The Kinetics and Modes of Gold Nanowire Breaking

Honghai Liu1, Enyong Jiang1,−, Haili Bai1, Ping Wu1, Zhiqing Li1, and Chang Q. Sun2,−∗

1 Tianjin Key Laboratory of Low Dimensional Materials Physics and Preparing Technology and Institute of Advanced Materials Physics, Faculty of Science, Tianjin University, Tianjin 300072, People’s Republic of China
2 School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798

Molecular dynamics calculations revealed that the operation temperature and the applied tensile stress (f) determine the kinetics, the mode, and the duration of Au nanowire breaking. In the stress range of 0.018 and 0.1 nN/atom, structure relaxation and transition occurs prior to the wire breaking at random positions with occasionally production of gold atomic chains containing 5–7 atoms. If the f is 0.1 nN/atom or higher, the wire breaks abruptly. However, when the f is 0.018 nN/atom or lower, no rupture occurs at all.

Keywords: Nanostructures, Rupture, Molecular Dynamics, Gold Nanowire.

1. INTRODUCTION

Metallic nanowires have attracted considerable interest in recent years due to their novel properties and potential applications in upcoming technologies such as nanoelectronic and mechanical devices.1−10 One of the most significant issues in nanowire applications is the structural stability of the wires under various conditions such as chemical, mechanical, and thermal stimuli.11−13 Generally, the extension of a nanowire is subject to two effects when the wire is under tension. The wire can be prolonged by pulling one or the two ends of the wire either in a constant speed under a non-constant tensile force14−19 or in different speed under a constant tensile stress.20,21 The latter in practice is more reasonable and practical. Unfortunately, only a few works have been done on the constant force stretching. In order to understand the kinetics, the modes, and the breaking times of the wire breaking under different forces and temperatures, we have examined the possible breaking mechanism of a gold nanowire by stretching it with constant tensile forces in a molecular dynamics approach. Results show that the temperature of operating and the strength of the tensile force dominate the kinetics, the mode, and the lifetime of gold wire breaking. At higher temperatures and under stronger tensile forces the wire will break quickly. The nanowire breaks in different ways subjecting to the joint effect of the temperatures and the applied tensile forces.

2. PRINCIPLES AND METHODS

The interaction between the Au atoms in the nanowire is described by the many-body tight-binding potential,22

\[
E_i = -\left\{ \sum_j \xi^2 \exp\left[ -2q \left( \frac{r_{ij}}{r_0} - 1 \right) \right] \right\}^{1/2} + \sum_j A \exp\left[ -p \left( \frac{r_{ij}}{r_0} - 1 \right) \right] \tag{1}
\]

where \( r_{ij} \) is the distance between atom \( i \) and atom \( j \), and \( r_0 \) is the first-neighbor distance at equilibrium. The parameters \( A, p, q \) and \( \xi \) are related to measurement regarding the cohesive energy, lattice parameter, bulk and shear elastic modulus, respectively (Table I in Ref. [22]). Figure 1 illustrates the typical pair potential, the first order (curve F) and the second order derivative (curve D) of the pairing potential. The first order derivative corresponds to the force between the two atoms,

\[
F_{ij} = -\sum_{j \neq i} \left\{ \frac{\partial E_i}{\partial r_{ij}} + \frac{\partial E_j}{\partial r_{ij}} \right\} \tag{2}
\]

We may correspond the inflection point of the D curve

\[
D = \frac{\partial F_{ij}}{\partial r_{ij}} = -\sum_{j \neq i} \left\{ \frac{\partial^2 E_i}{\partial r_{ij}^2} + \frac{\partial^2 E_j}{\partial r_{ij}^2} \right\}
\]

to the maximal bond length before breaking.7

∗Authors to whom correspondence should be addressed.
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Fig. 1. Illustration of interatomic potential energy $E$, interactive force $F$, and the slope of $F$ ($D = \partial E/\partial r$) between two Lennard-Jones atoms. The turning point of the $D$ curve corresponds to the breaking limit of the bond.

Fig. 2. Illustration of the pulling scheme for the nanowire. The left end is fixed; the tensile force $f$ is exerted on each atom uniformly in the pulling region at the right end of the nanowire under various temperatures.

Fig. 3. (a) Temperature and (b) tensile strength dependence of the breaking time of the Au nanowire under constant force for (a) and constant temperature for (b). The inset zooms in the breaking time at smaller forces showing random fluctuations.

