

Mechanical properties of multilayer hexagonal silicon under uniaxial tension



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ABSTRACT

Molecular dynamics simulations have been performed to investigate the mechanical properties of the two-dimensional silicon films composed of plane and buckled layers. The results clearly show that the Young's modulus in the zigzag direction is slightly smaller than that in the armchair direction, but the fracture stress and the fracture strain in the zigzag direction are both larger than those in the armchair direction. Moreover, it is found that the silicon film with plane layers has larger Young's modulus and fracture stress than the buckled layer film, but the latter has larger fracture strain due to the stress-induced phase transition.

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1. Introduction

Since its discovery in 2004, graphene, a two-dimensional (2D) atomic layer of carbon with a honeycomb structure, has attracted a worldwide attraction due to its extraordinary properties and potential applications [1–8]. Inspired by the tremendous advancement in graphene, similar 2D materials composed of other group-IV element attracts considerable scientific interest. Recently, single-layer silicon, so called silicene, has been reported to successfully grow on Ag (100), Ag (110), and Ag (111) substrates [9–11]. Theoretical and experimental evidence has indicated that silicene with a buckled stable honeycomb structure is predicted to possess massless Dirac fermions and to exhibit a detectable quantum spin Hall effect, and other attractive properties [12,13]. Comparing with graphene, silicene has its own advantages. On the one hand, silicene could be used in field effect transistor (FET) operating at room temperature basing on the opening and controlling of the band gap, while the zero band gap limits the potential application of graphene in present electronic devices [14]. On the other hand, silicene may have more potential applications in future nanoscale devices due to its compatibility with conventional Si-based electronic technology. All these advantages open up new opportunities for 2D silicon for various fundamental science studies and electronic applications. Recently, some efforts have been devoted to

studying the formation of low-dimensional silicon confined in nano-slits. Morishita et al. [15,16] used molecular dynamics (MD) simulations to study the formation of nanowire, single- and double-layer silicon in slit pores and the stability is further confirmed by first principles MD calculations up to 300 K, which demonstrate the possibility of the synthesis of novel nanostructures by confinement in nanopores. Afterwards, the electronic and phonon properties of the double-layer silicon computed by Bai et al. [17] suggested that the bilayer hexagonal silicon is a quasi-2D semimetal.

While the 2D silicon has been investigated for potential application in electrical devices and micro/nanoelectromechanical systems, successful implementation in such nanodevices requires full understanding of its mechanical properties. Several theoretical studies about the mechanical behaviors of silicene have been reported currently [18–21]. Cranford et al. [22] have used full atomistic first-principles-based ReaxFF MD to quantify the elastic stiffness, limit states and bending stiffness of monolayer silicene. Their results indicate that the corrugated-like structure of silicene increases the bending rigidity compared to the similar system of graphene. Jing et al. [23] have used ab initio calculation and MD simulations to calculate the Young's modulus of bulk silicene and found that the Young's modulus depends strongly on the chirality and size of the silicene nanoribbon due to the edge effects. In addition, Meza-Montes et al. [24] have investigated the size, vacancy and temperature effects on Young's modulus of silicene nanoribbons.

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In this work, we perform MD simulations to study the mechanical properties of 2D silicon films under uniaxial tension. Different from previous study focusing on the monolayer silicene, this work attempts to study the tensile behavior of multilayer silicon films, which are formed in slit nanopores. The structural evolution, stress-strain relation and Young's modulus of the nanosheets in the armchair and the zigzag directions are explored. This work provides a good understanding about the mechanical and fracture behaviors of 2D silicon for the design and fabrication of electronic and engineering applications.

2. Methods

In this study, MD simulations are used to investigate the tensile behavior of 2D silicon films formed between two isolated and smooth walls. The modified Tersoff potential is employed to describe the silicon-silicon interaction, which is fitted to both the elastic constants and melting point by modifying the angular-dependent term of Tersoff potential function [25]. The model performs extremely well in describing the crystalline, liquid, and amorphous phases of silicon. In this work, we use the MD package LAMMPS to perform the simulations [26]. The Nosé-Hoover thermostat and barostat are used to control the temperature and pressure, respectively, and the velocity-verlet algorithm is used to integrate the equations of motion with a time step of 1 fs. Firstly, we structure the 2D silicene films between two walls. We utilize the 12–6 Lennard-Jones (LJ) potential, with a well depth $\varepsilon = 0.310$ kcal/mol and size parameter $\sigma = 3.804$ Å [27–30], to describe the silicon-wall interaction. The periodic boundary conditions are applied in the plane directions parallel to the wall, while in the vertical direction perpendicular to the wall, the slit size D between two walls is set to be 10.6 Å, 12 Å and 15 Å. For each D , the liquid silicon film is firstly equilibrated at 3000 K, followed by a cooling process to 300 K at a quenching rate of 0.1 K/ps and a consequent relaxation process for 200 ps at 300 K. The isothermal-isobaric (NPT) ensemble are used in this stage at zero pressure. Then, we select the ordered structures from the obtained films as supercells. After structure optimization, the supercells are used as repeated units to build larger free-standing 2D silicon crystal sheet. Thereafter, silicon films with the size of about $200 \text{ Å} \times 200 \text{ Å}$ (containing 10,976, 12,480 and 18,720 atoms, respectively) with periodic boundary in the plane directions are cut down from the silicon sheet, followed an relaxation process for 1000 ps at 300 K and zero pressure under the NPT ensemble. Finally, the crystal sheets are stretched at a strain rate of 0.0002/ps in the armchair and the zigzag directions under the canonical ensemble.

