Strain rate effect on tensile behavior of the helical multi-shell gold nanowires

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Abstract
A molecular dynamics simulation of the helical multi-shell (HMS) gold nanowires for tensile behavior has been carried out at 4 K temperature. HMS nanowires, not like bulk face centered cubic (FCC) structure, have a multi-shell helical structure. This work compares mechanical properties and deformation behaviors of the 7-1, 11-4 and 14-7-1 multi-shell helical structure under different strain rates. The results reveal that the different strain rate influence the maximum stress, Young’s modulus and deformation behaviors. The Young’s modulus and maximum stress of HMS nanowires are function of the ratio of numbers of surface atoms to the total number of atoms, but tubular 11-4 HMS nanowire is an exception. For different strain rate, many different deformation behaviors are appear which include sliding, multi-sliding, phase transformative, twisting, necking and brittle deformations before breaking.

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1. Introduction
One-dimensional nanowires have attracted great interest in recent years because they have broad applications in different areas, such as in nano-mechanical and nano-electronic devices. Metallic nanowires with well-defined structures of several nanometers in size have been fabricated by using various methods [1–12]. As the scale is reduced to nanometers, the surface, small size and quantum effect dramatically changes the physical and transport phenomena. Gold nanowire becomes quantization of electronic conductance as their diameter is reduced to 2 nm [2]. In recent works, helical multi-shell (HMS) structures have been observed in gold nanowires [1,2] by transmission electron microscopy (TEM). These gold nanowires consist of coaxial tubes with $n$, $n'$ and $n''$ helical atom rows, where $n$, $n'$ and $n''$ denote the number of atoms in the outer, middle and inner shells, respectively; moreover, tubes with an odd number of atoms present a helical structure, whereas those with an even number of atoms do not. The HMS gold nanowires diameters vary from 0.6 to 1.2 nm. The thinnest gold nanowire exhibits a 7-1 shell structure with a diameter of about 0.6 nm, and two other nanowires are 11-4 and 14-7-1. Therefore, the structures of the HMS gold nanowires are different from those of the face centered cubic (FCC) crystalline bulk, influencing mechanical properties and electrical transportation.

Some fundamental studies have investigated the physical properties of metallic nanowires, by simulating molecular dynamics [13–27]. For example, metal nanotubes or nanowires have been melted [13–15], and the interior melting temperature in ultrathin nanowires has been found to be lower than that at the surface. Ultrathin Cu nanotubes collapsed into the empty core at low temperature and this is the main mechanism for the transformation from ultrathin nanotube to nanowire [16]. The mechanical behavior of the copper nanowires in a tensile test has been studied [17,18]. Unusual pentagonal structure in Cu nanowires was found mechanical stretching [19,20]. The strain rate effect induced by amorphizations of Ni nanowires has also been investigated by using molecular dynamics simulation [21]. Moreover, the formation of single-atom chains consisting of metal atoms was observed and studied by experiments and molecular dynamics simulations [22–27].
This work applies molecular dynamics simulation to study the mechanical behavior and deformation behaviors of gold nanowires with three types of multi-shell helical structures, 7-1, 11-4 and 14-7-1 structures, under various strain rates. In this study, all simulations are set at a temperature of 4 K.

2. Molecular dynamics simulation

Ultrathin gold nanowires with a multi-shell helical structure have been recently fabricated [2]. In this simulation, the multi-shell helical structures are constructed and originating from Au(1 1 1) plane, being rolled up with certain helical angle. Fig. 1 presents three types of multi-shell structure, i.e., 7-1, 11-4 and 14-7-1. For 7-1 and 14-7-1, those multi-shell configurations have a single central strand of gold atoms and a tube structure formed from helices of atoms coiled around the axis of the tube; for 11-4, it could be presumed as a cannular type of nanowire.

The many-body tight-binding potential is employed to simulate the interatomic force between the gold atoms [28,29]. The main difference between the many-body potential model and a pairwise potential model is that the interaction between two atoms is considered in the former case to depend not only on two atoms, but also upon their local environment. The tight-binding potential model commences by summing the band energy, which is characterized by the second moment of the d-band density of state, and a pairwise potential energy of the Born–Mayer type. The cohesive energy is thus expressed as follows:

$$E_c = \sum_{i=1}^{n} \left\{ -\sum_j \xi^2 \exp \left( -2q \left( \frac{r_{ij}}{r_0} - 1 \right) \right) \right\}^{1/2} + \sum_j A \exp \left[ -p \left( \frac{r_{ij}}{r_0} - 1 \right) \right]$$

where $\xi$ is an effective hopping integral, $r_{ij}$ the distance between atom $i$ and $j$, and $r_0$ is the first-neighbor distance. The parameters $A$, $p$, $q$ and $\xi$ are determined by the experimental data concerning cohesive energy, lattice parameter, bulk modulus and shear elastic constants $C_{44}$ and $C' = 1/2(C_{11} - C_{12})$, respectively. Furthermore, the force as negative gradient of cohesive energy, the interaction force on atom $i$ is given by:

$$F_i = -\sum_{j \neq i} \left( \frac{\partial E_i}{\partial r_{ij}} + \frac{\partial E_j}{\partial r_{ij}} \right)$$

