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Pathway into the silicon nucleation on silicene substrate at nanoscale

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ABSTRACT

The solidification process of silicon atoms on the heterogeneous surface of silicene in different shapes, ranging from plane, curved to tubular substrates, is studied by means of molecular dynamics (MD) simulations. The shape of nucleus determines the stacking sequence of silicon atoms. Silicene plate induces strong ordered liquid layers while the silicene nanotube (SNT) makes the silicon imprint its cylindrical structure. In the confined nanospace between SNTs, the growth competition has been observed, which causes structural changes at the shared interface. The internal potential field around SNT is responsible for the formation of spiral structures and the growth competition. The ordering degree decays with increasing distances from the SNT, which is the result of the decreasing acting force from nucleus. This study provides an opportunity for comprehensive and satisfactory understanding of the heterogeneous nucleation at nanoscale.

1. Introduction

Heterogeneous nucleation at the atomic scale has been attracting continuously attentions in the field of material science [1–3]. The geometrical shape of heterogeneous nucleus affects crystallization and profoundly determines the final structure [4–8]. Researchers [9] found that the shape of graphite in liquid cast metal has remarkable heredity effect, since then, much research work [10–13] has been done to discover such phenomena. Some studies [14–16] addressing heterogeneous nucleation relied almost on the classical spherical cap model exclusively. Recent studies [17,18] on heterogeneous nucleation are mainly phenomenological and paralleled extensions of classical nucleation theory. Due to the importance of heterogeneous nucleation, its mechanism has been a long-standing concern. Such theories explain the system qualitatively, but lose their applicability when the size of nuclei is comparable to the interface size. In spite of the immeasurable technological significance, nevertheless, the behavior of heterogeneous nucleation has not been well characterized [19,20].

In recent years, silicon materials has received much attention for its extensive applications in integrated circuits, photovoltaic materials and nanoelectronic transistors [21–23]. In order to design the high-quality silicon materials theoretically, the growth orientation, defect density, morphology and size of crystal grains should be controlled well. The addition of graphite into silicon as the heterogeneous substrate has been studied sufficiently as a method to manufacture the monocrystalline silicon theoretically [24]. However, the technique introduces carbon impurities into the monocrystal silicon, causing serious technological problems. To overcome these puzzles, growth of silicon on the silicene substrate can be a promising method to control the heterogeneous nucleation at an atomic scale, preventing the adulteration into simple silicon materials. To our knowledge, the incorporation of silicene into Si melt to manufacture the silicon material with significant properties has not been reported until now.

The main purpose of this paper is to study the silicon freezing on silicene substrates with different shapes, providing crucial theoretical support to guide the fabrication of high performance silicon materials.

2. Method

In this work, the silicon solidification on heterogeneous surfaces of tubular silicene is studied by MD simulations [25]. The discover module of Materials Studio [26,27] is used for all calculations. We have noticed that the COMPASS force field [28,29] has been proven to be applicable in describing the mechanical properties of carbon nanotubes and graphene sheets [30,31]. The COMPASS development has extended the coverage to include inorganic materials: metals, metal oxides, and metal halides [32]. In addition, the parameters of –Si–Si– have been well parameterized and rigorously tested by COMPASS force field [32]. Therefore, the COMPASS is a relatively ideal force field applying in silicene–silicon system.

The COMPASS force field aims to achieve high precision in predicting the nature of complex mixtures and condensed phase materials [33,34], which some parameters are derived based on ab initio data [35–37]. The maximum iteration is chosen as 10 [5] steps and time step is 1.0 fs. Temperature is controlled by Nose thermostat and the NVT ensemble (the number of particles N, volume V, and temperature T are constant) is

