

A Possible Approach Towards Silicene on Nonmetallic Substrates

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[Introduction]

Due to stronger spin-orbit coupling (SOC) effect and possible applications in realizing **quantum spin Hall (QSH) effect**, a close sibling of **graphene** called **silicene**, where Si atoms substitute C atoms in a two-dimensional honeycomb lattice, has drawn much attention both theoretically and experimentally in the past few years. Since valence orbitals of silicon do not sp^2 hybridize as easily as those of carbon, silicene is expected to prevail in a **low-buckled** form, i.e. neighboring Si atoms are displaced out of plane. Although it is difficult to form, freestanding silicene has been predicted and examined to be stable [1-3]. However, so far **the reported experimental studies of silicene using ARPES and STM/STS have been performed mainly on the metallic substrate of Ag**, where the abundant electronic states from the substrate may easily couple with and alter those of silicene on top.

Here we fabricated **single-layered Si nanofilms on Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β** which has a large gap to minimize the substrate effect and to obtain a nearly free-standing structure, characterized them with **in-situ Scanning Tunneling Microscopy/Spectroscopy (STM/STS)**, and achieved both the atomic and electronic structures of these nanofilms.

[Results and Discussion]

1. Atomic Structure of Silicene

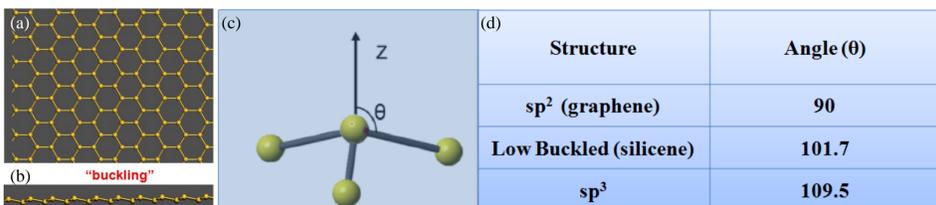


Fig. 1 Top view (a) and side view (b) of silicene. (c) Schematic of atomic arrangements with angle θ , which is defined as the angle between Si-Si bonds and Z direction normal to the plane. (d) Table of structure vs. angle θ .

2. Band Structure of Silicene

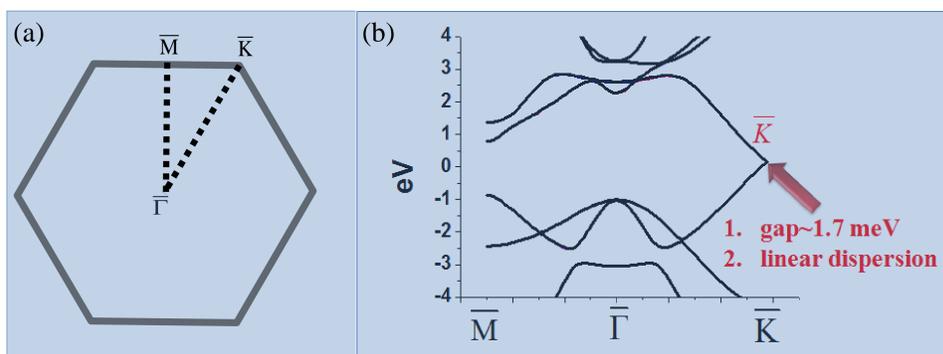


Fig. 2 (a) Schematic of the first Brillouin zone (FBZ) of silicene and its points of high symmetry. (b) Calculated band structure of silicene. Zero of energy is set at the Fermi level. There is a small bandgap (~ 1.7 meV) at \bar{K} , and bands are linear near the cross section point at \bar{K} .