Table 1 lists the parameters of the tight-binding potential associated with Au in the current simulation [29].

The loading state in the molecular dynamics simulation for the tensile test is as follows; the loading is applied along the axis, and top and bottom layers are set as fixed layers; the others are set as thermal controlled layers. The following scaling method is adopted to ensure that the temperature of the system remains constant during simulation [30]:

$$v_i^{\text{new}} = v_i \sqrt{\frac{T_D}{T_A}}$$

where $v_i^{\text{new}}$ is the velocity of particle $i$ after correction, $T_D$ and $T_A$ are the desired and actual temperatures of the system, respectively. This scaling method is applied during the simulation for a specific equilibrium temperature.

The stress in the atomistic simulation $\sigma_{mn}$ on $m$-plane and $n$-direction is calculated as:

$$\sigma_{mn} = \frac{1}{N_S} \sum_i \left[ m_i v_i^m v_i^n V_i - \frac{1}{2} V_i \sum_j \frac{\partial \phi(r_{ij})}{\partial r_{ij}} r_{ij}^m r_{ij}^n \right]$$

where $m_i$ is the mass of atom $I$, $V_i$ the volume assigned around to atom $I$, $N_S$ the number of particles contained in region S, where S is defined as the region of atomic interaction, $r_{ij}$ the distance between atoms $i$ and $j$, and $r_{ij}^m$ and $r_{ij}^n$ are the two components of the vector from atom $i$ to $j$. The first term of the right hand side of Eq. (4) represents the kinetic effect associated with atomic motion, and will be affected by temperature. The second term is related to the interactive forces and the distance between the atoms.
of the ultrathin gold nanowires can be obtained using Eqs. (4) and (5).

The Verlet algorithm [30] is employed to calculate the trajectories of the atoms and in the tensile test, the loading is applied to the Au nanowires after relaxation for 50 ps.

3. Results and discussion

This study addresses tensile tests of HMS gold nanowires with 7-1, 11-4 and 14-7-1 structures. The engineering stress and strain relationships and the morphologies of the deformation for different strain rates are shown in Figs. 2–5. The results reveal that the stress–strain relationships and deformed morphologies are strongly affected by strain rate. Figs. 2(a) and 3 show stress–strain relationship and deformed morphologies of 7-1 MHS nanowires for various strain rates. At a lower strain rate, 0.003% ps⁻¹, the stress–strain curve shows a zigzag of increase–decrease in stress as the strain is increased. The maximum stress is located at first yielding point, $\sigma_{33} = 7.0$ GPa and $\varepsilon = 0.07$, and the deformed zone are near to middle region. Increasing the strain rate of the tensile test, the stress–strain curves become smooth. The yielding stress increases first then decreases for large strain rate. When the strain rate is very high, there is no obviously yielding behavior in stress–strain curve. Snapshots of some critical deformed behavior after yielding are shown in Fig. 3(a)–(g). Fig. 3(a)–(d) show the deformed process at strain rate 0.003% ps⁻¹, (e) and (f) are at 0.833% ps⁻¹ and (g) is at 3.333% ps⁻¹. For the quite small strain rate, a zigzag

![Stress–strain relationships for (a) 7-1, (b) 11-4 and (c) 14-7-1 structure under tensile test.](image)

Fig. 2. Stress–strain relationships for (a) 7-1, (b) 11-4 and (c) 14-7-1 structure under tensile test.
stress–strain curve implies successive yielding process. From Fig. 3(a), the atomic configuration of cross-section is transformed from that of the 7-1 structure to that of 6-1 structure after yielding. The 6-1 structure suffuses the nanowire gradually as the strain is increased to 0.13, and the stress raises to near $\sigma_{33} = 5 \text{ GPa}$. Basically, the helical angle between the two areas apart from the sliding zone remains. Continuing to increase the strain, the 7-1 nanowire is necked and the atomic configuration of cross-section changes. Fig. 3(b)–(d) show the snapshots which the cross section of the 7-1 nanowire neck to a width of four, two and one atom chains at different strains, respectively. The dynamics evolution of this quadruple strand, double strand and single strand can be experimentally observed [2]. For the

