APPLICATION OF MOLECULAR DYNAMICS SIMULATIONS TO MODELLING OF INDENTATION

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ABSTRACT

A three-dimensional large-scale molecular dynamics (MD) model of indentation of a pyramidal diamond indenter into a copper single crystal will be described. The attention will be focused to the formulation of a new updating algorithm of non-fixed list of neighbouring atoms of each updated atom in a MD-simulation. This algorithm saves computational time due to the simple fact that only neighbouring atoms laying in the cut-off radius of given atom are taken into account to compute acting forces. The list of neighbouring atoms is dynamically changed during simulation. Therefore, arbitrary large deformations can be simulated without loss of numerical preciseness. Linear dependence of simulation time on the number atoms involved is proved, up to one million of atoms, for this algorithm. It will be shown that the penetration of a diamond indenter into a copper single crystal leads to force hysteresis. The shape of hysteresis curves which represents the dependence of the normal acting force on the penetration depth is strongly affected by the size of the simulation block. The proposed concept of handling of neighbouring atoms can be easily applied to different types of MD-models as for example scratch tests.

KEYWORDS

Indentation, molecular dynamics simulations, scratch test.

INTRODUCTION

The devolopement of experimental instruments with atomic resolution enables us to study and measure surface and bulk material properties at nanoscale. Analytical studies yield interatomic potentials, such as pair, three-body, and embeded atom. Those potentials give the possibility to perform numerical simulations of material behaviours at the atomic-scale. Molecular dynamics (MD) simulations have been proven as a suitable method to determine instantaneous material properties. Atomic simulations are used to model adhesion, indentation, cutting, etc. in recent MD studies [1].

By indentation we understand penetration of an indentation tool into a tested material. Indentation at nanoscale is used to determine surface properties of different materials with or without suface improvements. It donot destroy the tested material (cf. details in [2-4]).

Generally there are two commonly used techniques of computation of forces affecting an atom under consideration. In the first one, it is assumed that all atoms involved in a simulation influence an atom under consideration. This is the simplest technique that is extremely computationally inefficient and leads to the parabolic dependence of simulation time on the total number of atoms. In the second one, all atoms lying in some restricted neighbourhood called cut-off radius only influence an atom under consideration. It stems from the assumption that influence of atoms that have bigger distance then some prescribed radius is negligible. A fixed list of neighbouring atoms of every atom involved in a simulation is used.

It is evident that such a fixed list of atoms can leads to incorrect results in the case of large deformations. In this case, atoms can be mixed, and therefore a fixed list of neighbouring atoms cannot be used. Therefore, a completely new algorithm ensuring us that actual neighbours of an atom are taken at any particular time of a simulation for arbitrary deformation will be proposed. Preliminary results of this model with new updating algorithm of non-fixed list of neighbouring atoms were published in [5].

MODEL

A three-dimensional molecular dynamics model of indentation of a pyramidal diamond indenter into a copper single crystal will be described in this section. A new updating algorithm of non-fixed list of neighbouring atoms will be explained in the next section. Initial positions of copper atoms are located at the theoretical crystalographical positions of face centred cubic (fcc) lattice. Positions of copper atoms are not fixed. The diamond lattice prescribes positions of carbon atoms creating the indenter that move as a compact body because the diamond indenter is rigid.

Forces defined by interactions with other atoms influence movement of an atom under consideration. In our case, those forces result from two-particle potentials, i.e. potentials between the atom under consideration and different atoms laying in the cut-off radius. Only two types of potentials are present in our simulations, namely, Johnson potential of copper-copper, and Born-Mayer potential of copper-carbon interactions.

