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Mechanical properties of kinked silicon nanowires

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ABSTRACT

Molecular dynamics simulations are used to investigate the mechanical properties of KSiNWs. Our results show that KSiNWs have a much larger fracture strain compared to straight SiNWs. The effects of the periodic length of KSiNWs with symmetric arms and the arm length of the KSiNW with asymmetric arms on the mechanical properties of KSiNWs are studied. The fracture stress of KSiNWs decrease as the periodic length increases. However, the fracture strain of KSiNWs is not dependent on the short periodic length and the fracture strain of KSiNWs will abruptly increase to very large value and then vary slightly as the periodic length increases. In addition, the fracture stress is not dependent on arm length while the fracture strain monotonically increases as the arm length increases. We also investigate the fracture process of KSiNWs. The results in this paper suggest that the KSiNWs with larger fracture strain can be a promising anode materials in high performance Li-ion batteries.

1. Introduction

One-dimensional semiconductor nanowires and nanotubes are attracting much attention because of their great potential of application in nanoscale devices [1,2]. Among various one-dimensional nanostructures, silicon nanowires (SiNWs) appear to be an especially appealing choice due to the importance of silicon in the modern electronic industry [3]. Recently, SiNWs have been synthesized by different methods such as solution techniques [4] and a metal-catalytic vapor–liquid–solid method [5–7]. As potential building blocks for field-effect transistors [8–11], resonators [12], and biosensing application [13–15], SiNWs have been intensively explored. To fabricate novel devices with fewer welding joints and improved electric connections, SiNWs with controlled shape are needed to realize their full potentials. Recently, kinked silicon nanowire (KSiNW) was synthesized by Lieber et al. [16]. It is able to adjust the arm length of the kink and turning angle. To date, many correlative investigations from both experiments [17–22] and theoretical calculations [23,24] have been performed. In most of the work, the attentions were mainly paid on the growth mechanisms of the kinks in SiNWs. The application of KSiNWs as nanoelectronic bioprobes has been demonstrated in recent experiment [25]. The conductance properties of kinked nanowires were studied by first-principles transport calculations [26]. In addition, the reduction in the thermal conductivity by kinks in SiNWs was investigated by using molecular dynamics (MD) simulations, which indicated the KSiNWs could be a promising candidate for thermoelectric materials [27]. Materials with different mechanical, thermal, and electronic properties are needed to design smart and functional nanodevices. However, the study of mechanical properties of KSiNWs is also necessary and timely. Now the studies on the mechanical characters of KSiNWs are little reported [28].

In this paper, we perform MD simulations to investigate the mechanical properties of KSiNWs and compare it to that of straight SiNWs. The effects of the arm length of the kink on the mechanical properties are investigated. We also study the fracture process of KSiNWs.

2. Simulation details

Fig. 1 shows the configuration for two kinds of KSiNWs of 3.3 nm in diameter. One is the KSiNW with symmetric arms and the other is the KSiNW with asymmetric arms. The growth direction changes from one [100] to another [100] direction at the kink. The angle between these two [100] direction is 90°. The periodic boundary condition is applied in the axial direction, and the free boundary condition is applied in the lateral direction. The atomic interactions are described using the Stillinger–Weber (SW) potential [29]. The empirical SW interatomic potential consists of two- and three-body interaction terms and was originally fitted to describe the crystalline and liquid silicon phases. The SW potential

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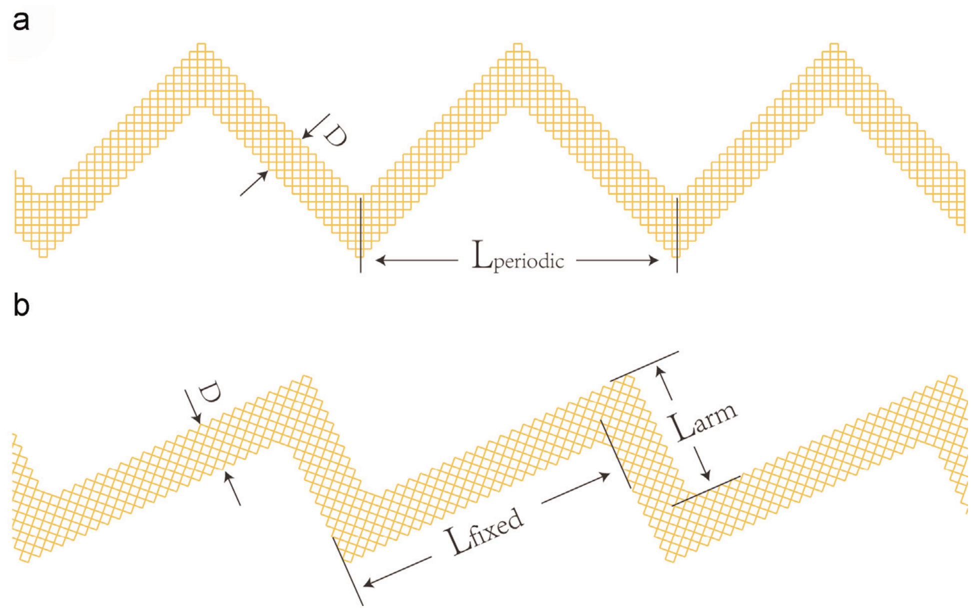

Fig. 1. Configuration for KSiNWs with cross-sectional width (D), periodic length ($L_{periodic}$), arm length (L_{arm}), and fixed arm length (L_{fixed}). (a) KSiNWs. (b) KSiNWs with asymmetric arms.

has been used in MD simulations of straight SiNWs and found to give good results for nanowire properties [30–33]. Therefore, the SW potential should be reliable to study the mechanical properties of KSiNWs.

