In situ Transformations of Gold Contacts Studied by Molecular Dynamics Simulations

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ABSTRACT

We apply molecular dynamics methods for simulation of in situ processes in new combined TEM/SPM technique. The atomic structure transformations of a gold nanobridge between two contacts are studied in processes of loading-unloading and friction cycles, vertical, lateral, diagonal and zigzag motion. In all cases only a single-atom contact is broken at the final stage of deformations. The deformation process strongly depends on the velocity of fracture and schemes of motion.
Keywords: molecular dynamics simulation, TEM-SPM

1 INTRODUCTION

Contact phenomena between metallic and ceramic nanoparticles play a key role in the processes of adhesion, seizure, friction, indentation, sintering, recrystallization, deformation, etc. Till recently the nanocontact phenomena studies were limited only to observations and analysis of transformations ex situ. Recently developed TEM/AFM technique [1,2] allows us to visualize an atomic structure of contacts under deformation in situ in couple with a simultaneous measurement of driving tip-sample nN-forces. However, mechanism of contact deformations during such experiments is not sufficiently understood.

Modeling and simulation is an effective theoretical method for observation of a cantilever and tip motion in SPM [3-9]. Molecular dynamics (MD) simulations were widely used for calculation of nanowires deformation with picosecond resolution during lateral and normal motion of tips [3-4,6,8]. The purpose of this report is to investigate the mechanisms of atomistic transformations of gold nanocontacts under lateral, normal and zigzag motion. We combined theoretical MD technique and experimental TEM/AFM [1,2] to study contact phenomena at the nanolevel for gold.

2 CALCULATION METHODS

To simulate the dynamical evolution of the contact we used original SIDEM software . MD simulation was performed using original empirical short-range pair potential for Au. The potential ensures the stability of fcc gold lattice. We modeled the contacts by two different ways.

The first modeling was the loading-unloading and friction cycles calculations of gold-tip with different radii and gold surface. An example of contact of Au-tip of 4 nm in radius with Au (100)-surface is shown in fig.1.a. The loading-unloading cycle was simulated by moving of the tip by a step of 0.01a to the sample (1-200 steps) and then away from it (201-400 steps), were a=0.408 nm - lattice period for Au. The friction cycles were modeled by moving of the tip with the same step size along the surface (1-200 steps) and backwards (201-400 steps) at the different heights.

The second modeling is the nanobridge deformations calculations. The calculated gold nanobridge of 8X8X8 lattice period total contains 2433 atoms. The nanobridge consists of two grains or parts, upper and lower. The all 1132 atoms of upper part at each step undergo the the following displacement: (i) in lateral direction with a step of 0.01a, (ii) in normal direction with the step 0.01a, 0.1a, 0.3a, (iii) in diagonal direction with a step of 0.014a and (iv) zigzag motion with the step 0.01a. Cases (i) and (ii) correspond to shear and strain deformations, respectively. Case (iii) corresponds to more complex deformation with both components. Case (iv) corresponds to motion with lateral vibration. The total numbers of displacement steps were 1000.

For both calculations at every step a sufficient time was given for the tip-surface or nanobridge system relax in a stable state. Dynamical relaxation was carried out after each displacement step. The structures of contact as well as radial distribution function were calculated also after each step of the relaxation. The process of dynamical evolution in all cases is represented as the series of snapshots. The snapshots image of all atoms in the narrow plane dy=(0,a), crossing the centre of tip-surface or nanobridge in plane (x,z). Atoms in the (0, a/2) and (a/2, a) planes are shown by open and black circles, respectivelyallowing the evolution of two central atomic planes may be analyzed. We did not use any thermostat for

calculation of temperature dependences. There were not any important differences between the results obtained at 12 K and 290 K in the resent molecular dynamics experiments [6].

3 RESULTS

3.1 Loading-unloading and friction cycles

The results for loading-unloading cycle are presented at fig.1. At the loading ther "adhesion avalanche" instability was oserved .Neighboring tip and surface atoms jumps abruptly to meet each other at a height of 0.46 nm. A number of contact bonds changes from 16 to 905, adhesion force drops from -1.6 nN to -50 nN. The radius of created contact equals to ~1 nm, closely to experimental ones. The contact is compressed (at loading) and stretched (at unloading) so as the interaction type is elastic. Then, at subsequent unloading several instabilities and reorganization of contact appear. Calculated values of yield strength at the points of contact reorganizations (points A, B, C and D in fig.1.c) equal to 3-6 GPa, which is consistent with experimental values of 5 GPa calculated by us in the TEM/AFM experiment [2]. At the final image a reorientation of tip structure from (001) to (111) are observed (fig.1.b).