Johnson type potential of copper-copper (*Cu-Cu*) interactions for the bulk material has the form

$$\varphi_{Cu\text{-}Cu} = b_3 \cdot (r - r_0)^3 + b_2 \cdot (r - r_0)^2 - d_1 , \tag{1}$$

where b_3, b_2, r_0 and d_1 are constants of $-1.09 \cdot 10^{11}$ [J/m^3], 13.69 [J/m^2], $2.56 \cdot 10^{-10}$ [m], and $3.20 \cdot 10^{-20}$ [J] respectively. Constant r_0 represent the equilibrium distance of copper atoms. The value of cut-off radius r_C is defined by the point where the space derivative of this potential reach the value of zero ($\partial \varphi_{Cu\text{-}Cu} / \partial r = 0$) and is equal to 0.94 of Cu lattice constant. Such size of the cut-off radius causes that twelve neighbouring atoms influence an bulk atom under consideration. The force is repulsive for distances smaller than r_0 and attractive above this value up to the cut-off radius.

Born-Mayer potential of copper-carbon (*Cu-C*) for the interaction of copper with a diamond indenter

$$\varphi_{Cu\text{-}C} = c \cdot \exp[-2\alpha (r - r_0)] - d_2 , \tag{2}$$

where c, α, r_0, and d_2 are constants of $7.37 \cdot 10^{-20}$ [J], $9.55 \cdot 10^{9}$ [1/m], $2.56 \cdot 10^{-10}$ [m], $2.40 \cdot 10^{-22}$ [J] respectively. The cut-off radius $r_{Cu\text{-}C}$ is equal to $1.5 \cdot r_0$. This force is repulsive for any distance of copper and carbon atoms.

Constant d_1 and d_2 are taken in such way that appropriate potentials reach the value of zero at the distance equal to the cut-off radius. Otherwise, it leads to step-like force when an atom approaching the atom under consideration cross the cut-off radius and those potentials do not reach zero value at the cut-off radius.

Force acting on an atom under consideration, computed from potentials, cause movement of atoms involved in the simulation. We just use the well-known equation of force F

$$F = - \text{grad} (\varphi) \ , \tag{3}$$

where the potential φ is expressed by the following sum of two-particle potentials

$$\varphi = \Sigma_{\{i \in N\}} \varphi_i \ . \tag{4}$$

N represents the set of all atoms that are used to compute potentials acting on an atom under consideration.

The resulting force F enters the following equation of motion that is used to compute displacement of an atom under consideration. Equation of motion has the form

$$F = m \cdot a \ , \tag{5}$$

where m is the mass of an atom and a is the acceleration of given atom. For simplicity, no damping is used in the equation of motion. Such damping term should be a function of velocity of given motion. We know that acceleration a is the second time derivative of displacement s of the atom

$$a = d^2s / dt^2 \ . \tag{6}$$

New positions of atoms are computed from old positions of atoms and forces acting on them. Simply we insert equations 3 and 4 in equation 5. Mass m of a copper atom is known. Therefore, a new position of an atom can be computed by integration of equation 6.

External forces affecting a particular simulation should be defined. We consider that a vertical movement at the bottom of the simulated atomic structure is not allowed. Movement of the rigid indenter defines the other external force. The indenter moves compared to the deformed atomic structure with a constant velocity. Movement of the indenter inserts energy into the system.

UPDATING ALGORITHM OF NON-FIXED LIST OF NEIGHBOURING ATOMS

We assume that the three-dimensional finite space is divided into a fixed and uniform grid of cuboids that completely fill the finite space occupied by atoms involved in the MD-simulation. The size of a cuboid is half of the cut-off radius in the x and y direction, and the cut-off radius in direction z. Therefore statistically one atom is located in one particular cuboid. Any atom belongs to the only one cuboid from all possible cuboids. None, one, or more than one atom can be located in one cuboid. Let us take one particular atom under consideration. This atom belongs to one specific cuboid of the grid. Let us draw balls with

radius equal to the cut-off radius from every point of this cuboid in which the atom lays. All cuboids that are fully or partly located in any of those balls belong to the neighbourhood of given cuboid; such neighbourhood is uniform in the space. It is assumed that all atoms located in neighbouring cuboids are neighbouring atoms of an atom under consideration and have to be used to compute the force F. It has to be tested to which cuboid this atom belongs every time when a new position of given atom is computed. The reason is that the atom can cross the border of the cuboid.