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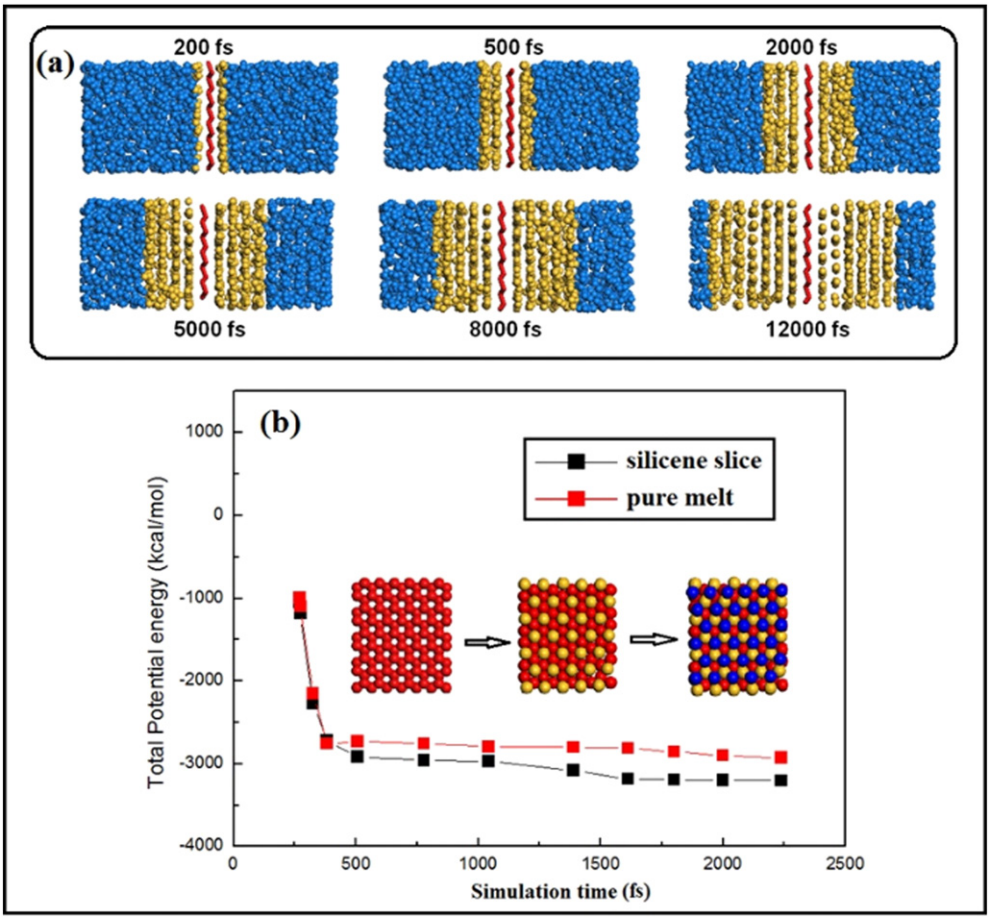

Fig. 1. Silicon layer formation on the silicene slice and the total potential energy variation: (a) process of silicon atoms solidification on sheet silicene at different relaxation time, (b) potential energy variation as a function of time, the inserted graph shows the layer-by-layer distribution of melt atoms adjacent to the sheet silicene.

chosen. The Verlet algorithm is employed to calculate the velocity, and initial velocities of silicon atoms follow a temperature-dependent Boltzmann distribution. To achieve the growth process of silicon on heterogeneous surfaces of tubular silicene, several procedures should be done. Firstly, the standard crystal of silicon is heated and melted to liquid state at the temperature of 1800 K. Finally, the heterogeneous

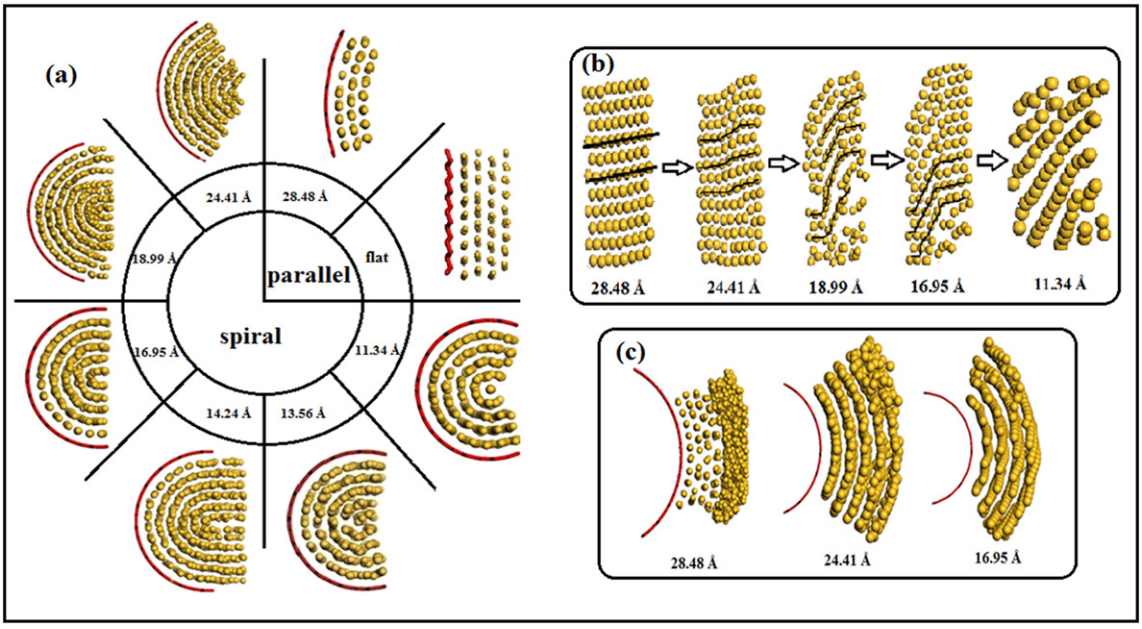

Fig. 2. Silicon atom formation on the curving silicene: (a) solidification on the curving silicene with fixed arc length (61.25 Å) but with different curvature radii (ranging from 28.48 Å to 11.34 Å), (b) side view of the silicon atoms layer close to the curving silicene, (c) final structures of droplets outside the curving silicene.