Computational Materials Science 152 (2018) 331–336

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Atomistic study of the bending properties of silicon nanowires

X.R. Zhuo[a], H.G. Beom[b,*]

[a] College of Mechanics and Materials, Hohai University, Nanjing 210098, China
[b] Department of Mechanical Engineering, Inha University, Incheon 402-751, Republic of Korea

ARTICLE INFO

Keywords:
Molecular dynamics simulation
Silicon nanowires
Bending deformation
Young's modulus
Size effect
Shape effect

ABSTRACT

Molecular dynamics simulations are conducted to investigate the mechanical properties and deformation mechanism of silicon nanowires (SiNWs) under pure bending, with a focus on the effects of nanowire diameter, orientation, and cross-sectional shape. The results show that the nanowire diameter and cross-sectional shape do not influence the yield mechanism but the orientation does. In contrast to [1 0 0] and [1 1 0] SiNWs whose yield mechanism is dislocation nucleation, [1 1 1] SiNWs yield by a direct crystal-to-amorphous transition. Moreover, the activated slip plane for [1 0 0] and [1 1 0] SiNWs is different, i.e., {1 1 0} and {1 1 1} plane for [1 0 0] and [1 1 0] SiNWs, respectively. The Young's modulus of [1 0 0] and [1 1 1] SiNWs is dependent on the nanowire diameter and cross-sectional shape, whereas that of [1 1 0] SiNWs is insensitive to these factors. Furthermore, only the nanowire orientation and cross-sectional shape influence the critical bending strain of [1 0 0] and [1 1 1] SiNWs. The results presented in this work may provide valuable information for the design of nanodevices based on SiNWs.

1. Introduction

Due to their unique piezoelectric [1], optical [2], electrical [3], thermal [4], and mechanical [5] properties, one-dimensional nanomaterials are considered as essential building blocks for future nanotechnology applications. Silicon nanowires (SiNWs) are of particular interest as they are compatible with conventional silicon-based technologies. SiNWs have been demonstrated to have potential applications in a broad range of nanoelectromechanical systems such as logic gates [6], field effect transistors [7], battery anodes [8], light-emitting diodes [9], and nanosensors [10]. The integrity and reliability of these nanodevices depend primarily on the mechanical properties of the SiNWs, which differ from bulk silicon because of their large surface-to-volume ratio. Therefore, a thorough understanding of the mechanical properties of SiNWs is of vital importance.

Numerous experimental techniques have been devised to investigate the mechanical properties of SiNWs, including tensile testing inside a scanning electron microscope (SEM) [11], three-point bending using atomic force microscopy (AFM) [12], bending tests of a cantilevered nanowire using AFM [13], nanoindentation testing [14], and resonant frequency testing [15]. Both elastic and plastic properties of SiNWs have been demonstrated to differ from those of bulk silicon. The Young's modulus decreases, whereas the fracture strength increases, as the nanowire width reduces, up to a value comparable with the ideal strength of silicon [16,17]. In addition, the deformation mechanism of SiNWs shows size-dependence. In tensile tests, the fracture mechanism was observed to change from brittle to ductile when the nanowire diameter decreased to a critical size of around 60 nm [18]. Similar behavior was observed during compression tests, but the critical diameter was between 310 and 400 nm [19]. Fruitful results were obtained from these experiments; however, they were unable to reveal the detailed atomic deformation mechanisms.

Atomistic simulations have been broadly employed to investigate the deformation behavior of nanomaterials, since they can provide detailed information about the first stages of plasticity or crack nucleation. Previous atomistic simulations on SiNWs focused mainly on the mechanical properties and deformation mechanisms under uniaxial tension or compression. Little attention has been paid to the deformation of SiNWs under pure bending. The stress distribution on the cross-section of a SiNW is relatively uniform under a tensile or compressive loading, whereas a stress gradient is induced across the cross-section under pure bending, which may lead to different mechanical responses.