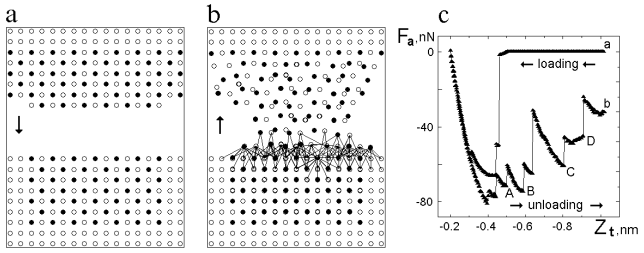

Fig.1. Snapshots of gold tip-surface contact before loading (a) and after unloading (b) and calculated adhesion force variations (c). Open and black circles show atoms in adjacent (001)-planes.

The frictional cycles were modeled for different heights, namely 0.3a, 0.5a, 0.6a, 0.7a, 0.9a. It was found that the critical height was 0.6a. If the height of scanning was below of this critical value the tip was blunting and wearing. In this case the scanning run with the defect formation, such as blocks, twins and cracks formation and its healing. The effect of subsurface atoms seizure by tip apex atoms was observed. This “subsurface seizure” effect consists in formation of ideal crystalline structure of subsurface atoms with apex atoms and cracks in subsurface itself. The contact structure in this case is an atomic "iceberg" submerged in the surface "ocean". These findings allow us to find a more effective mode of the TEM holder motion.

3.2 Nanobridge deformations

Just before breaking of nanobridge in TEM/AFM experiment the forces up to 10 nN was observed, see [2]. Junging from this breaking force the number of breaking atoms could have correspond to ten. Beside this the creation of the double neck was observed. We tried to explain these results. For this purposes we modeled the elongation of nanobridge in three different directions: [100], [010] and [110] and employed several different schemes of upper grain motion, including vibration.

In all cases strong rearrangements of the nanobridge are observed. The nanobridge thins step by step with defect formation, such as vacancies, twins, grain boundaries, surface steps. At the final stage of the deformation only single atom contact is broken in any cases. But the mechanism of deformation differs for different cases. During strain deformations reorientation from (100) to (111) planes for all atoms of nanobridge take place with formation of zig-zag vacancy cavities like in loading-unloading modelling (fig1.b). During shear deformations the tilt and slips along (110) plane take place with formation of twins. During shear and strain deformations rotation of grains take place with formation of several grain boundaries, vacancies and steps (fig.2).

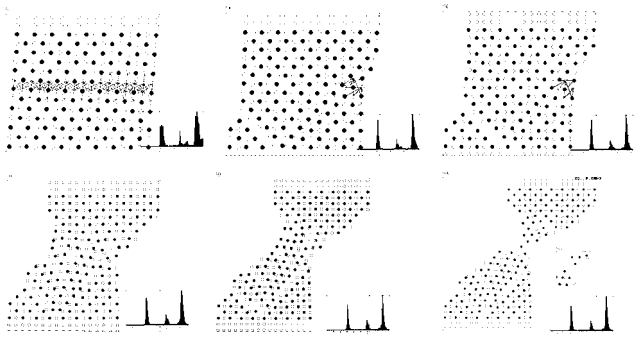

Fig.2. Snapshots of the nanobridge during shear and tensile strains at N-steps DX=0.01a and DY=0.01a.

It should be noted that Marszalek at. al. [9] experimentally confirmed the sliding of crystal planes within the gold nanowires with changing of the local structure from fcc to hcp. Such reconstraction during strength are well known for plastic deformation of fcc metals [10].

The velocity influences on the deformations were studied. For study of speed effects on the deformation process we have studied the tensile strain with different step, namely 0.01a, 0.1a and 0.3a. If the velocity of atomic relaxation more then the velocity of fracture than plastic behaviour takes place. If the velocity of fracture more then the velocity of an atomic relaxation the brittle behaviour takes place.

We modelled the lateral vibration of TEM holder as zigzag motion of upper grain. The motion at every step were modelled as total displacement in the elongation direction, summarized from two diagonal motion. During vibration we observed formation of two nanobridges so as in the real experiment [1,2].

CONCLUSION

We may conclude that the process of nanocontact deformation is more complex in comparison with the well known MD simulations [3-8]. During modelling of nanocontact evolution we must take into account the directions of deformation (not only parallel or perpendicular directions), the velocities of deformation and the velocities of atomic relaxation, the vibration and temperature effects. If velocity of atomic relaxation greater then velocity of fracture than plastic behaviour takes place, including twining, reconstruction, sliding and nanocracks healing. If the velocity of fracture greater then the velocity of an atomic relaxation the brittle behaviour takes place, including formation of vacancies, their clusters, nanockracks and formation of free surface. The schemes of deformation may be represented as "tilt-slip-tilt-slip-thining" for shear strains, "elongation-recrystallisation-elongation-thining" for tensile strains, "tilt-slip-step formation-tilt-slip-thining" for diagonal strain and more complex with rotation of grains for zigzag motion. In all schemes at the final stage of demormations only a single-atom contact is broken.

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