The remaining task is the way of updating the list of atoms that belong to a cuboid. Generally, there are two possible ways solving this problem. The first one requires massively parallel computers that are not accessible yet. In this case, the position of every atom is updated by a processor that belong to this atom only that is independent from other atoms and processors. It means that processors are distributed. The same is valid for memory. The second possible way is to use a special transformation function which enable us to simulate a virtual parallel computation on the classical von Neumann type of computer. This leads to the definition of *hash* and *heap* vectors that are used in the proposed MD-model.

Firstly, let us define the hash vector that is composed of pointers. The position of pointer in the hash vector uniquely defines the number of the cuboid. Numbering of cuboids should go in direction of dominant deformation otherwise computational load increase dramatically. Cuboids are fixed during the whole simulation.

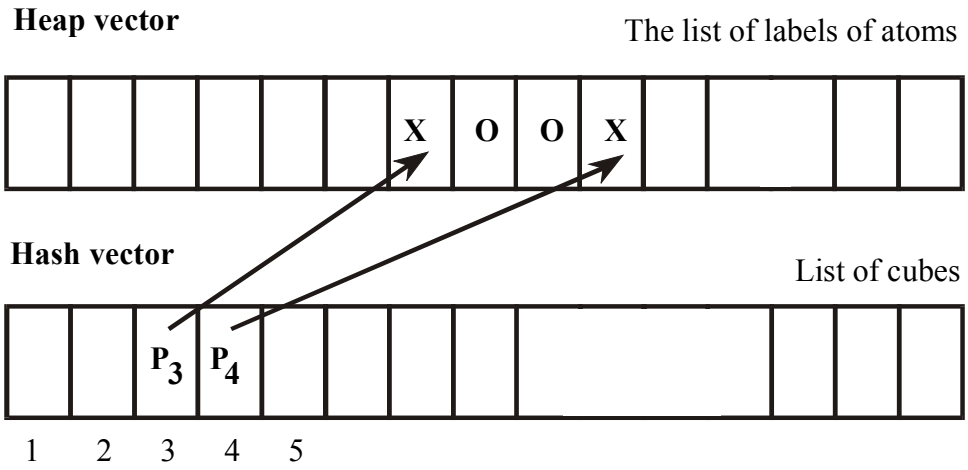

Fig. 1. Schematic description of the algorithm using the hash and heap vectors that updates the list of labels of atoms that belongs to arbitrary cuboid. End of list of atoms belonging to one cuboid is marked by symbol X.

Secondly, let us define the heap vector in which labels of every atom are stored. Those labels uniquely define every atom. Pointers from the hash vector points to labels of atoms in the heap vector. The heap vector is composed of blocks of atoms (of size 1,2,3,…) belonging to one particular cuboid. Every pointer points to the end of a block. Therefore, the end of the previous block uniquely defines the beginning of the block. If an atom changes the position during a simulation step and cross the border of the cuboid then the heap and hash vectors have to be updated. If necessary the atom is moved into different block of atoms belonging to different cuboid. This algorithm is schematically described in Fig. 1.

It have been tested that simulation times are linear up to 1 065 000 atoms what was the highest simulated number of atoms for the proposed algorithm. The total simulation time of the sample with 1 065 000 atoms and simulated for 2000 time steps is 12.8 hours. Higher numbers of simulated atoms requires larger portion of RAM memory than 128MB otherwise swapping of RAM occur which destroy the linear dependence of the total simulation time on the total number of atoms.

