

Atomic structure of silicon nanoribbons on Ag(110)

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Abstract. Silicon nanoribbon (NR) growth on Ag(110) substrate is reinvestigated using scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Deposition of a single silicon monolayer at 230 ° C results in the formation of one-dimensional 1.6 nm wide silicon nanoribbons into a well-ordered compact array with a nanometer scale of only 2 nm. Based on STM analysis, we obtained an atomic model of silicon nanoribbons (NRs) in which they are essentially twisted, and the quantum confinement of electrons in NRs contributes to the electron density of states.

1. Introduction

Substantial efforts have been focused recently on the electronic properties of two-dimensional (2D) materials in the perspective of their integration new devices [1]. Given the impact of graphene over the last few years [2], the isomorphic silicene [3] and germanene [4] are now considered to be promising novel materials with the advantage of being compatible with existing semiconductor technology [5]. Theoretical investigations of free-standing silicene show that these two novel materials have electronic structures with band structures presenting a linear crossing at the K and K' points of the surface Brillouin zone indicative of semi-metallic character, and massless Dirac fermion character. These result in similar properties such as a large charge carrier mobility and Hall effect [4,6-8]. For the moment, the primary method for growing silicene and germanene is on solid substrates, in particular silver: Ge/Ag [9-12] and Si/Ag [3, 13-15] and recently on gold [16] and iridium [17]. On Ag(111), silicene forms a continuous sheet [15], with at least three distinct ordered phases [18-21], depending on the deposition conditions. Free-standing silicon sheets only exist as silicon nanotubes [22] or multilayer silicene from chemical methods [23]. Now, nanoribbons are very interesting because of their potential for 1D dispersion effects with directional conductivity. A perfectly well defined edge structure is required and the coherent electron confinement will lead to observable effects such as quantum interference channeling at their edges [24]. To achieve this, graphene nanoribbons have to be synthesized chemically [25, 26], and Bi nanolines on Si(001) require a high formation temperature (600 °) [27], while Si nanowires on SiC did not show any 1D conductivity [28]. On the Ag(110) surface, one-dimensional silicene nanoribbons (NRs) [13] can be grown. The isolated NRs show a low

reactivity to molecular oxygen; oxidation occurs only at the Si NRs terminations and develops along the $[-110]$ direction indicating that their edges are not reactive to molecular oxygen [29]. In response to this remarkable observation, we present Scanning Tunneling Microscopy images of a compact parallel assembly of silicene nanoribbons on Ag(110). The NRs are 1.6 nm wide with a well-defined edge structure and an electronic contribution is visible in the STM images taken at different voltages.

2. Experiments

The standard tools for surface preparation and characterization were used: an ion gun for surface cleaning, a low energy electron diffraction (LEED) instrument, and a scanning tunneling microscope (STM) for surface characterization at the atomic scale. The STM experiments were performed at room temperature (RT). The Ag(110) sample was cleaned by several cycles of sputtering (600eV Ar^+ ions, $P = 5 \cdot 10^{-5} mbar$) followed by annealing at 400 °C until a sharp $p(1 \times 1)$ pattern was obtained. Silicon was evaporated by a direct current heating of a piece of Si wafer, and deposited onto the Ag(110) surface held at 230 °C.

3. Results and discussion

Figure 1a shows the bright sharp (1×1) LEED pattern of the clean bare Ag(110) surface. The deposition of silicon on the silver substrate is done at a constant flux and the LEED patterns are regularly monitored. We found that during silicon deposition on the Ag(110) substrate held at 230 °C, a (2×5) LEED pattern appears and becomes brighter as we approach a Si coverage of 1 monolayer (ML), as clearly seen in Figure 1b. The $(x2)$ periodicity is along the $[\bar{1}10]^*$ while the spots along the $[001]^*$ direction show a $(x5)$ periodicity relative to the bare substrate. To guide the eye, the $(x5)$ and the $(x2)$ spots are highlighted by white circles. This clear LEED pattern is a signature that 1ML of silicon forms an extended periodic superstructure on Ag(110).