3. Substrate: Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β Reconstructed Surface

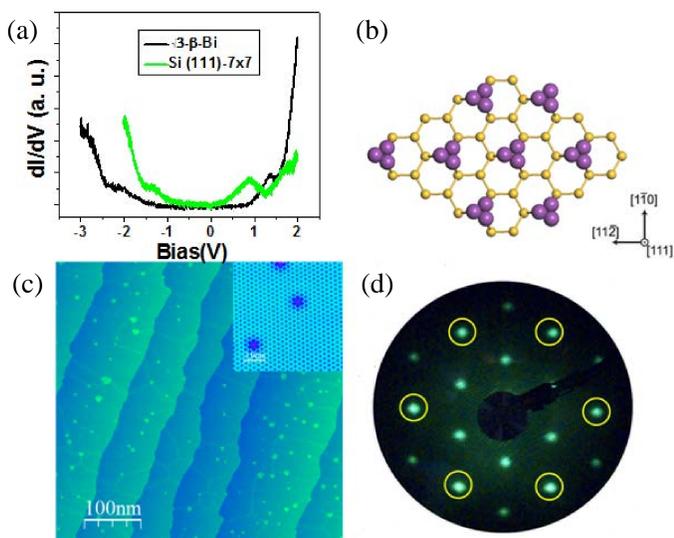


Fig. 3 (a) STS of Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β (black line) and Si(111)-7 \times 7 (green line). The reconstructed surface can fully passivate the dangling bands on the surface and thus induce less DOS near E_F . (b) Structural model of β -phase with trimer Bi atoms adsorbed on the T4 positions. Yellow balls represent Si atoms while the purple ones represent Bi atoms. (c) Surface of Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β with the inset showing the atomic resolution image of 15 nm \times 15 nm. (d) LEED pattern of Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β . Si 1 \times 1 spots are marked by yellow circles for reference.

4. $\sqrt{3}\times\sqrt{3}$ Reconstructed Silicene Nanofilms on Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β

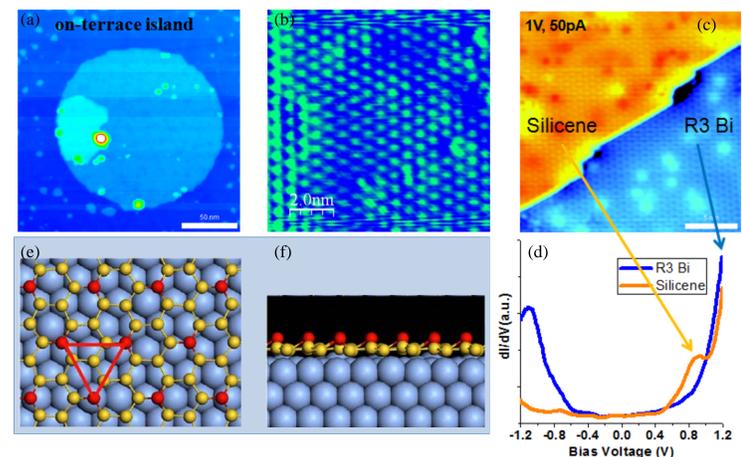


Fig. 4 (a) STM image shows a round silicene island forms on Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β . (b) Atomic resolution image taken on the island indicates $\sqrt{3}\times\sqrt{3}$ reconstruction of silicene. (c-d) Comparison of two different 3×3 reconstructions: silicene on top and Bi- β below. Besides the differences in the atomic resolution image (c), i.e. silicene are solid spots while Bi- β are honeycomb, STS (d) also shows different LDOS distributions. (e-f) Adapted from Ref. [3]. Top views (e) and side views (f) of $\sqrt{3}\times\sqrt{3}$ structures of silicene. Color code: Yellow and red spheres denote Si atoms in lower layer, and Si atoms in higher layer, respectively.