![Fig. 3. Morphology of the deformed 7-1 nanowire in different strain at various strain rate of (a)–(d) 0.003% ps$^{-1}$; (e)–(f) 0.833% ps$^{-1}$; (g) 3.333% ps$^{-1}$. The strain of all snapshots are (a) $\varepsilon = 0.122$; (b) $\varepsilon = 0.204$; (c) $\varepsilon = 0.27$; (d) $\varepsilon = 0.451$; (e) $\varepsilon = 0.104$; (f) $\varepsilon = 0.242$; (g) $\varepsilon = 0.152$, respectively.](image-url)

stress rate of 0.833% ps$^{-1}$, the maximum stress, $\sigma_{33} = 7.2 \text{ GPa}$, is higher than that of 0.333% ps$^{-1}$, and the stress–strain curve is more smooth. At this strain rate, the 6-1 structure are formed near end of wire after yielding and then necking deformations occur at both end side of the wires, as shown in Fig. 3(e) and (f). Moreover, at very high strain rate, 3.333% ps$^{-1}$, the maximum stress is lower than that at low strain rate. From the stress–strain curve, there is no obviously yielding point at high strain rate. Due to very high strain rate, the kinetic energy interaction among the atoms in the deformed zones has not enough time to transfer to others. The brittle type of deformation at two end zones is formed and others retain the original 7-1 structure such as shown in Fig. 3(g).

![Fig. 4. Morphology of the deformed 11-4 nanowire in different strain at various strain rate of (a)–(c) 0.003% ps$^{-1}$; (d)–(e) 0.833% ps$^{-1}$; (f) 3.333% ps$^{-1}$. We can see in perspective (a) of the right hand side, the inner shell (black sphere) neck before the out shell (gray sphere) produces after first yielding. The strain of all snapshots are (a) $\varepsilon = 0.049$; (b) $\varepsilon = 0.051$; (c) $\varepsilon = 0.090$; (d) $\varepsilon = 0.166$; (e) $\varepsilon = 0.299$; (f) $\varepsilon = 0.14$, respectively.](image-url)

![Fig. 5. Morphology of the deformed 14-7-1 nanowire in different strain at various strain rate of (a)–(d) 0.003% ps$^{-1}$; (e)–(f) 0.833% ps$^{-1}$; (g) 3.333% ps$^{-1}$. The strain of all snapshots are (a) $\varepsilon = 0.074$; (b) $\varepsilon = 0.106$; (c) $\varepsilon = 0.246$; (d) $\varepsilon = 0.115$; (e) $\varepsilon = 0.250$; (f) $\varepsilon = 0.655$; (g) $\varepsilon = 0.096$, respectively.](image-url)
Figs. 2(b) and 4 presents stress–strain relationship and deformed morphologies of 11-4 MHS nanowires for various strain rates. For small strain rate, 0.003% ps$^{-1}$, the maximum stress is near to $\sigma_{33} = 4$ GPa at strain 0.047. Comparing to the 7-1 nanowire, the maximum stress is much lower. From the morphology of deformation at low strain rate as shown in Fig. 4(a)–(c), it can be found that the tubular wires are necked in the inner shell just after maximum stress. This behavior is not the same as 7-1 nanowire. This kind of behavior is due to instability of tubular wire under tension. Again, increasing the strain, the wire begins to slide, and the structure reconstruct to a tight structure at strain 0.05, as show in Fig. 4(b). Continuing to increase the strain, the stress is rise again, and the stress is approach to $\sigma_{33} = 3.6$ GPa at strain 0.09. After strain 0.09, the sliding and necking deformation is observed in Fig. 4(c). Owing to the fact that the 11-4 structure can be treated as a hollow tube, the wire becomes unstable as the side deformation increases. Therefore, the 11-4 structure of a nanotube, because of its tubular structural characteristics, yields more easily than 7-1 and 14-7-1 structure. In Fig. 4(d and e), we show the snapshots of the system at strains for a higher strain rate 0.833% ps$^{-1}$, the deformation behaviors is also different from that of thinnest 7-1 structure. The tight atom of surface structure of 11-4 nanowire is extended to a FCC structure at both end side of the wire as show in Fig. 4(d). Moreover, the phase transform cause the 11-4 nanowire to have a higher maximum stress. The new structure allows the system to support a higher stress. Increasing the strain, the wire necked at both side, showing in Fig. 4(e), through breaking. At very high strain rate, 3.333% ps$^{-1}$, the maximum stress is lower than that at low strain rate. From the stress–strain curve, there is no obviously yielding point at high strain rate just like the 7-1 nanowire. The brittle type of deformation at two end zones is formed and others retain the original 11-4 structure shown in Fig. 4(f).