In this work, we investigate the mechanical properties and deformation mechanisms of SiNWs under pure bending. To this end, a molecular dynamics (MD) simulation technique was employed. The evolution of the atomic configuration was visualized in detail to reveal the deformation mechanisms. The Young's modulus and critical bending strain were evaluated, and their dependence on a variety of factors including nanowire size, nanowire orientation, and cross-sectional shape were examined.

* Corresponding author.
E-mail address: hgbeom@inha.ac.kr (H.G. Beom).

https://doi.org/10.1016/j.commatsci.2018.06.009
Received 30 March 2018; Received in revised form 31 May 2018; Accepted 4 June 2018

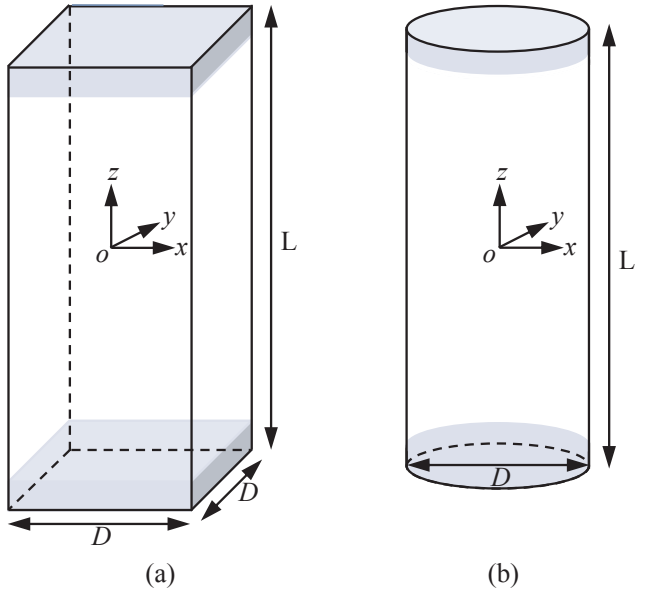

Fig. 1. Atomic model for silicon nanowires, where the shaded areas denote the frozen atoms and the transparent area represents the active atoms. (a) Square cross-sectional SiNWs. (b) Circular cross-sectional SiNWs.

2. Simulation method

SiNWs with two kinds of cross-sections were considered, as shown in Fig. 1. For simplicity, square and circular cross-sectional SiNWs are labeled S-SiNWs and C-SiNWs, respectively. SiNWs with different growth directions have been successfully synthesized. To clarify the role of the crystallographic orientation, we considered three longitudinal axes (z axis in Fig. 1): [0 0 1], [1 1 0], and [1 1 1]. The origin of coordinates is located at the gravity center of SiNWs; the crystallographic orientations of coordinate axes are shown in Table 1. The aspect ratio (length/diameter) of all SiNWs was fixed to three, which has been broadly used in previous works [20–22]. Here, the width of S-SiNWs is regarded as their diameter. To examine the size effect, four diameters (D = 2.7, 4.6, 7.7, 9.6 nm) were considered in this work. The number of atoms for each SiNW is shown in Table 2.

A reliable potential plays a central role in ensuring the accuracy of simulation results. There is no doubt that *ab initio* calculations are the most reliable approach, however, their application is limited to small systems because of the heavy calculation burden. A variety of empirical potentials, such as the environment-dependent interatomic potential (EDIP) [23], the Tersoff potential [24], the modified embedded atom method (MEAM) potential [25], and the Stillinger-Weber (SW) potential [26], have been constructed for simulating silicon. However, SW and Tersoff potential cannot predict room temperature brittle fracture observed experimentally, while MEAM potential can. In addition, EDIP and SW potential may yield non-physical plastic deformation [27,28]. Therefore, MEAM potential was employed in this study. The pair cutoff was set to be 0.6 nm, consistent with previous works [29–32], and other required parameters were obtained from Ref. [31].