All MD simulations are performed using LAMMPS package [34]. The velocity-Verlet algorithm is employed to integrate the equations of motion. All molecular systems were equilibrated at a constant pressure of 1 atm and a temperature of 300 K using constant number of particles, pressure, and temperature (*NPT*) for 100 ps with a timestep of 0.1 fs. The strain is then applied along the uniaxial direction to perform uniaxial tensile tests. The applied strain rate is 0.001/ps. The pressure component vertical to the loading direction is controlled to maintain the uniaxial tensile condition. The strain increment is applied to the structure after every 10,000 time steps. All the MD simulations are carried out at 300 K and the temperature is controlled by employing the Nosé–Hoover thermostat [35].

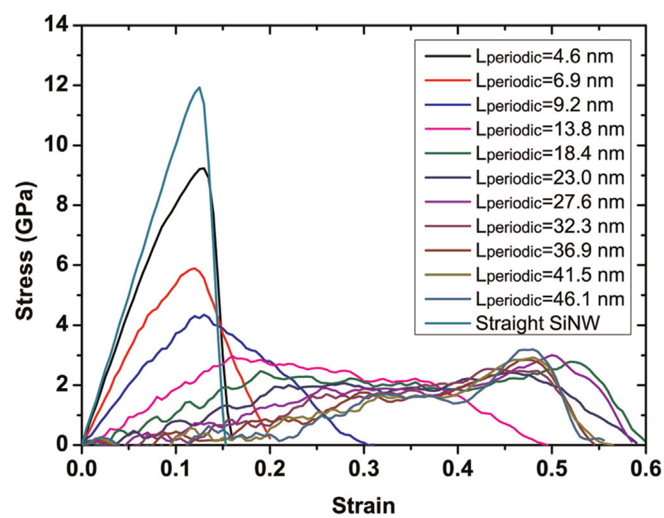

Fig. 2. The stress–strain curves for the KSiNWs with the various periodic length. The stress–strain curve for straight SiNW is shown for comparison.

3. Results and discussion

Fig. 2 shows the axial stress–strain curves for the KSiNWs with the various periodic length. The periodic length ($L_{periodic}$ indicated in Fig. 1a) varies from 4.6 to 46.1 nm. For comparison we also show the axial stress–strain curve of straight SiNWs. The Young's modulus is evaluated using the expression, $Y = \sigma/\varepsilon$ in the elastic region (the strain≤5%), where σ and ε are the stress and strain, respectively. The Young's modulus of straight SiNW is estimated as 90.5 GPa, which is consistent with the experimental results of 93–180 GPa of SiNWs [36–38] and our previous MD simulation results with the same SW interatomic potential [32]. The results in the figure indicate that the Young's modulus of KSiNWs is lower than that of straight SiNW. When the periodic length is less than 10 nm, the axial stress–strain curves of KSiNWs are similar to that of straight SiNW, which means that the tensile deformation process of KSiNWs is similar to that of straight SiNW as shown in our previous results [33]. Fig. 3 shows the variations of fracture stress and strain with the periodic length for KSiNWs. The fracture stress of KSiNWs decrease as the periodic length increases. When the periodic length is larger than 10 nm, the fracture stress vary slightly. However, the fracture strain of KSiNWs is not dependent on the periodic length when the periodic length is less than 10 nm. When the periodic length is larger than 10 nm, the fracture strain of KSiNWs will abruptly increase to very large value and then also vary slightly. Specifically, when the periodic length is about 41.6 nm, the fracture stress of the KSiNWs is about 73% lower than that of straight SiNW, while the fracture strain of the KSiNWs is higher than that of straight SiNW by about 284%. These results indicate that when the periodic length is larger than 10 nm, the tensile deformation process of KSiNWs is different from that of straight SiNW. We will investigate this in detail in the last sections.

To further investigate the effects of the arm length of the kink on the mechanical properties of KSiNWs, we construct some KSiNWs with asymmetric arms as shown in Fig. 1b. One arm length of 19.5 nm is fixed and the other arm length varies from 5.4 to 19.5 nm (L_{fixed} and L_{arm} indicated in Fig. 1b). Fig. 4 shows the axial stress–strain curves for the KSiNWs with the various arm length. It can be seen that the stress–strain curves are different for KSiNWs with different arm lengths. As the arm length increases, there is an obvious hardening stage in the stress–strain curves.