Figs. 2(c) and 5 shows the stress and strain relationships for the 14-7-1 nanowire at various strain rates. The stress–strain relationship of 14-7-1 nanowire is like as that of 7-1 nanowire. It could be found that the maximum stress increases as strain rate increasing for low strain rate, however, decreases as strain rate increasing for high strain rate. Snapshots of some critical deformed behavior after yielding are shown in Fig. 5(a)–(b). In Fig. 5(a)–(c), snapshots of the system at several strains for strain rate 0.003% ps$^{-1}$ are shown. The sliding deformation occurs at strain 0.074 after first yielding as shown in Fig. 5(a). Further increasing the strain to 0.106, the necking deformation causes the wire pack to a cross section of 10-4 structure as shown in Fig. 5(b). Finally, the wire is necked to one atom width before breaking. At a higher the strain rate 0.833% ps$^{-1}$, the deformation behaviors is different from the other two molded HMS nanowires. The multi-sliding occurred after yielding as show in Fig. 5(d). Increasing strain again, the necked deformation happen at both end side, and then one atom chain also could be found before breaking as shown in Fig. 5(e and f). For very high strain rate, 3.333% ps$^{-1}$, no more obviously yielding can be found. The brittle deformation at both end of the wire is also observed in 14-7-1 nanowire as shown in Fig. 5(g).

Fig. 6 shows the effect of strain rate on maximum stress at temperature 4 K. The maximum stress of 7-1, 11-4 and 14-7-1 nanowires are almost unchanged over a large range of strain rate, and the values of maximum stress are near to 7, 4 and 4.8 GPa, respectively. General speaking, the maximum stress is function of the ratio of numbers of surface atoms to the total number of atoms, and increases with smaller cross-section [24,31]. However, owing to the 11-4 HMS nanowire can be treat as a nanotube, which will be easily buckled at inner shell under tension, the strength of 11-4 nanowire is lower comparing to 14-7-1 nanowire. Up to a strain rate of $10^9$ s$^{-1}$, the maximum stress have a slightly increase, because the different deformation behavior from lower strain rate are occur as previous description. However, the maximum stress decrease after a very high strain rate of $10^{10}$ s$^{-1}$, and the brittle deformation are formed at small area and others retain the original structures on 7-1, 11-4 and 14-7-1 nanowires. The stress concentration is observed near the top and bottom sides, and the interaction among the atoms in the deformed zones has not enough time to transfer to other atoms. In Fig. 6, the engineering stress and engineering strain are adopted. This could not present the true state of the stress concentration exactly.

Fig. 7 displays the effect of strain rate on Young’s modulus at 4 K. In this article, the force approach is adopted to evaluate the Young’s modulus of the nanowires. The Young’s modulus derived from the engineering approach which so call engineering Young’s modulus, and it can be determined from the results of tensile and compressed tests for the strain $\varepsilon < 2\%$ using linear regression [32]. The Young’s moduli are almost unchanged over a large range of strain rate for 7-1, 11-4 and 14-7-1 HMS structures, and the values are 147, 112 and 100 GPa, respectively. The Young’s moduli of HMS nanowires are higher than that of FCC structure [24]. However, up to a strain rate of $10^{10}$ s$^{-1}$, the Young’s modulus is decrease as the strain rate is increased, because the engineering stress is employed.
Fig. 7. Young’s modulus vs. strain rate for HMS nanowires at 4 K.

4. Conclusion

The molecular dynamics simulation is applied to study the stress–strain relationship of the HMS gold nanowires at temperature 4 K for various tensile velocity. The results show that the 7-1 structure has the highest maximum stress, and the maximum stress of 7-1 and 14-7-1 structure with a diameter of 0.6 and 1.0 nm, respectively, are stronger than that of tubular 11-4 structure with a diameter of 0.8 nm. The strain rates affect Young’s modulus, maximum stress and deformation behaviors. For various strain rates, the deformation behaviors are different on different type HMS nanowires. The HMS nanowires formed a close packing structure after failure at a strain rate lower than $5 \times 10^8$ s$^{-1}$, two or more deformation zones appear at a higher strain rates, and brittle deformation zones are obtained at a very high strain rates.

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