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Effect of surface roughness on elastic limit of silicon nanowires

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ABSTRACT

Effect of surface roughness on deformation mechanism and yielding strength of silicon nanowires under tension are investigated by using molecular dynamics simulation. By varying opening angle and depth of surface notches, different periodic V-type notches models are created on {1 0 0} or {1 1 0} side surfaces to simulate different types of surface roughness. The results show that the presence of rough surface can significantly reduce the initial elastic limit of silicon nanowires. The yield stress of rough wires with a certain cross-sectional size depends on the surface notch depth and is independent of the opening angle. We also investigated the size effect on this notch depth dependence, and observed that the yield stress becomes less sensitive when the wire height increases. In addition, the influence of surface orientation on the surface roughness effect was discussed.

1. Introduction

Silicon nanowires (Si-NWs) are of potential applications in nanoscale electrical devices such as electrochemical biosensors [1,2], field-effect transistors (FET) [3,4], photo detectors [5,6] and photo-voltaic solar cells [7]. The reliability and stability of these silicon nanowire-based emerging nanoelectronic devices are largely dependent on their mechanical properties, like elastic properties, elastic limit, failure behavior and etc. Recently, many experimental and computational investigations have been performed to study the fracture behaviors of Si NWs [8,9]. Brittle fracture behaviors of silicon nanowires have been reported by some experimental researches [10], whereas ductile deformation have also been observed at room temperature [11–13]. By using molecular dynamics simulations, ductile responses beyond yielding have been reported by Kang and Cai [14], while the axial orientations dependence of different fracture behaviors have been discovered by the current authors [15]. This ductile vs. brittle dispute had attracted extensive researches on failure behavior of Si-NWs. Among these researches, both experimental and computational results exhibited scattered at elastic limits.

Some of the strength fluctuation may be attributed to the uncertainties in different experimental conditions; some may be due to the inaccuracy of computational models, for almost all the previous reports considered nanowires as ideal cylindrical or square rods. In practice, realistic Si-NWs were usually covered by defective surfaces, surface contamination, amorphous shells or silicon oxide layers according to their synthesis methods [16–18]. It was reported that deformation mechanism of Si NWs under tension was largely determined by its surface effect [19]. Thus, it is expected that the role of surface or interface defects may play a key role in determining the mechanical properties of Si NWs when their sizes are reduced to several nanometers. Some works have been done to study the effect of such surface defects, i.e. typical single surface step. However, there are still no systematic researches with respect to the role of surface defects distribution (surface roughness) on the elastic limits of Si NWs.

Recently, surface engineering had attracted extensive interests owing to that they can affect the mechanical and physical properties of some semiconductor nanostructures [20–22]. It was reported that Li–Si reaction rate in lithium battery anode is crystallographic orientation dependent [23]. The variation of surface orientation may determine the key lithiation direction of silicon rods. Some researchers also reported thermal conductivity reduction by creating periodic saw-tooth faceting on Si-NWs sidewalls [18,21]. Additionally, surface roughness scattering mechanism was found to affect the size dependence of low-field electron mobility [24] in silicon nanowires. Given that physical properties of Si NWs can be dramatically altered by the variation of surface roughness, taking the influence of surface roughness into account is therefore needed for investigation of their elastic limits, which may provide potential applications for surface engineering.

To model surface roughness, we artificially create simplified Si NW models with a uniform rectangular cross-section and periodic notches on a pair of parallel side surfaces. In this way, rough

