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Size effects on the fracture behavior of amorphous silica nanowires

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ABSTRACT

Size effects on deformation behavior and fracture mechanism of amorphous silica nanowires (NWs) were studied by molecular dynamics simulation with reactive force field ReaxFF. We analyzed the evolution of voids during the tension deformation, and focused on the role of voids played in the fracture process of amorphous silica NWs. Our study shows that the smaller diameter NWs damage only from localized necking and the small growth of voids has no effect on its fracture behavior. While for the larger diameter NWs, there exists growth and coalescence of void inside the NWs and crack propagation on the surface of NWs. It is the combined action of these two mechanisms that leads to the final fracture. The evolution of the size of biggest void (BV) displays three distinct regions, which are corresponding to the different deformation stages of NWs. The voids begin to grow significantly after the yielding point, and the size of BV in the fracture stage increases much more quickly owing to the coalescence of voids. Moreover, the critical radius of BV at the start point of fracture stage increases from 2.6 Å to 3.8 Å with the increase of diameter of amorphous silica NWs.

1. Introduction

Amorphous silica nanowires are the promising functional and structural nanobuilding blocks in nanoelectronics. To integrate these nanowires into functional nanodevices, a fundamental understanding of their mechanical properties and deformation behaviors is of significant importance, because mechanical failure of these nanobuilding blocks may lead to malfunction or even fatal failure of the entire devices.

Size effects on the mechanical properties of amorphous silica NWs have been studied by many researchers using experiment method [1–6] and MD simulation [5,7–9]. However, most of them focused on amorphous silica NWs' elastic response and elastic modulus as a function of diameter. Only limited studies cared about the plastic and fracture process of amorphous silica NWs. Brambilla and Payne [1] measured the ultimate strength of glass silica NWs with diameter $D = 60–300$ nm, which were manufactured by the so-called "modified flame brushing technique". The measured ultimate strength is in excess of 10 GPa and increases for decreasing nanowire diameter. Scanning electron micrographs of the broken fragments show flat fracture surfaces and there is no evidence of diameter tapering or corrugated fracture surfaces. Yuan and Huang [8] studied amorphous silica NWs under uniaxial tension using MD simulation. They carefully investigated the choice of simulation parameters to correctly predict the fracture behavior of amorphous silica. With proper simulation parameters, they found that amorphous silica NWs remain brittle fracture when the diameter shrinks down to 2 nm.

Amorphous silica is a typical brittle material, where crack propagation leads to an abrupt break without significant deformation. However, when analyzed the fracture behavior at the nanometer scale with an atomic force microscope, Celarie et al. [10] and Bonamy et al. [11] revealed the presence of nanoscale damage cavities ahead of a crack tip in amorphous silica, and cracks advance via the coalescence of the cavities. This fracture behavior, which seems to contradict the traditional view of brittle material, is further confirmed by MD simulation. Muralidharan et al. [12] and Pedone et al. [13] studied the tension deformation and fracture process of amorphous silica bulk using MD simulation. A striking similarity between both simulation and experiments is that the growth and coalescence of nanoscale voids leads to final failure.

In this work, MD simulations of amorphous silica NWs under uniaxial tension were carried out to study the size effect on mechanical properties and fracture behavior. We also studied the evolution of size of voids and critical size of voids during the tension and fracture process. A deep fundamental understanding of the deformation and failure behavior will provide important information for better application of amorphous silica NWs.

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2. Computational methods

In our simulation, we used a reactive force field ReaxFF developed by van Duin et al. [14]. ReaxFF can accurately describe the bond breaking and formation behavior in large silicon and silicon oxide systems, which is essentially important for tension and fracture simulation of amorphous silica NWs. Amorphous silica bulk sample was prepared by initially melting a 133,056 atom system of α-quartz at 4000 K in NVT ensemble for 50 ps until the system was completely melted, and then quenching the melt to 300 K with a quenching rate of 25 K/ps using NPT ensemble. The melting and annealing processes were repeated twice using the same preparation parameters. Finally, the system was equilibrated at 300 K in NPT ensemble for 30 ps. After these procedures we got a uniform block of amorphous silica with dimensions of $12.5 \times 12.5 \times 12.6\ nm^3$. Nosé–Hoover thermostat and Berendsen barostat were utilized to control the temperature and pressure of the simulation system. Pressure was maintained at a constant of 1 atm in NPT ensemble. All simulations were performed with a time step of 0.5 fs, and periodic boundary conditions (PBC) were imposed on the surfaces in three directions. Table 1 shows the structural properties obtained from the amorphous silica bulk sample, which are in good agreement with the previous simulation results and experimental data.

Five independent bulk samples of the same size ($12.5 \times 12.5 \times 12.6\ nm^3$) were prepared using the above method. By cutting along its z-axis and around its center of x–y plan, we carved out a series of NWs samples with diameter from 2.23 nm to 10.23 nm from each of bulk samples. So we also got five independent amorphous silica NWs samples for each diameter (D = 2.23–10.23 nm). Before tension simulation, these NWs were completely equilibrated at 300 K in NVT ensemble for 40 ps to eliminate surface effect as much as possible. Uniaxial tension tests were conducted at 300 K in NVT ensemble with PBC along the axial line direction and free boundary conditions on the surrounding surface. The engineering strain rate was $10^9\ s^{-1}$. We also carried out uniaxial tension simulations for amorphous silica bulk to present data for comparison. For amorphous silica bulk, NPT ensemble was adopted and PBC were applied on three directions. All the simulations were carried out with LAMMPS [15] package.

