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Understanding the tensile behaviors of ultra-thin ZnO nanowires via molecular dynamics simulations

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By using molecular dynamics (MD) method, the tensile behavior of ultra-thin ZnO nanowires in <0001> orientation with three different diameters have been investigated respectively. Through the numerical simulations, the tensile properties including Young’s modulus and yielding stress are obtained as functions of strain rates, temperatures and diameter sizes. The simulation results indicate that the nanowire Young’s modulus and yielding stress would decrease with the increasing of diameter size. In addition, a significant dependence of tensile properties on temperature was also observed with the Young’s modulus and yielding stress decreasing on average by 8% and 18% respectively, while the temperature rises from 0.1 K to 400 K. However, in our simulations the Young’s modulus and yielding stress have no obvious change with different strain rates. Lastly, the structure of ultra-thin ZnO nanowires could be transformed at the strain of ∼7%-11% while the nanowires eventually fracture at the strain of nearly 15%.

I. INTRODUCTION

Being a unique nanomaterial, zinc oxide (ZnO) exhibits semiconducting, piezoelectric and pyroelectric multiple properties,1 of which the nanostructures have a variety of morphologies, such as nanowire, nanocage, nanobel, nanocube, nanohelix/nanospring, nanoring or nanoplate. With reduction in its size, mechanical, thermal, electronic, optical and magnetic properties are introduced, which are mainly believed to be the result of surface and quantum confinement effects and have been increasingly attracting the attention of researchers in the concerned fields2,3 in the past two decades. There are three well-known polymorphs of ZnO, including wurtzite(WZ), rocksalt and zinc blende. Under ambient conditions, WZ is the most commonly and stable phase of the three.4 Nowadays, WZ-structured ZnO nanowires are generally synthesized through the solid-vapor phase thermal sublimation technique5,6 and widely used in the researches of their mechanical properties which are of critical relevance to the design and reliability of devices based on ZnO nanowires.

The characterization of mechanical properties of the 1-D nanostructure can be achieved through the methods of experiments and computational simulations.7 The major experiment methods, including atomic force microscopy (AFM) testing, in situ scanning electron microscopy (SEM) testing and in situ transmission electron microscopy (TEM) testing are widely utilized in the test of mechanical properties of ZnO nanowires. Hoffmann and Michler8 measured the fracture strength of ZnO nanowires with diameters ranging from 60nm to 310nm in tensile and bending experiments.
with a nanomanipulator inside a SEM, and they found that the Young’s modulus could be extracted to be about 100GPa, which is much lower than that from numerical simulations. Huang et al. studied the mechanical properties of individual ZnO nanowires by TEM, and the results indicate that the elastic bending modulus of individual ZnO nanowires were measured to be about 58GPa. Apart from experimental tests, many researchers also carried out computational simulations of the mechanical properties of ZnO nanowires. Dai et al. performed MD simulations of ZnO nanowires under tensile loading and compared it with the simulations of TiO2 wires to present size-dependent mechanical properties and super ductility of metal oxide wires. They found large surface-to-volume ratio is responsible for their size effects. Chen et al. analyzed the size dependence of the Young’s modulus of ZnO nanowires in <0001> orientation, and the result shows that the Young’s modulus of nanowires with diameters smaller than 120nm is increasing dramatically with the decreasing diameters, and is significantly higher than that of the larger ones whose modulus tend to that of bulk ZnO. Additionally, Wen et al. investigated the mechanical properties of ZnO nanowires that range in diameter from 18 to 304 nm, and the ultimate strength of small diameter wires was found to increase, and exhibits values up to 40 times than that of bulk. As reported in the work of Wang, a phase transformation for WZ-structured ZnO nanowires in <0001> orientation would occur during uniaxial tensile process when stress is above 7 GPa and the stress-induced phase transformation has an important impact on the electronic, thermal, and mechanical responses of ZnO. Meanwhile, Xu et al. carried out both experimental and theoretical investigations of the elastic and failure properties of ZnO nanowires under different loading modes, and conducted the buckling tests on ZnO nanowires along the polar direction <0001>. The results indicate that both tensile modulus and bending modulus were found to increase as the decreasing nanowire diameter, but the phase transformation was not observed in their experiments.