3. Results and discussion

To begin with, we investigate the solidification behavior of liquid silicon films confined in nano-slits with different sizes (D). Fig. 1 shows the change of potential energy (E_p) per atom and average coordination during the cooling process. It could be found that both the E_p and average coordination strongly depend on the temperature and the slit size. As plotted in Fig. 1(a), the tendency of E_p versus temperature for different slit sizes is similar, where the E_p drops slowly with the decrease of temperature except a sudden decline when the phase of system transfers from liquid to solid. The transition points are 1650 K, 1570 K and 1230 K at $D = 10.6$ Å, 12 Å and 15 Å, respectively. Fig. 1(b) shows the average coordination as a function of temperature. The coordination number of each atom counts neighbors within a radius of 3 Å, which is closely related to the geometry of the local structure and is extremely useful in the analysis of the various covalent bonding struc-

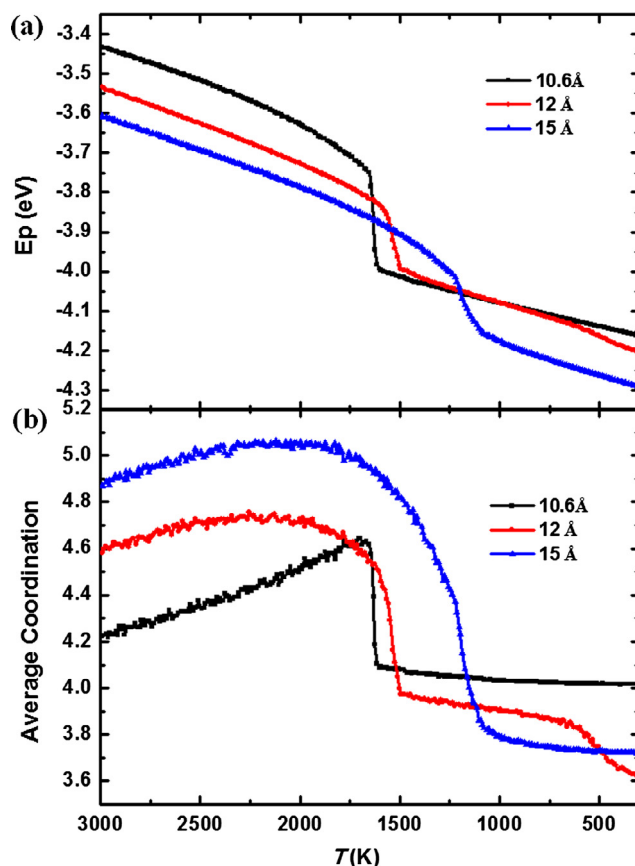


Fig. 1. Freezing process of liquid silicon films confined in slits with different sizes. (a) Potential energy (E_p) per atom and (b) average coordination as a function of temperature.

tures [31–33]. It can be found that the average coordination first increases and then decrease slowly with the decreasing temperature. In the stage of liquid-solid phase transition, the average coordination decrease sharply. It is worth noting that the average coordination of the three films at 300 K are quite different from each other, indicating these films have different structures.

To further clarify the structural details of silicon films, the microscopic structures of silicon films at 300 K are displayed in Fig. 2. It can be found that the solidification structure is very different at different slit sizes. At $D = 10.6$ Å, despite the disordered structure and a few topologic defects, the 2D silicon is composed of two plane layers (2PL). Each layer exhibits a hexagonal structure composed of tetracoordinated atoms (TETRACAs) as shown in Fig. 2 (a), much different from the tricoordinated atoms (TRICAs) dominated graphite, due to the strong atomic interaction between two layers [34,17]. At $D = 12$ Å, the silicon film is composed of two buckled layers (2BL). As shown in Fig. 2(b), each layer of the silicon film prefers a low-buckled hexagonal structure. The atoms in the hexagonal structure arrange alternatively in two sub-layers. The outer sub-layer is composed of TRICAs while the inner sub-layer is composed of TETRACAs because the atoms in the inner sub-layer get bonding with those in the inner sub-layer of the other main layer. Similarly, the silicon film is composed of three buckled layers (3BL) at $D = 15$ Å as shown in Fig. 2(c). It is worth nothing that the middle layer has a diamond structure composed of TETRACAs, while the other two surface layers has similar structure with those $D = 12$ Å. The atoms in two sub-layers of the middle layer get bonding with the atoms in the two surface layers, respectively. Fig. 2(b) shows the density profile at different slits, which is measured by calculating the atomic number density within a thin slice

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