RESULTS AND DISCUSSION

The first and the most important result of the proposed MD-model, i.e. the dependence of the total simulation time t on the number of atoms N involved in the simulations for the fixed number of 2000 simulation steps reads

$$t = a\,N + b\ , \tag{7}$$

where constants a and b, reached by linear regression, are equal to 80.2161 and 0.0430, respectively. The regression coefficient is equal to 0.9998. All computations were carried out on a 400 MHz Pentium III PC. This linear dependence of total simulation time t on the number of atoms N enables us to use normal PC to simulate extra large samples for relatively short times.

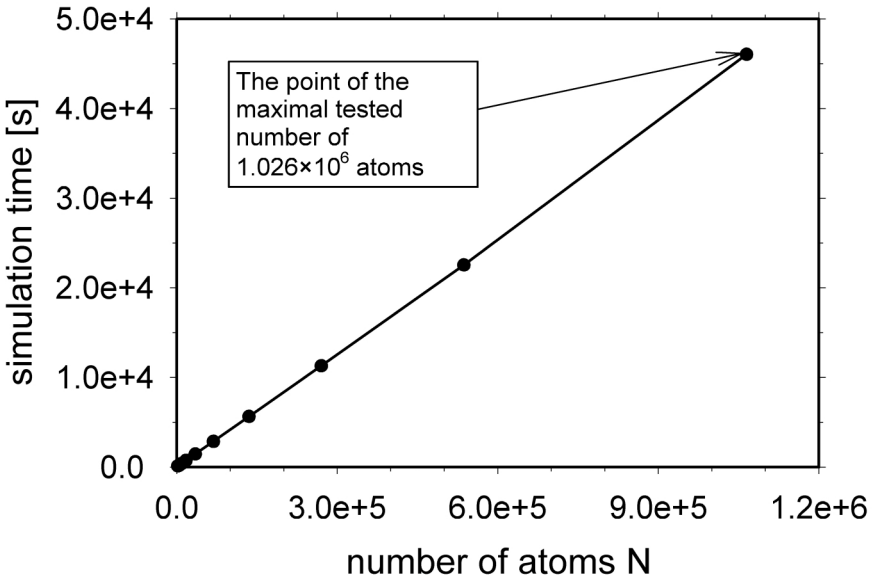

Fig. 2. Dependence of the total simulation time t on the number of atoms N involved in the simulations for 2000 simulation steps.

Firstly, the developed MD-model has been applied to indentation of diamond indenter into a copper single crystal of different sizes. Cuboids of different sizes of 128, 512, and 1026 thousands of atoms, namely, were taken. Loading algorithm of indentor have three parts: (i) loading in direction perpendicular to the surface by the velocity 200 ms^{-1} for 1000 simulation

steps, (ii) stop for 500 simulation steps, (iii) the direction of movement is instantly reversed with the same velocity of 200 ms^{-1} for 500 simulation steps.

If one would like to compare simulated data to experimental data then the best way, in our case, is to take dependence of acting force F on the penetration depth h of the indenter. Despite the fact that a relatively small sample is used the resulting force curve has same hysteresis shape as experiments on bigger samples. Small size of the sample and the indenter leads to small resulting force. Force gradually increase during loading and gradually decrease during unloading (cf. Fig.3). The curve is not smooth because of irregular movement of atoms. Larger samples lead to more smooth curves.