3. Results and discussion

3.1. Stress–strain curve

Fig. 1 shows the tension stress–strain curves of amorphous silica NWs (D = 2.23–10.23 nm, L = 12.6 nm) and silica bulk. On the stage of linear elastic deformation, the stress–strain curves become steeper and steeper with the increase of the diameter of NWs. The peaks of the stress–strain curves for NWs also become higher and higher with the increasing of diameter, but are always much smaller than silica bulk. According to these stress–strain curves, the amorphous silica NWs and bulk all exhibit brittle fracture behavior.

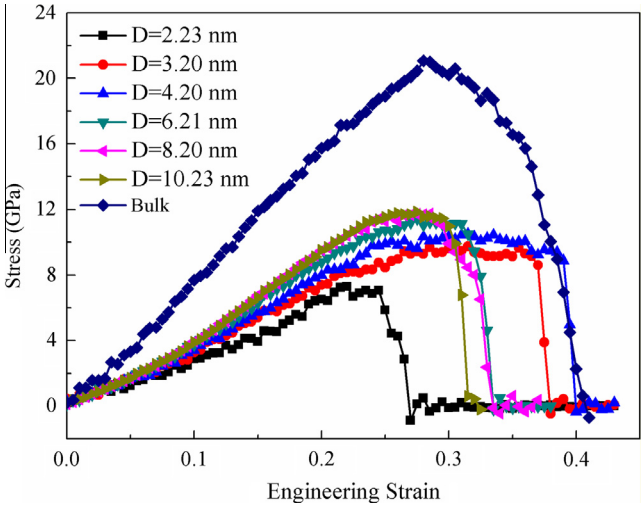

Fig. 1. Stress–strain curves of uniaxial tension for the amorphous silica NWs (D = 2.23–10.23 nm, L = 12.6 nm) and silica bulk.

Amorphous silica has a very strong nonlinear elasticity [18]. Due to the strain dependence of elastic modulus, the resulted Young's modulus when extracted from a linear fit to the stress–strain curve, is very sensitive to the strain range used for linear fit. Therefore, we calculated the zero-strain Young's modulus from the third-order polynomial fitting to the stress–strain curves in the strain range of 0–12%. The same extraction method has also been used by Yuan and Huang in their MD simulations [9] and by Gupta and Kurkjian in their experiments [18]. Fig. 2 shows the Young's modulus of amorphous silica NWs as a function of diameter, including the data calculated in this paper and those found in the literature. The error bar of Young's modulus of our MD results in

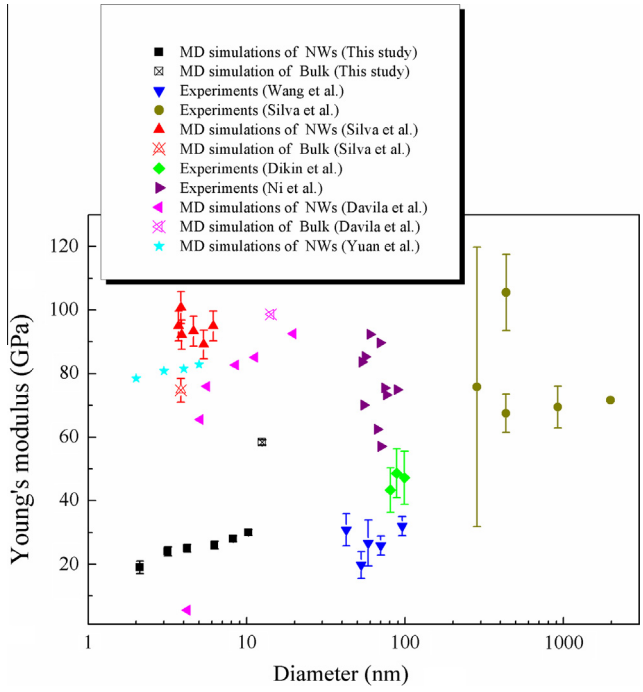

Fig. 2. Young's modulus of amorphous silica NWs as a function of diameter, adapted from Ref. [7].

Table 1
Structural properties of the bulk amorphous silica sample.

Property	This study	ReaxFF MD[a]	Experiment[b]
Density (g cm^{-3})	2.24	2.14	2.20
O–Si–O angle (°)	108.73	109.2	109.5
Si–O–Si angle (°)	154.06	150	153
Si–Si dist. (Å)	3.05	3.0 ± 0.2	
O–O dist. (Å)	2.61	2.7 ± 0.3	2.65
Si–O dist. (Å)	1.60	1.59 ± 0.07	1.61 ± 0.004

[a] Results from Ref. [16].
[b] Results from Ref. [17].