Due to the limitation of fabrication techniques and experimental conditions, it’s difficult for us to test the mechanical properties of ultra-thin ZnO nanowires experimentally. And in some situations, the atomic configuration of nanowires should also be obtained to analyze the change of their internal structure during the tensile process. Therefore, our work has been carried out based on MD simulations and WZ-structured ZnO nanowires in <0001> orientation of different diameter sizes are utilized to investigate the dependence of tensile properties including Young’s modulus and yielding stress on the temperature and strain-rate, which is rarely involved and important in the nanotechnology research.

II. PHYSICAL MODELING AND MD SIMULATION

A. Physical modeling

The ZnO nanowires with WZ structures studied in present study are generated by repeating a WZ unit cell along the <0001> orientation and the lattice parameters respectively are \(a = b = 0.3296\) nm and \(c = 0.52065\) nm. Three models of ZnO nanowire with different diameters, including \(\Phi 8.5\) Å, \(\Phi 15.6\) Å and \(\Phi 35.5\) Å, are constructed with the same initial length of \(~13\) nm and the corresponding number of atoms is 1200, 4050 and 18350, respectively. Fig. 1 gives the sketch map of the ZnO nanowires with the diameter of 15.6 Å and the parameter \(\Phi\) is defined as the diameter of the cross-section’s inscribed circle. It’s worth noting that the elastic properties of Young’s modulus and yielding stress observed in present research are actually independent of the nanowire length. In addition, the cross section of ZnO nanowires prepared in this paper is hexagon instead of round. Due to the low coordination number of edge atoms and the shrinking relaxation of its body, the cross section of ZnO nanowires will become smooth after a full relaxation process during MD simulations, and it could be regarded as round.

B. MD simulation

During the process of MD simulation, atoms, molecules and other basic unit constituting matter in a simulated system are treated as particles, and the external force applied on each particle is calculated according to the interaction potential functions between those particles. The primary
condition for the success of MD calculation is the choice of availability interatomic potentials to describe the interaction between atoms in the crystalline lattice. Note that the Zn-O bond has also a covalent besides an ionic character. Zn belongs to a d-block metal group 12 and behaves more like an alkali metal.\textsuperscript{16} Coulomb plus Buckingham potentials are known to work well for alkali and alkaline earth metal compounds.\textsuperscript{17,18} In the present MD simulations, the interatomic interaction not only contains long-range coulombic interactions but also short-range non-coulombic interactions. The non-coulombic interactions between Zn–O and Zn–Zn are mostly repulsive and the potential of Buckingham is chosen to describe them. The potential of Morse is chosen to describe the non-coulombic O-O interaction and the Coulombic pair potential is chosen to describe the coulombic interaction of all the particles.\textsuperscript{19}

In the system, the total energy is computed by summing all pair interactions of the form:

\begin{align*}
\phi(r_{ij}) &= \frac{q_i q_j}{4 \pi \varepsilon_0 r_{ij}} \\
\phi(r_{ij}) &= A \exp\left(-\frac{r_{ij}}{\rho}\right) - C/r_{ij}^6 \\
\phi(r_{ij}) &= A \left[\left(1 - \exp\left(-C(r_{ij} - \rho)\right)\right)^2 - 1\right]
\end{align*}

where \(r_{ij}\) is the distance between two ions with charges \(q_i\) and \(q_j\), \(\varepsilon_0\) is the permittivity of the free space. The parameters \(A\), \(\rho\) and \(C\) are obtained by empirical fitting to the structure and properties of WZ-structured ZnO,\textsuperscript{20} as listed in Table I. Equ.(1) considers the long-range Coulomb pair interactions, while Equ.(2) and Equ.(3) correspond respectively to Buckingham and Morse potentials. A cutoff radius of 12.0 Å was set for all short-range non-Coulombic interactions, and the Ewald method\textsuperscript{21,22} was used to calculate the long-range Coulombic interactions in both real and reciprocal space.

**TABLE I.** Short-range potential parameters of ZnO used in simulations.

<table>
<thead>
<tr>
<th>Source</th>
<th>(A) (eV)</th>
<th>(\rho) (Å)</th>
<th>(C) (eV Å(^6))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn-O</td>
<td>257600.0</td>
<td>0.1396</td>
<td>0.0</td>
</tr>
<tr>
<td>Zn-Zn</td>
<td>78.91</td>
<td>0.5177</td>
<td>0.0</td>
</tr>
<tr>
<td>O-O</td>
<td>0.1567</td>
<td>3.405</td>
<td>1.164</td>
</tr>
</tbody>
</table>

FIG. 1. Sketch map of the model of ZnO nanowire with WZ structures along <0001> orientation: (a), side view, \(\Phi\) denotes the diameter of ZnO nanowire; (b), cross section; (c), axial direction. Notes: The red balls present Oxygen atoms, and the light blue ones present Zinc atoms.
TABLE II. Strain rates versus stretching speeds.

