -k & 0 & k \end{bmatrix} \begin{pmatrix} u_{ix} \\ u_{iy} \\ u_{jx} \\ u_{jy} \end{pmatrix} = \begin{pmatrix} f_{ix} \\ f_{iy} \\ f_{jx} \\ f_{jy} \end{pmatrix} \tag{23}$$

where: $k := f_{ij}(r_{ij})/r_{ij}$.

This system of equations describing one atomic bonding, is nonlinear and must be transformed into the form, which can be solved using an iterative method. After some transformations, system of equations can be expressed as:

$$\begin{bmatrix} k & 0 & -k & 0 \\ 0 & k & 0 & -k \\ -k & 0 & k & 0 \\ 0 & -k & 0 & k \end{bmatrix} \begin{pmatrix} u_{ix} \\ u_{iy} \\ u_{jx} \\ u_{jy} \end{pmatrix} - \begin{pmatrix} k(x_i - x_j) \\ k(y_i - y_j) \\ k(x_j - x_i) \\ k(y_j - y_i) \end{pmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \tag{24}$$

or

$$\mathbf{L}(\mathbf{u}) = 0 \tag{25}$$

where

$$\mathbf{L}(\mathbf{u}) = \begin{Bmatrix} L_1 \\ L_2 \\ L_3 \\ L_4 \end{Bmatrix} \equiv k \begin{Bmatrix} (u_{ix} - u_{jx}) - (x_i - x_j) \\ (u_{iy} - u_{jy}) - (y_i - y_j) \\ (u_{jx} - u_{ix}) - (x_j - x_i) \\ (u_{jy} - u_{iy}) - (y_j - y_i) \end{Bmatrix} \tag{26}$$

The system of nonlinear Eqs. (25) is solved iteratively, using the Newton-Raphson method:

$$\mathbf{u}^{(n+1)} = \mathbf{u}^{(n)} - \left[\mathbf{L}'(\mathbf{u}^{(n)})\right]^{-1} \mathbf{L}(\mathbf{u}^{(n)}) \tag{27}$$

where:

$$\mathbf{L}' = \begin{bmatrix} \frac{\partial L_1}{\partial u_{ix}} & \frac{\partial L_1}{\partial u_{iy}} & \frac{\partial L_1}{\partial u_{jx}} & \frac{\partial L_1}{\partial u_{jy}} \\ \frac{\partial L_2}{\partial u_{ix}} & \frac{\partial L_2}{\partial u_{iy}} & \frac{\partial L_2}{\partial u_{jx}} & \frac{\partial L_2}{\partial u_{jy}} \\ \frac{\partial L_3}{\partial u_{ix}} & \frac{\partial L_3}{\partial u_{iy}} & \frac{\partial L_3}{\partial u_{jx}} & \frac{\partial L_3}{\partial u_{jy}} \\ \frac{\partial L_4}{\partial u_{ix}} & \frac{\partial L_4}{\partial u_{iy}} & \frac{\partial L_4}{\partial u_{jx}} & \frac{\partial L_4}{\partial u_{jy}} \end{bmatrix}. \tag{28}$$

The Jacobian matrix **L'** and the vector **L** 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 **L'** and **L**, the constraints are applied using elimination method. The main concept is to assume some initial positions of molecules (eg. undeformed lattice) and obtain final, stable equilibrium configuration of atoms with appropriate boundary conditions.

## 4. The multiscale model

The construction of the multiscale model is shown in Fig. 5. The discrete model occupies only rather small area of the model $\Omega_a$, where the simulation at the nanoscale should be performed. The rest of the structure $\Omega$ is modelled by BEM.

