Molecular dynamics simulation of timescale effect and lattice transformation of copper nanorod under bending

H. A. Wu*, X. X. Wang**, G. R. Liu*

*Singapore-MIT Alliance, National University of Singapore,
10 Kent Ridge Crescent, 119260, Singapore, smawha@nus.edu.sg
**Department of Modern Mechanics, University of Science and Technology of China, Hefei, 230026, China

ABSTRACT

Mechanical behaviors of materials and structures at nanoscale are essentially different from those at macroscale, resulting from surface effect, size effect and time scale effect. In some experimental research at nanoscale, the bending displacement of nanorod is measured and used to gain the lateral force. In our present work, the bending behavior of metal Cu nanorod is simulated by molecular dynamics method. Embedded-atom potential is employed to represent the atomic interactions.

The simulation results show that the bending behavior of metal nanorod is significantly loading rate dependent and nonlinear. It is found that in the elastic bending process, crystal lattice can transform from FCC structure to HCP structure. After such lattice transformation, metal nanorod is thickened and shortened. Its bending stiffness is remarkably strengthened. Whether lattice transformation occurs or not depends on both the loading magnitude and the loading rate.

Keywords: molecular dynamics, nanorod, mechanical behavior, timescale effect, lattice transformation

1 INTRODUCTION

Owing to the progress of techniques and technology with high performance and high efficiency, fundamental understanding of their phenomena and functions from the elementary processes of molecular motion has increasingly been required. This leads to the introduction of molecular mechanical engineering which forms a bridge between microscopic molecular understanding and macroscopic continuum engineering [1]. Microelectromechanical systems (MEMS) have been widely studied for decades, and great progresses have been achieved in the field of commercial application. Nanoelectromechanical systems (NEMS) are now evolving, with new scientific studies and technical applications emerging. Mechanical devices are shrinking in length size to reduce mass, increase resonant frequency, and lower the force constants. Advances in the field include improvements in fabrication processes and new methods for actuating and detecting motion at the nanoscale [2]. The mechanical properties of structures and materials with nanoscale, such as Young's modulus, strength and toughness, are important to proposed applications of nanodevice.

Wong et al. [3] measured the dependence of deflection of a cantilevered nanotube upon an external force applied at different locations along the nanotube, and they then obtained the Young's modulus by fitting their data with a force-deflection relation resulting from the linear elastic mechanics analysis of cantilevered beams. In Poncharal et al.'s experiment [4], deflection was measured as an indirect value to compute the electric force. However, a very important caveat must be kept in mind: is linear elastic theory still reliable at nanoscale?

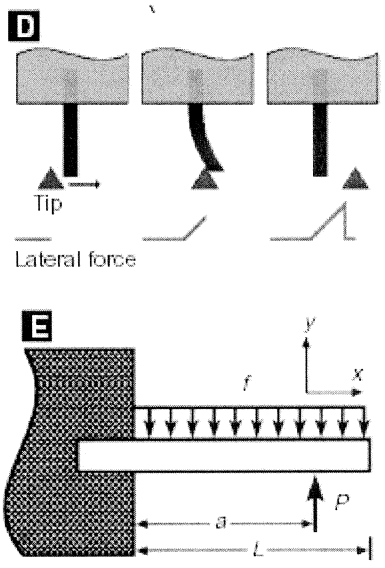

Fig.1 Schematic of beam bending with an AFM tip[3]

At nanoscale one can no longer think of the material as continuum, rather one has to consider that it is formed from discrete atoms. This requires one to analyze how the elements of normal design change as the scale is reduced from millimeter to micron to nanometers. With the Dreiding and universal force fields, Cagin et al. have optimized the structures of the two planetary gear designs and the neon pump with atomistic simulation [5]. This is a good example of computer-aided molecular mechanical engineering. Metal nanowires (nanorods) have received considerable attention for its potential application and theoretical research. Due to the big surface-to-volume ratio, the differences from bulk materials are dramatic. The extension properties, deformation and fracture mechanisms have been widely studied by molecular dynamics simulation [6-9]. High strain rates can even induce amorphization/melting in homogeneous elastically strained fcc single crystal nanowires [9].

In our present work, the bending behavior of metal nanorod is simulated by molecular dynamics method, and some results are discussed. We hope the atomistic simulation results can give much understanding when the mechanical properties of nano-structures are predicted.

2 SIMULATION METHOD

We consider copper nanorod with rectangular section, as figure 2 shows. The size is 1.62nm×1.62nm×20.22nm. The initial atomic configuration is positioned at the fcc lattice sites.