5. Armchair and Zigzag Edge States of $\sqrt{3}\times\sqrt{3}$ Silicene

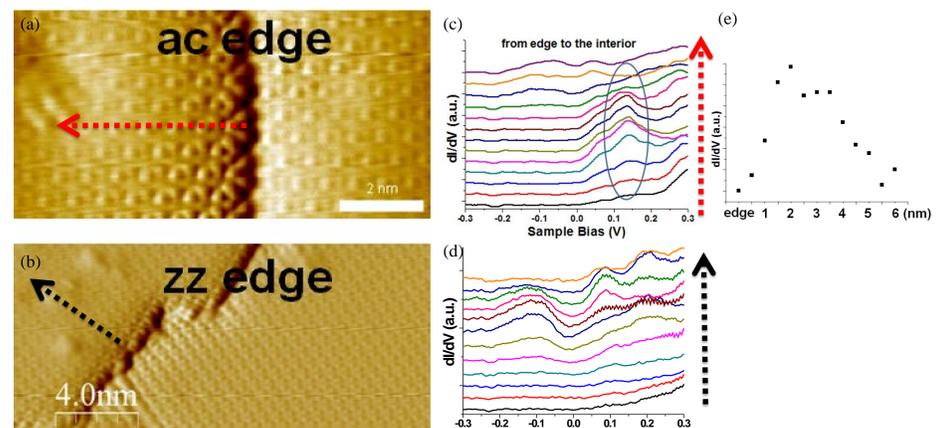


Fig. 5 (a-b) Atomic resolution images show the detailed structures of armchair (a) and zigzag (b) edges of silicene, respectively. (c-d) A series of STS taken on the perpendicular directions of ac edge (c) and zz edge (d). (e) LDOS intensities at 131 meV at the ac edge are extracted to identify the position where peak values show up. Notice no such obvious trends exist in the zz case.

6. 2×1 Reconstructed Silicene Nanofilms on Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β

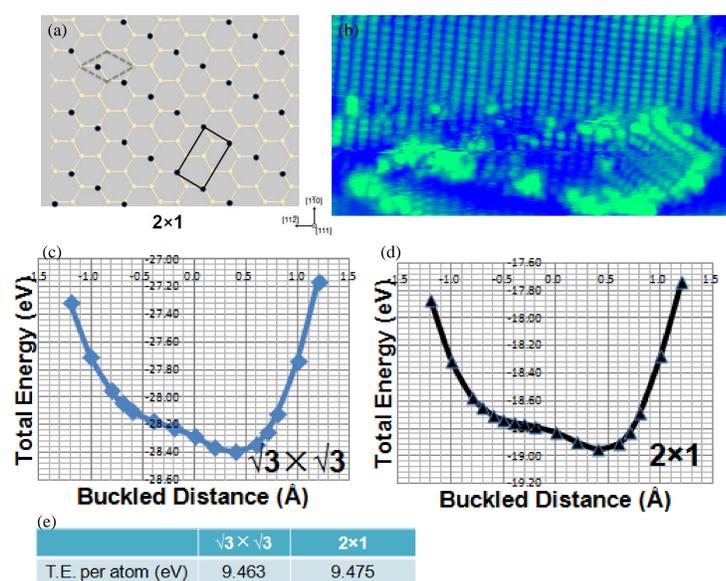


Fig. 5 (a) Schematic of 2×1 reconstruction of silicene. (b) 20nm \times 10nm image shows the 2×1 . There are two orientations within two nearby domains, whose angle is 60° . (c-e) Total energy as a function of buckle distance in two kinds of reconstructions based on DFT calculations. Due to the comparable total energy per atom, phase transition between the two structures is highly possible.

[Conclusions]

Silicene islands can be formed on the nonmetallic substrates, Si(111)- $\sqrt{3}\times\sqrt{3}$:Bi- β . Armchair and zigzag edges exhibit different electronic features, indicating different natures of two kinds of edge states. Additionally, 2×1 reconstruction is also present in the system. We confirm the stability of those two phases by DFT calculations as well. Our results demonstrate a well-defined basis for further studies of silicene on semiconducting substrate, offering a possible approach for silicene-based device architecture in the practical field.

[References]

- [1] Meng, L. et al. Buckled Silicene Formation on Ir(111). Nano Lett. 13, 685-690, (2013).
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- [3] Lin, C.-L. et al. Substrate-Induced Symmetry Breaking in Silicene. Phys. Rev. Lett. 110, 076801 (2013).