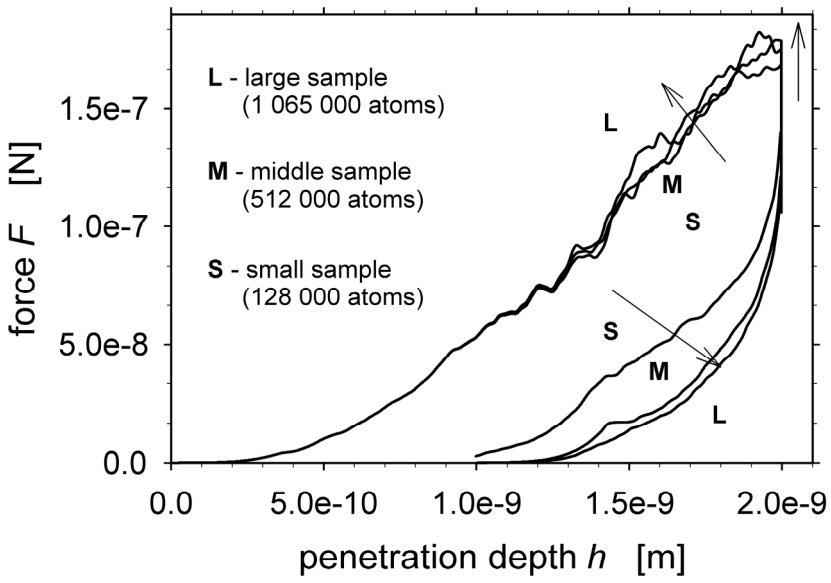

Fig. 3. Hysteresis curves resulting from sequential loading and unloading of samples by indenter where dependence of force F acting on the penetration depth h is displayed for three different sizes of samples, i.e. 128, 512 and 1 065 thousands of atoms.

Arrows in Fig. 3 marks the directions of shifts of different parts of hysteresis curves as the size of sample increase. The unloading branch of hysteresis curve is substantially shifted down as the crystal size increase. The loading branch is less influenced than unloading one as the size of simulated crystal increase. Saturation of hysteresis curve, as the size of crystal increase, has not been observed. It is expected that even bigger crystals are necessary to reach saturation.

A larger sample is less deformable. It has been observed that larger samples attain higher local deformation compared to small samples that move almost as a rigid body. Therefore the indenter is more penetrated into a larger sample what results in the increase of the maximal force at the turning point of indentation (cf. arrow pointing up in Fig. 3).

Dependency of potential E_P and kinetic E_k energies on simulation step compared to force F is displayed in Fig. 4 for simulation with 1 065 000 atoms. The initial increase of potential

energy is followed by almost constant energy during stop of indentor and then by a decrease when the direction of movement of indentor is reversed. Potential energy is transformed into kinetic one. Fig. 4 clearly reflects the loading algoritm.

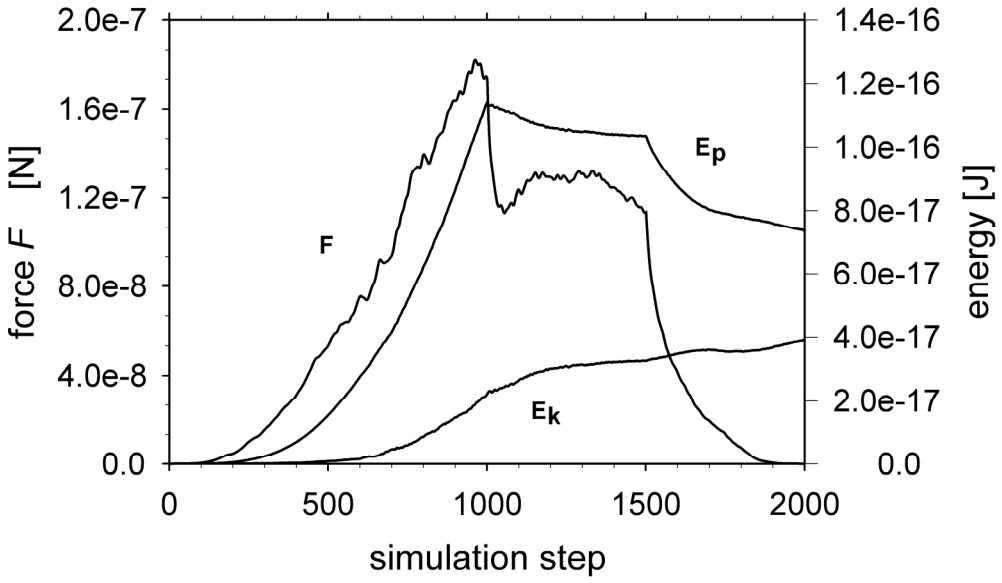

Fig. 4. Dependencies of potential E_P and kinetic E_K energies on simulation step compared to force F for the crystal of size of 1 065 000 atoms. The initial increase of the potential energy is transformed into the kinetic one.