The nanorod is relaxed for 1 ns before the bending loading is applied. In this free relaxation process, the surface atoms move slightly because of losing some of their neighbor atoms, thus the total energy minimizes and the system reaches a stable state. Then one end is fixed by fixing the atomic displacements of four layers. Lateral force is applied at the other end. The force is distributed uniformly to the atoms of two layers. The loading is applied in an incremental way, 0.2pN/(atom·step), ten steps in total. The loading is kept constant during the period of each loading step. The relaxation time of each step varies from 0.02ns to 20ns, which represents different loading rate.

Fig.2 Simulation model of copper nanorod

The EAM potential for copper presented by Johnson [10] is employed as atomic interaction potential. The simulation temperature is kept constant at 0.01K by using velocity scaling method. This is only to ignore the complex influence and focus on the main mechanical mechanisms. The Gear algorithm used to integrate Newton's equations of motion uses up to the 5'th time derivative of the atom positions. The timstep is 0.01ps.

3 RESULTS AND DISCUSSION

The loading-deflection curves of different loading rates are shown in Figure 3. From the figure it is obvious that the bending behavior is remarkably loading-rate dependent. Figure 4 shows the curves of deflections varying with time for different loading rates.

It is found that the result can be considered as a quasi-static one for the loading rate of 20ns/step, because the deflection converge to a stable value during the period of each loading step. For other cases of different loading rates, the deformation does not converge, and the results are considered as dynamical or impact ones. Timescale effect is well illustrated. The deformation of nanorod results from the motion of atoms, and the motion of atoms is dependent on time. If the loading rate is too fast, the motion of atoms is inadequate since lack of time. The nanorod is in a non-equilibrium state during the loading steps.

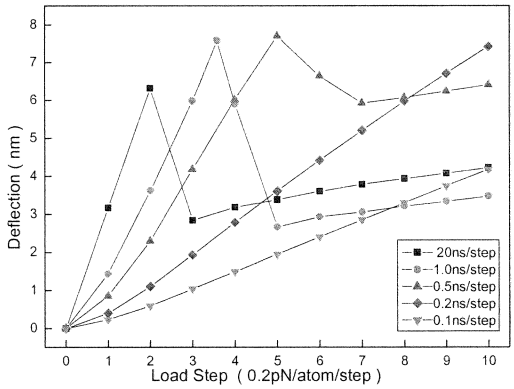

Fig.3 Deformation-load curves under different loading rates

The curves exhibit an abnormality that the deflection decrease with increasing bending loading, which conflicts with what predicted by continuum mechanics. The change of mechanical property of material must result from the change of its micro-structure. From the atomic images, it is found that crystal lattice of the metal nanorod changes when the bending reaches a critical extent. Figure 5 shows atomic images before and after the crystal lattice transformation for the loading rate of 20ns/step.

As a response to the further external bending loading, the crystal lattice of copper nanorod transforms from fcc structure to hcp structure. After such transformation, the nanorod is thickened and shortened. The bending stiffness

is remarkably strengthened. This is the microstructure mechanism which results in the decreasing of deflection of nanorod. From the view of the evolvement of atomic configuration, crystal lattice transformation starts from normal fcc structure, via fast dislocation processes of formation, movement and annihilating, and finally normal hcp crystal lattice structure is produced.

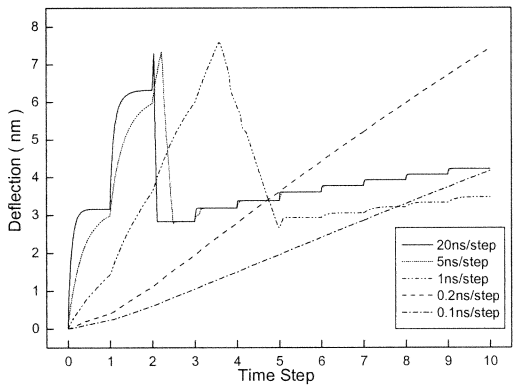

Fig.4 Displacement-time curves under different loading rates

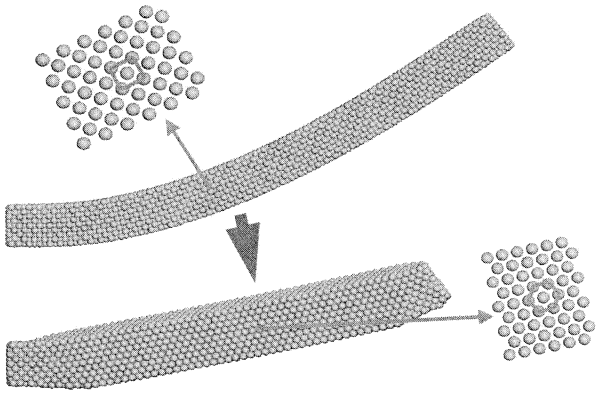

Fig.5 Crystal lattice transformation from FCC to HCP

Before the lattice transformation, the bending behavior of nanorod is elastic, which means that the nanorod will return to its original deformation state once the applied force is removed. The relation of deflection to loading is strictly linear for the quasi-static loading case, which is illustrated by the curve of 20ns/step in Figure 6. When the loading is in a dynamics or impact way, the curves of loading-deflection are not strictly linear, which is illustrated by the other two curves in Figure 6. It exhibits an initial stiffening character, i.e. the bending modulus of initial stage is bigger.