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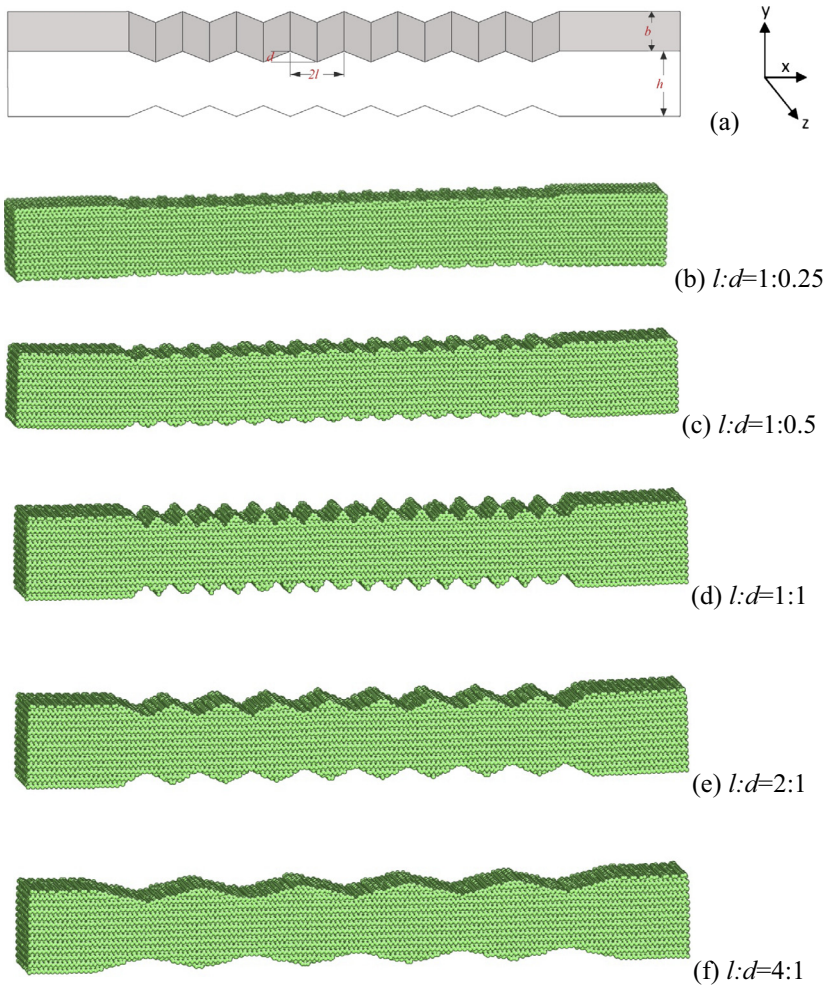

Fig. 1. (a) Schematic of silicon nanowires with two opposite rough surfaces. The wire length, width and height are L_0, b and h, respectively. Typical snapshots of initial silicon nanowires with different tilt factors l:d at (b) 1:0.25, (c) 1:0.5, (d) 1:1, (e) 2:1 and (f) 4:1.

Table 1
Si NW models and the corresponding lattice orientation along each direction.

Model name	x	y	z
⟨100⟩a	[100]	[010]	[001]
⟨100⟩b	[001]	[110]	[$\bar{1}$10]
⟨110⟩a	[$\bar{1}$10]	[001]	[110]
⟨110⟩b	[110]	[$\bar{1}$10]	[001]
⟨111⟩b	[111]	[1$\bar{1}$0]	[11$\bar{2}$]

surfaces with different notch geometries, i.e. surface notch depths and opening angles, can be created systematically on a specific surface. We should also bear in mind that Si NWs were commonly observed with hexagonal and nearly cylindrical cross-sections. This cross-sectional difference may affect elastic limits at yielding to some extent. By ignoring the cross-sectional shape effect here, we only focus on the effect of surface roughness on the elastic limit. By using molecular dynamics simulations, tensile deformations of Si NWs with and without surface notches are performed. We present the results about effects of surface notch depth and surface opening angle on the variation of elastic limits. Explanations of the notch depth sensitivity and opening angle insensitivity on yield strength are provided based on the underlying deformation mechanisms. Finally, we will discuss the effects of surface roughness based on surface energy calculations.

2. Methods

In this work, the influence of surface roughness on the deformation and fracture behaviors related to Si NWs stretching was studied by performing molecular dynamics simulations. As an alternative way, molecular dynamics simulation can be performed to uncover the detailed deformation mechanism that experiments cannot capture. The Modified Embedded Atom Method (MEAM) potential [25] developed by Timonova and Thijsse (2011) was used to account for the interactions among silicon atoms. This potential was well fitted to cohesive energy, equilibrium lattice, bulk modulus, surface energy, cubic elastic constants, vacancy formation energy, and screw dislocation Peierls stress. A detailed validation of the MEAM potential and the comparison between this potential and other classic potentials can be found in existed literatures [14,15,26].

Si NWs were usually manufactured with different axial orientations, cross-sectional shapes and wire sizes due to different synthesis techniques [22,27]. For simplicity, all wires are modeled of the same length but different axial orientations and surface roughness. All wires were cut from bulk crystal silicon with a rectangular cross-section. The length L_0 is aligned along x direction, height h along y direction, and width b along z direction, as shown in Fig. 1. Free boundary conditions are applied in all three directions. According to their axial orientation, we classified the modeled wires into three typical groups: ⟨100⟩, ⟨110⟩, and ⟨111⟩. To