We employed a piece of Au nanowire with a $0.816 \times 0.816$ nm$^2$ or $4 \times 4$ atoms cross-section along the FCC(100) direction in the computation. After a 30-ps relaxation at 50 K, the FCC structure of the wire was evolved into the body centered tetragonal (BCT) structure that is relatively stable. We then investigated the breaking kinetics of the relaxed wire under the applied force $F$ at different temperatures, as illustrated in Figure 2. It would be easier in calculations to use the stress $f = F/n$ than to use the $F$ that is shared equally by all the $n$ atoms in the pulling region.

3. RESULTS AND DISCUSSION

First, we calculated the lifetime ($t$, or force holding time before breaking) of the wire by exerting a continuous constant tensile stress amounted at $f = 1$ nN/atom along the wire axis under various temperatures ($T$). The $t - T$ profile in Figure 3(a) shows clearly that the lifetime of the nanowire becomes shorter as relatively higher temperatures. Next, by keeping the temperature at 50 K, we changed the tensile force $f$ to see the lifetime and the breaking mode of the wire. Results in Figure 3(b) show that the lifetime of the wire varies with the $f$ applied. A larger $f$ value will cause the wire to break in a shorter time, e.g., at $f = 0.05$ nN/atom, the wire breaks in 47.1 ps; at $f = 0.1$ nN/atom the wire breaking time turns to be 14.7 ps. It is interesting to note that the curve in Figure 3(b) could be divided into three regions: (i) in the region of $f > 0.1$ nN/atom, the wire lifetime decreases gradually when the the applied force is increased; (ii) within the force region of 0.018 and 0.1 nN/atom, the wire lifetime changes irregularly; (iii) in the region of $f < 0.018$ nN/atom, no breaking occurs to the Au wire even in a longer time (140 ps).

Since the breaking of a chemical bond is a process of increasing the separation between the related atoms to the maximal extent, the breaking time of the chemical bond is determined by speed of the atomic separating. Therefore, the speed of atomic motion along the wire axis determines the lifetime and the kinetics of the wire breaking. The atomic motion depends on the force applied and the ambient temperature of operation. If the operating temperature is higher, the bond will become weaker and break more easily under the same force. A stronger pulling force will speed up the atomic motion along the force direction without sufficient time for structure relaxation. Therefore, at
rapidly and therefore increase the atomic distance quickly. This will cause the atoms in the pulling region to move more quickly. The relaxation is limited by atomic motion. A strong force hand, the diffusion of the pulling effect on the structure is limited. The force direction is at a finite velocity. On the other hand, the diffusion of the pulling effect on the structure of the entire nanowire is limited. However, the monatomic chain appearing and breaking randomly, which is responsible for the fluctuation in the curve of Figure 3(b). In the region of \( f > 0.1 \text{ nN/atom} \), the structure transition from the BCT to the FCC occurs near the pulling region with a scale length \( L \approx f \) depending on the \( f \) value. The transition diffuses into the neighboring region and the transition distance increases as the \( f \) is decreased. The structure transition prolongs the life of the entire nanowire. However, the monatomic chain appears and breaks randomly, which is responsible for the fluctuation in the curve of Figure 3(b). In the region of \( f < 0.018 \text{ nN/atom} \), the tensile force is too weak to break the bond.

One may wonder how the strength of the tensile force could influence the structure of the Au nanowire. As can be seen from Figure 1, the interatomic force acting on an atom depends on the separation between the neighbouring atoms, and hence the atomic motion along the force direction is at a finite velocity. On the other hand, the diffusion of the pulling effect on the structure relaxation is limited by atomic motion. A strong force will cause the atoms in the pulling region to move more rapidly and therefore increase the atomic distance quickly. There will be no sufficient time for the diffusion of structure transition, resulting in a bond rupture nearby the pulling region, without apparent structural transition being resolved (Fig. 4, \( f = 1 \text{ nN/atom} \)). As the tensile force is decreased, the atomic motion becomes slower, which provides sufficient time for larger-scale structure transition diffusion. The lifetime of the wire becomes longer. Because of the diffusion of the structure relaxation, the wire breaks at random points. Therefore, it is difficult to predict accurately the position and time of wire breaking when monatomic chain appears. However, the results may provide guidelines for us to make atomic chains at the strictly controlled temperature and stretching force.

4. CONCLUSION

It is found that the kinetics, the mode, and the lifetime of Au nanowire breaking are sensitive to the strength of the tensile force and the temperature of operating. The wire breaks abruptly at higher temperatures and under stronger forces. If the force is weak enough, no rupture occurs. In the intermediate force region, the wire breaks after a structure transition with the length scale of diffused transition being subject to the force applied. The similar effects might exist in other kinds of materials in nanoscale such as nanobelts and nanoclusters.

Multimedia movie illustration: the breaking kinetics and modes under the forces of 0.1 and 0.04 nN/atom at 50 K.

References
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