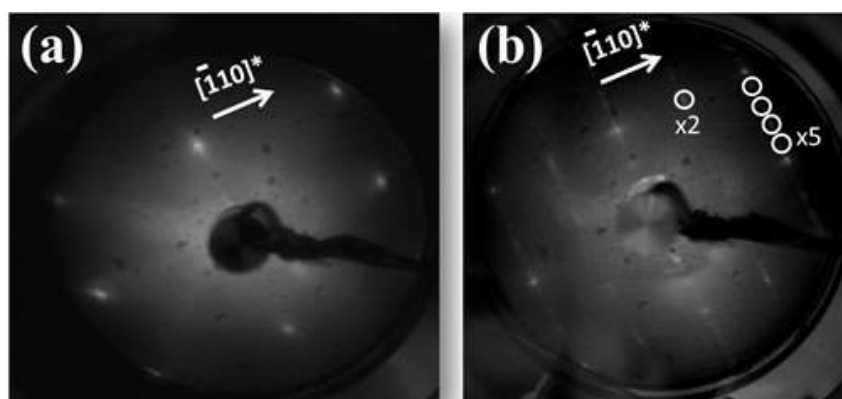


Figure 1. LEED patterns recorded at $E_p = 50eV$ corresponding to: a) the (1×1) reconstruction of the bare Ag(110) surface, b) the (2×5) superstructure obtained after the deposition of 1 Si ML on Ag(110) held at 230 °C. The $(x2)$ and $(x5)$ spots are highlighted by white circles.

We performed STM measurements at several imaging conditions to probe atomic structure of this (2×5) silicon superstructure in more detail. The (2×5) superstructure STM image (Figure 2a), obtained at a sample voltage $V = -80$ mV and a constant current of 2.2 nA, shows a well-ordered and compact array of self-assembled silicene nanoribbons (NRs). All these silicene NRs are aligned along the $[-110]$ direction of the bare Ag(110). By scanning large areas of the surface, we noted that their length is limited only by the size of the terraces. In order to quantitatively

determine the structural characteristics of the silicon NRs, several line scans were analyzed and shown in Figures 2b and 2c. The line scans reveal NRs with a width of 1.6 nm, corresponding to $4a_{Ag}$ where $a_{Ag}=0.409$ nm, and they are evenly spaced with a separation of 2.0 nm corresponding to a (x5) periodicity along the Ag [100] direction (Figure 2b). In the STM image, the NRs are composed of an ordered array of protrusions (bright spots) with a spacing along the Ag [-110] direction corresponding to a (x2) periodicity (Figure 2c). The distance between two neighbor protrusions along the Ag $[\bar{1}10]$ direction is equal to 0.58 nm corresponding to $2a_{[\bar{1}10]}$, in good agreement with the (x2) periodicity shown in the LEED pattern along the Ag [-110] direction.

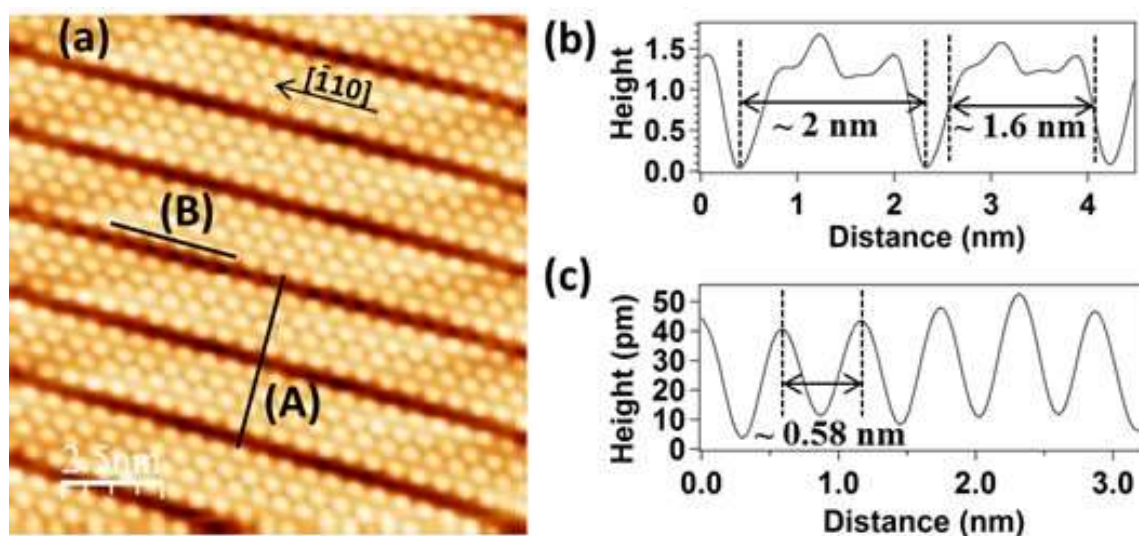


Figure 2. a) STM image of silicene NRs grown at 230° C on a Ag(110) surface ($12.5 \times 12.5 \text{ nm}^2$, $V = -80$ mV, $I = 2.2$ nA), b) line scan A across the NR showing the (x5) periodicity, c) line scan B along the NR showing the (x2) periodicity.