After the crystal lattice transformation, the loading-deflection curves are still linear, but the curvatures are much smaller, as showed in Figure 3. The bending modulus is much increased. During the period of each loading step, the deflection converges quickly, even the loading rate of 0.5ns/step can also be considered as quasi-static loading. This shows that timescale is much different for different structures at nanoscale.

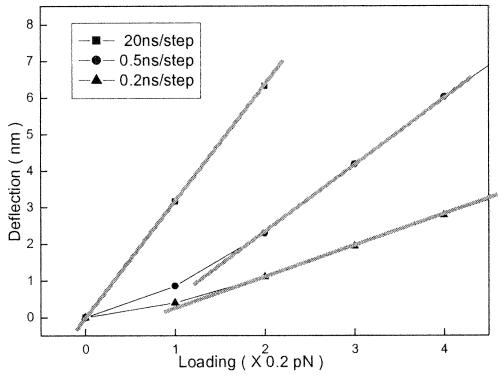

Fig.6 Elastic displacement-loading cruves

It should be noticed that deflection decrease does not occur in the curve of 0.2ns/step loading rate. We owe it to two possible reasons. One is the lack of time to produce transformation, and the other is that the bending does not reach the critical value to produce transformation. To verify it, another two models are simulated. Model (A) can be presented as: first free relaxation to a stable state, then apply 10 loading step, keeping the loading constant, relaxation from another 20 step. Model (B) can be presented as: first free relaxation to a stable state, then apply 10 loading step, keeping the loading constant, relaxation from another 20 step. Each step time is 0.2ns, and each step loading is 0.2pN/atom. The size and boundary conditions are the same as previous presented. The loading-deflection curves are illustrated in Figure 7.

Two models exhibit different deformation mechanisms after the first 10 loading steps. For model (A), during the period of loading steps from 10 to 12, the deflection increases, though the loading is kept constant. This is because during the first 10 steps, the motion of atoms is not inadequate, which results from fast loading and lack of time. Then dislocations emitting and movement result in plasticity. There is a oscillation in the deflection. Plasticity results in the decrease of bending modulus of nanorod, so the deflection increases without any further loading. Finally the deflection converges to a stable value. For model (B), the case is much different. Deflection increases with the increasing loading, then during the period of 13th loading step crystal lattice structure transforms from fcc to hcp. At the same time, dislocations emit and move. Finally the deflection also converges to a stable value. Compare model (A) with (B), it is very interesting that the deflection of (A)

is larger than model (B), while its loading is smaller than model (B), which results from the crystal lattice transformation in model (B). Microstructure decides the property. The comparison of these two models shows that whether the lattice transformation occurs or not is dependent on both the loading magnitude and the loading rate.

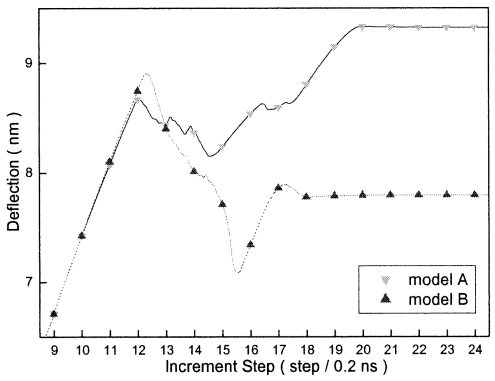

Fig.7 Contrast curves between crystal lattice transformation and dislocation mechanism

It should be specially noted that the mechanical behaviors of metal nanorod is also dependent on the lattice orientation. The bending moduli of nanorod with different lattice orientation are different. The lattice orientation system changes after the crystal lattice transformation.

4 CONCLUSIONS

The understanding of mechanical behaviors of nano-structures is crucial to the engineering design of nano-devices. Molecular dynamics simulation can help me investigate the physical mechanisms of deformation, motion, failure, etc. At nanoscale, due to small size effect and surface effect, the mechanical properties are much different from those at macroscale. The traditional continuum mechanics is not reliable to materials and structures with length size of nanoscale.

The bending behavior of metal nanorod exhibits remarkable loading rate dependence and nonlinearity. In the elastic bending stage, crystal lattice can transform from FCC to HCP. After such lattice transformation, the metal nanorod is thickened and shortened. The bending stiffness is dramatically strengthened. Whether the lattice transformation occurs of not depends on both the loading magnitude and the loading rate.

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