MD simulations of the pure bending of SiNWs were performed at 300 K using the open source molecular dynamics program called the large-scale atomic/molecular massively parallel simulator (LAMMPS) [33]. A time step of 1 fs was used in all simulations. A Nose-Hoover thermostat was used to control the temperature of the simulation system. SiNWs were created by removing all atoms outside a certain region of a bulk silicon matrix. Non-periodic boundary conditions were used in all directions. The simulation model was divided into three parts: an upper boundary region, an active region, and a lower boundary region, as shown in Fig. 1. The shaded areas represent the two boundary regions, where the length of each area is larger than the pair cutoff of the MEAM potential. After being generated, SiNWs were relaxed to a minimum energy state by the conjugate gradient method. Then, the two boundary regions were frozen and the active region was equilibrated at 300 K in the NVT ensemble for 50 ps. After equilibration, pure bending was simulated by rotating the two boundary regions around the y axis of SiNWs at a rate of 9×10^{-5} degree per time step. The maximum strain occurs on the outer surface of SiNWs and the corresponding strain rate is $5.2 \times 10^{8}\,s^{-1}$. During the bending process, the temperature of the active region was maintained at 300 K. Such a loading method has been widely applied to simulate pure bending deformation of carbon nanotubes [34] and metal nanowires [35]. The structural evolution of the SiNWs was visualized using the software Atomeye [36].

Table 1
Crystallographic orientation of coordinate axes for silicon nanowires.

	x	y	z
[0 0 1] SiNWs	[1 0 0]	[0 1 0]	[0 0 1]
[1 1 0] SiNWs	[0 0 1]	[1 $\bar{1}$ 0]	[1 1 0]
[1 1 1] SiNWs	[1 $\bar{1}$ 0]	[1 1 $\bar{2}$]	[1 1 1]

Table 2
Number of atoms in SiNWs as a function of diameter, orientation, and cross-sectional shape.

D(nm)	Type					
	[0 0 1] S-SiNW	[0 0 1] C-SiNW	[1 1 0] S-SiNW	[1 1 0] C-SiNW	[1 1 1] S-SiNW	[1 1 1] C-SiNW
2.7	3917	2861	3867	3087	3917	3178
4.6	17,309	13,813	17,745	12,353	15,050	12,068
7.7	72,705	58,753	75,411	57,345	74,052	58,139
9.6	139,267	111,435	143,987	113,901	146,454	114,510

3. Results and discussion

3.1. Strain energy-bending angle curves

In order to characterize the mechanical response of SiNWs to the applied bending, the relationship between the stored strain energy (U) and the bending angle (θ) was examined. The strain energy is defined as the change in the potential energy of SiNWs resulting from the applied bending moment. Only the U-θ curves for SiNWs with a diameter of 7.7 nm are plotted in Fig. 2 since their overall trends were not affected by nanowire diameter. The U-θ curves exhibit a similar trend regardless of nanowire orientation and cross-sectional shape. Specifically, the U-θ curves can be divided into two distinct regions: an elastic and inelastic region. In the elastic regime, the strain energy varies in a near-quadratic manner with the applied bending angle. At the end of the elastic region, a discontinuity is observed, which is attributed to the yield of the SiNWs. In the inelastic regime, the strain energy exhibits a near-linear dependence on the bending angle. Similar behavior has been reported for the bending deformation of carbon nanotubes [34]. At the end of the inelastic regime, a second discontinuity is observed. To reveal the deformation mechanism corresponding to the two discontinuities, visualizations of the evolution of atomic configurations are presented in the following section.

3.2. Deformation mechanism of SiNWs

The deformation mechanism of SiNWs under bending was insensitive to the cross-sectional shape and nanowire diameter. The atomic configurations of [1 0 0], [1 1 0], and [1 1 1] SiNWs with a diameter of 7.7 nm corresponding to different bending angles are