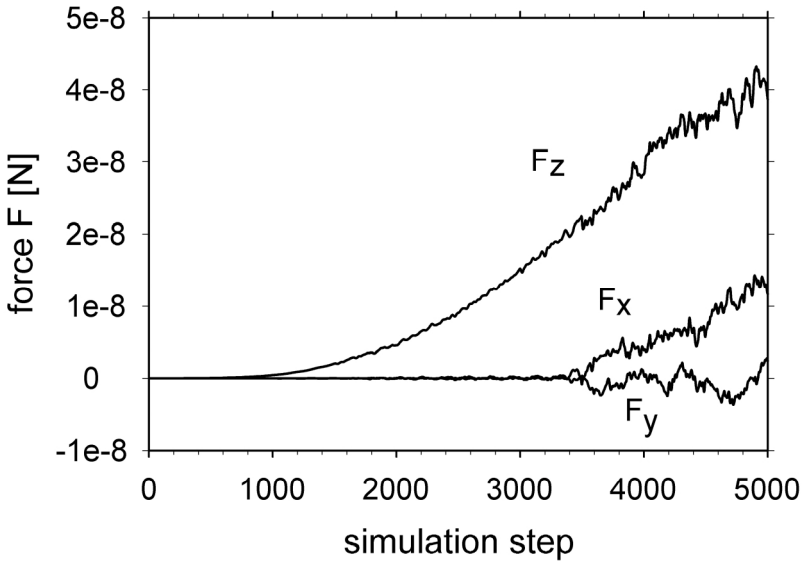

Fig. 5. Forces F_x, F_y, F_z that act on the tool with dependence on simulation step. Fluctuations for larger penetrations of indenter are observed. Relatively large fluctuations are present for F_x and F_y .

As the second application, the MD-model has been applied to the following scratch test. Copper surface of a single crystal has been scratched by a diamond tool, having the same size as in the case of indentation, with the velocity of 200 ms^{-1} in the direction parallel to the surface of the crystal (x direction), and with the velocity of 20 ms^{-1} in the direction perpendicular to the surface of the crystal (z direction).

Forces F_x, F_y, F_z that act on the tool with dependence on simulation step can be seen in Fig. 5. Force F_z stems from the repulsive reaction of the crystal on the penetration of the indenter, and therefore reach the highest value from all forces. Fluctuations for larger penetrations of indenter are observed. Relatively large fluctuations are present for F_y . The reason is simple; no external force acts in direction y. Force F_y results from local deformations of deformed crystal on scratching process.

CONCLUSIONS

A three-dimensional large-scale molecular dynamics (MD) model of indentation of pyramidal diamond indenter into a copper single crystal have been proposed in this work. The attention has been focused to the formulation of a new updating algorithm of non-fixed list of neighbouring atoms of each updated atom in MD-simulation. Linear dependence of simulation time on the number atoms involved is proved for the maximum of one million atoms. Higher numbers of simulated atoms requires larger portion of RAM memory than 128MB. The total simulation time of the sample with 1 065 000 atoms and simulated for 2000 time steps is 12.8 hours.

As an example of application of this new algorithm, indentation a copper single crystal by a diamond indenter have been simulated. Force hysteresis is observed as expected from experiments. A strong dependence of force F, potential energy E_P, and kinetic energy E_K on the size of the crystal and loading algorithm has been observed. The concept explained in this paper which saves computational load can be easily applied to different applications of MD-simulations. Scratch tests were performed as the second application of MD-model.

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