<table>
<thead>
<tr>
<th>Strain rates (s$^{-1}$)</th>
<th>Stretching speeds (ms$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.63 × 10$^7$</td>
<td>1</td>
</tr>
<tr>
<td>3.81 × 10$^8$</td>
<td>5</td>
</tr>
<tr>
<td>7.63 × 10$^8$</td>
<td>10</td>
</tr>
<tr>
<td>1.52 × 10$^9$</td>
<td>20</td>
</tr>
</tbody>
</table>

After geometric construction, we performed a series of relevant MD simulations. During the process of simulation, NPT conditions using the Nose-Hoover thermostat were imposed in the system. The time step is set as 1 fs and the system temperatures are set as 0.1 K, 100 K, 200 K, 300 K, and 400 K to study the temperature effects on tensile properties of ZnO nanowires. The periodicity of boundary conditions is required for the Ewald solver that is introduced. In order to ensure that the initial system is close to equilibrium state with lowest energy, 50 ps are set up to achieve the natural balance without imposing any external force on the theoretical model to relax the system.

According to the existing literatures,$^{23-25}$ most of the stretching speeds range from 1 m/s to 1000 m/s. In present research, the deformation process of the nanowire will be conducted in the axial direction with different strain rates as shown in Table II, including 7.63 × 10$^7$ s$^{-1}$, 3.81 × 10$^8$ s$^{-1}$, 7.63 × 10$^8$ s$^{-1}$ and 1.52 × 10$^9$ s$^{-1}$, and the corresponding stretching speeds are 1 m/s, 5 m/s, 10 m/s and 20 m/s respectively. The tensile strain was applied uniformly with a constant increment in its total length to obtain the specified strain rate and the average stress in the specimen was computed following each applied strain increment.$^{26}$ A numerical method named velocity Verlet algorithm is adopted to work out the spatial positions of particles at different time, the state of motion and so on.

III. SIMULATION RESULTS AND DISCUSSIONS

A. Stretching process

As for the stretching process of WZ-structured ZnO nanowire in MD simulations with the diameter of 15.6 Å, the surface morphologies of the nanowire are shown in Fig. 2(a). And Fig. 2(b) shows the corresponding stress-strain curve, in which the points indicate the four states: (i) the original state of nanowires; (ii) initiation of structure transformation; (iii) completion of the transformation; (iv) the rupture state.

![Fig. 2](image-url)
As observed in Fig. 2(b), one can get that the deformation process of ZnO nanowires would be divided into four stages: initial elastic stretching, structural transformation from WZ to body-centered tetragonal (BCT) (as shown in the two insets of atomic configuration), elastic stretching with a new modulus and finally fracture. In the elastic deformation zone, the stress changes with strain in a straight line before the phase transformation of ZnO nanowire, which occurs with a combination of the breaking of every other Zn-O bond along the <0001> direction and the formation of an equal number of Zn-O bonds along the same direction next to the broken bonds. After the structural transformation, the nanowires would experience the process of elastic stretching again and eventually shear failure. It’s worth pointing out that the structural transformation of ZnO nanowires seems irreversible. When the nanowires are unloaded at the stage of iii-iv as shown in Fig. 2(b) during the stretching process, it would retain the BCT structure and the stress would be induced to zero with a new modulus. Further research on the underlying mechanism of this phenomenon remains needed.

B. Results and discussions

Through the MD simulations of the ultra-thin WZ-structured ZnO nanowires (Φ8.5 Å, Φ15.6 Å and Φ35.5 Å), it can be found that all the nanowires experience the similar stretching process as shown in Fig. 2, and the stress-strain curves have the similar variation tendencies, except for some numerical distinctions. In this paper, we will concentrate on the dependence of tensile properties on temperature, strain-rate and diameter size, as shown in the following figures.