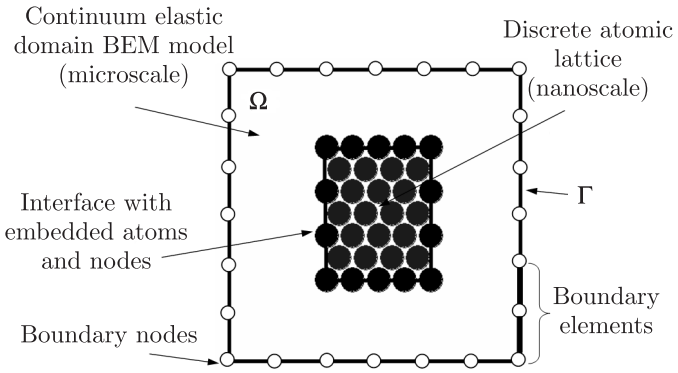


Fig. 5. The coupled BEM-atomic multiscale model

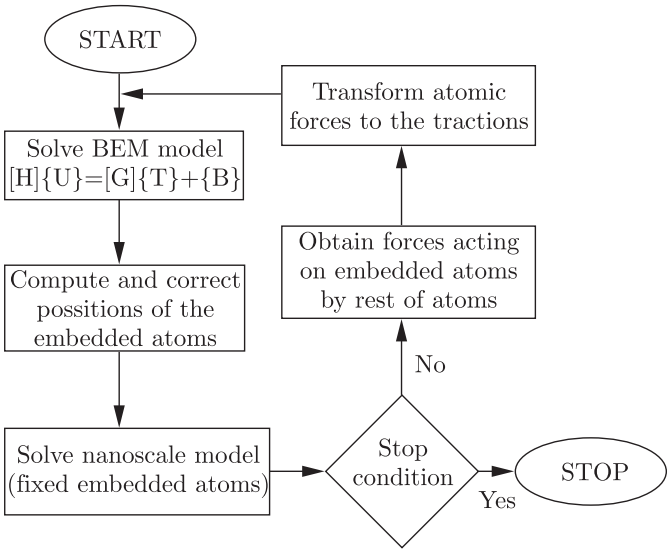


Fig. 6. The algorithm of solving coupled atomistic-BEM model

The interface $\Gamma_a$ 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 Fig. 6.

In the first step, the microscale boundary conditions are applied and the BEM model is solved (Fig. 6). 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 previous section. Finally, forces acting on interface atoms are computed and introduced as a tractions nodal values to the BEM model. These computations are repeated iteratively until the 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) $\varepsilon$.

## 5. Numerical examples

Some numerical simulations were performed using the technique described in above sections. In the first example the plate witch the u-shape notch under the shear load is presented (Fig. 7a):

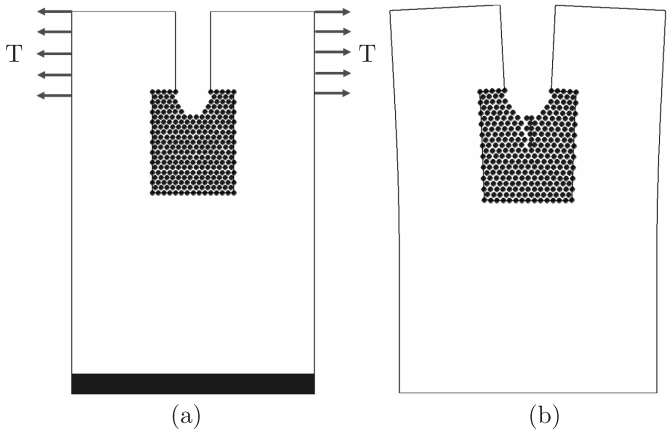


Fig. 7. The plate with the notch under the tensile load: initial equilibrium without any load (a), equilibrium state of the loaded plate (b)

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 18×12 nm. The continuum model contains 61 quadratic elements and 244 degrees of freedom. The atomic model contains 282 atoms, 546 degrees of freedom. The Lennard-Jones potential was used with the following parameters: $\sigma$ = 0.2575 nm, $\varepsilon$ = 0.1699 nN*nm, r0 = 0.289 nm, values are taken from [12]. The potential describe material with properties close to the aluminum.

Figure 7b shows the result of the numerical simulation. The atoms displaced to the new equilibrium positions under the loaded continuum model. It can be observed that a crack at the centre of the notch is arising.

The next example shows a plate with the U-shape notch (Fig. 8a):

The bottom of the plate is constrained and the shear load is applied on the right side. Dimensions of the plate are 40×27 nm. The continuum model contains 113 quadratic elements. The atomic model contains 884 atoms (1768 degrees of freedom). The parameters and material properties are the same as in previous example.

Results of the numerical simulations are presented in Fig. 8b. The atoms moved to find a new equilibrium state. Opening of the cracks at the corners of the notch can be observed.

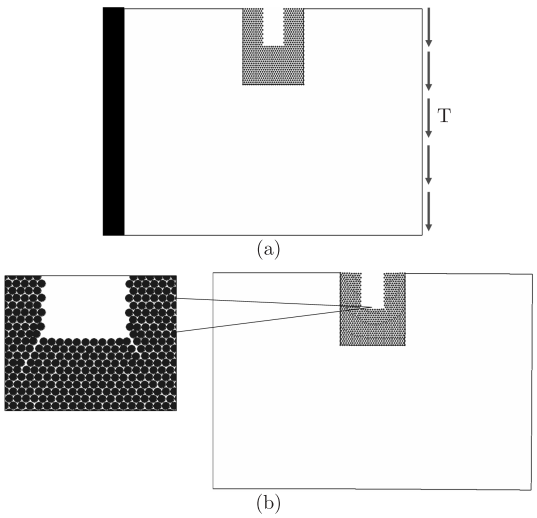


Fig. 8. The plate with U-notch under the shear load: initial equilibrium without load (a), equilibrium state under shear load (b)

## 6. Final remarks

This kind 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 more realistic results can be obtained using EAM potential. The presented examples can be treated as benchmark problems. 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 from 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. [13]. The applications of these algorithms in prediction of atoms distribution give a great probability of finding the global optimal solutions but this kind of 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 [12]. In this case the continuum BEM model will be described by the application of the second order gradient stress theory [14].

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