Before structural transformation, the nanowire is stretched linearly and Young’s modulus is defined as the slope of the stress-strain curve. Fig. 3 shows the variation of Young’s modulus with the temperature and the typical vertical error bar in the curves represents the corresponding standard deviation. As observed in Fig. 3, it can be obtained that the Young’s modulus of WZ-structured ZnO nanowires is significantly higher than the bulk ZnO (\(\sim 170\) GPa), and would decrease with the increasing of temperature. According to the theory of thermodynamics, the total kinetic energy of all the atoms of the system generally satisfies the following equation:

\[
E_k = \frac{1}{2} \sum_{i=0}^{N} m v_i^2 = \frac{3}{2} N K_B T
\]

where \(E_k\) is the total kinetic energy of the system; \(N\) is the total number of atoms; \(K_B\) is the Boltzmann constant; \(T\) is the thermodynamic temperature. The higher the temperature is, the more

![FIG. 3. Young’s modulus as a function of temperature of ZnO nanowires with different diameter size at the strain-rate of 7.63 \times 10^7 \text{s}^{-1}.](image-url)
active the atoms become, and it will be more easily for the atoms to escape from their equilibrium position, resulting in lattice defects. Consequently, the lattice defects of the nanowires are more intense at higher temperature at the same strain, so that the nanowires are more easily to reach their yielding limits. Therefore, the Young’s modulus at lower temperature will be higher than those at higher temperature.

Fig. 4 shows the dependence of Young’s modulus and yielding stress on different stretching speeds for ZnO nanowires of three diameter sizes. It could be found that the strain rate has little impact on the Young’s modulus and yielding stress. The stress-strain curves of ZnO nanowires with different strain rates are almost overlapping before the structural transformation. Meanwhile, all the structural transformation occurred at the strain of about 7%-11% in different rates, and the nanowires eventually fracture at the strain of ~15%, which is in accordance with the work of Wang. A Buckingham-type potential with charge interactions is also used by him in the MD simulations to describe atomic interactions. The nanowires analyzed in the simulations have different diameters from nearly 40 Å to 90 Å and the temperature of system is set at 300 K. In his work, the phase transformation from WZ to BCT is also observed, and for the particular nanowire of 65 Å which is described as an instance in his paper, the transformation occurred at the strain of 7.5% and the nanowire eventually fractured at the strain of 16.9%.
TABLE III. Young’s modulus of WZ-structured ZnO nanowires at different strain-rates and temperatures.

<table>
<thead>
<tr>
<th>Strain rates (s(^{-1}))</th>
<th>Diameters (Å)</th>
<th>Young’s modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.1 K</td>
<td>100 K</td>
</tr>
<tr>
<td>7.63×10(^7)</td>
<td>8.5</td>
<td>337.0</td>
</tr>
<tr>
<td></td>
<td>15.6</td>
<td>236.4</td>
</tr>
<tr>
<td></td>
<td>35.5</td>
<td>202.5</td>
</tr>
<tr>
<td>3.81×10(^8)</td>
<td>8.5</td>
<td>336.8</td>
</tr>
<tr>
<td></td>
<td>15.6</td>
<td>236.5</td>
</tr>
<tr>
<td></td>
<td>35.5</td>
<td>202.3</td>
</tr>
<tr>
<td>7.63×10(^9)</td>
<td>8.5</td>
<td>336.5</td>
</tr>
<tr>
<td></td>
<td>15.6</td>
<td>236.6</td>
</tr>
<tr>
<td></td>
<td>35.5</td>
<td>202.2</td>
</tr>
<tr>
<td>1.52×10(^9)</td>
<td>8.5</td>
<td>336.6</td>
</tr>
<tr>
<td></td>
<td>15.6</td>
<td>236.5</td>
</tr>
<tr>
<td></td>
<td>35.5</td>
<td>202.3</td>
</tr>
</tbody>
</table>

TABLE IV. Yielding stress of WZ-structured ZnO nanowires at different strain-rates and temperatures.

<table>
<thead>
<tr>
<th>Strain rates (s(^{-1}))</th>
<th>Diameters (Å)</th>
<th>Yielding stress (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.1 K</td>
<td>100 K</td>
</tr>
<tr>
<td>7.63×10(^7)</td>
<td>8.5</td>
<td>29.3</td>
</tr>
<tr>
<td></td>
<td>15.6</td>
<td>24.2</td>
</tr>
<tr>
<td></td>
<td>35.5</td>
<td>20.9</td>
</tr>
<tr>
<td>3.81×10(^8)</td>
<td>8.5</td>
<td>29.8</td>
</tr>
<tr>
<td></td>
<td>15.6</td>
<td>23.8</td>
</tr>
<tr>
<td></td>
<td>35.5</td>
<td>20.5</td>
</tr>
<tr>
<td>7.63×10(^9)</td>
<td>8.5</td>
<td>30.5</td>
</tr>
<tr>
<td></td>
<td>15.6</td>
<td>23.6</td>
</tr>
<tr>
<td></td>
<td>35.5</td>
<td>20.3</td>
</tr>
<tr>
<td>1.52×10(^9)</td>
<td>8.5</td>
<td>30.2</td>
</tr>
<tr>
<td></td>
<td>15.6</td>
<td>24.0</td>
</tr>
<tr>
<td></td>
<td>35.5</td>
<td>20.3</td>
</tr>
</tbody>
</table>

For the purpose to make it easier to observe, we can get some approximate and useful datum from different strain-stress curves. Tables III and IV list the tensile properties including Young’s modulus and yielding stress respectively of the ultra-thin nanowires under different conditions.

As observed in Table III, the Young’s modulus would decrease with the rise of temperature, and for the nanowire of 8.5 Å, it will decrease by 9.2% from 337.0 GPa to 305.7 GPa as temperature increases from 0.1 K to 400 K. In addition, with the increase of temperature, it will be difficult for the nanowires to maintain stability during the stretching process when temperature exceeds 800 K despite that it’s lower than the melting point of ZnO. Corresponding to Fig. 4, the Young’s modulus as well as the yielding stress is almost an invariable value with the increase of strain rate.

During the stretching process for thinner nanowires, a higher proportion of atoms with incomplete lattice effects will greatly reduce the strength of nanowires and quickly enter their yielding state. Therefore, one can make a conclusion that the smaller the diameter of the nanowire, the lower the modulus. However, the elastic modulus of nanowires reported in this article isn’t in correspondence with the principle above, as shown in Fig. 5.
FIG. 5. Stress-strain curves of different diameters at the temperature of 0.1 K and at the strain rate of 7.63×10^8 s⁻¹.

Fig. 5 shows the stress-strain curves of ZnO nanowires with the three diameter sizes. The system temperature is set as 0.1 k and strain rate as 7.63×10^8 s⁻¹. A significant dependence of elastic properties on size is observed. It is found that the Young’s modulus of WZ-structured ZnO nanowires decreases by 39.9% and the yielding stress decreases by 33.4% over the range of lateral dimension from 8.5 Å to 35.5 Å, which is similar to the trend reported by Agrawal. In his work, the <0001> oriented ZnO nanowires with diameters ranging from 5 nm to 20 nm were prepared for the MD simulations, which were performed with a Buckingham type potential and long-range ionic interactions. A obviously dependence of elastic properties on size can also be found in his simulation, but the decreasing degree of the yielding stress and the Young’s modulus isn’t that great with the increasing of diameter.

Much work has been done hitherto to explain the size effects and several mechanisms have been proposed. Zhang and Huang found that the surface bond saturation was caused by an increased electron density rather than bulk nonlinear elastic effects, which may be responsible for the size effects. Chen et al. proposed an approximate core-shell composite NW model based on the surface stiffening effect that results from the gradually shortened bond lengths from the bulk core to the outmost surface, through which the size effect was well explained. Meanwhile, surface-stress-induced internal compressive stress has been indicated to be in inverse proportional to the lateral dimension of the nanowires, effectively resulting in the size effect observed here.

When the dimension of cross section is sufficiently large, the surface-stress-induced compressive stress is very small and the surface effects are insignificant, as a result of which the material approximately exhibits bulk behavior.

IV. CONCLUSIONS

In this work, a molecular dynamics study has been carried out to investigate the tensile properties of ultra-thin WZ-structured ZnO nanowires in <0001> axial orientation. Through the numerical simulations under different conditions, an evident size dependence was observed in the elastic responses. The Young’s modulus and yielding stress would decrease significantly with the increasing of diameter size. This phenomenon may be attributed to surface-stress-induced internal compressive stress which is inversely proportional to the lateral dimensions. Furthermore, the elastic modulus was also found to be temperature-dependent with the temperature ranging from 0.1 K to 400 K, which could make the lattice defects of the nanowires more intense. However, the Young’s and yielding stress have no obvious change with different strain rates. These findings of ZnO nanowires indicated in this paper highlight the advantage of their applications in nanodevices, such as nanosensors, nanogenerators and nanoresonators.
ACKNOWLEDGEMENTS

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Author Contributions

All of the authors made important contributions on this work. Specifically, WW proposed the project and analyzed the simulation results. ZP and FL contributed to the MD simulation processes. WW and YL composed the manuscript. All the authors participated in the discussions of the results.

Conflicts of Interest

The authors report no conflicts of interest. The authors alone are responsible for the content and writing of the paper.