In Figure 2, the lateral size of the protrusions within the NRs is too large to correspond to single silicon atoms. So the silicon NRs were imaged under different conditions from those of Figure 2. At a surface voltage of -0.2 V and a constant current of 1.9 nA, we observed a honeycomb arrangement (highlighted in red in Figure 3a) indicative of a quasi-atomic resolution. The pattern is clearly quite different from that in Figure 2. An analysis of the line scans shows that the distance between the nearest-neighbor protrusions forming this honeycomb structure (red hexagons) is equal to 0.335 nm. This distance is much larger than the expected nearest-neighbor Si-Si distance of 0.235 nm, indicating that the protrusions observed in the STM image do not correspond to neighboring Si atoms. Based on these experimental observations, we derived a structural model, which is displayed in Figure 3b. In this model we assign the protrusions observed in STM to the two second-neighbor silicon atoms of an armchair-terminated silicene nanoribbon. Now, the 0.58 nm wide hexagons are commensurate with the (x2) periodicity along the Ag direction, giving a measured lateral distance of 0.335 nm between the two second nearest silicon atoms. This results in an in-plane lateral separation between nearest-neighbor Si atoms of 0.193 nm. There are two explanations why not all the silicon atoms in the NRs are visible in the STM images. The first is that the silicon atoms in the nanoribbon are substantially buckled, as recent studies on silicene have reported [21, 29] with a buckling between 0.04 and 0.12 nm. The reported Si-Si bond length in silicene sheets varies between 0.20 and 0.25 nm, which implies that the projected in-plane Si-Si distances are close to

the 0.193 nm value measured in this study and previously [15, 29].

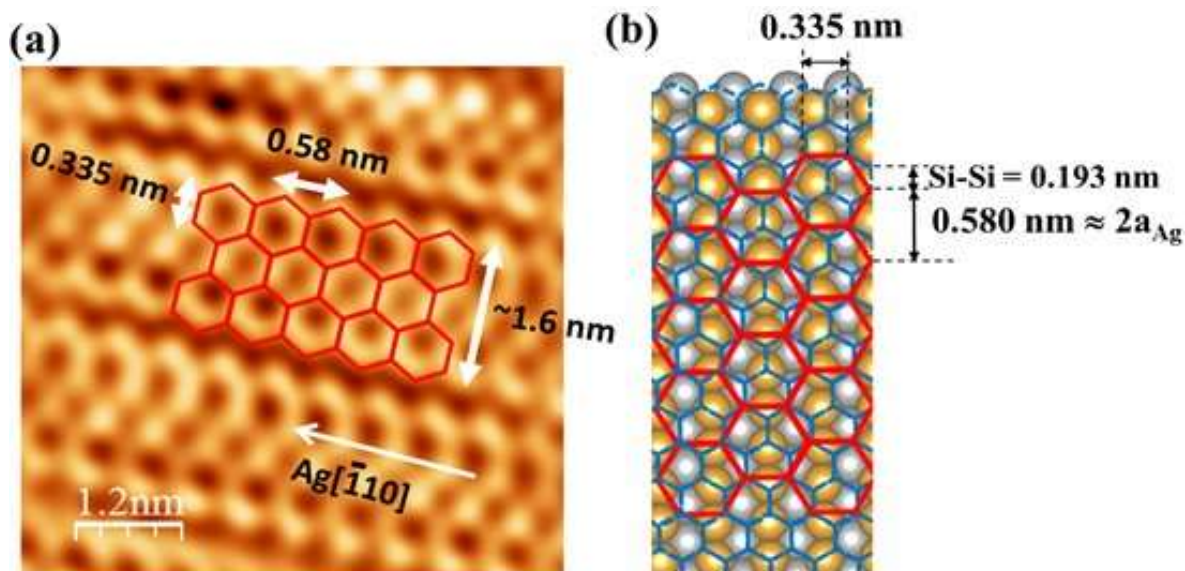


Figure 3. a) Atomically resolved filled-states STM image of silicene NRs grown at 230 °C on a Ag(110) surface ($6 \times 6 \text{ nm}^2$, $V = -0.2 \text{ V}$, $I = 1.9 \text{ nA}$). b) Proposed model where the grey and yellow atoms correspond to the first and the second silver layers, respectively. The blue honeycomb structure corresponds to the internal structure of silicene NRs while the red one corresponds to the structure observed in the STM image.

The second explanation is an electronic contribution to the periodic structure in the STM images, which is controlled by the interaction between the atoms of the silicene and the rows of underlying Ag atoms. The graphene and silicene honeycomb structure has a Bravais lattice containing two atoms which leads to an inequivalence between the sub-lattices "a" and "b". Inspection of Figure 3a immediately shows that the red hexagons occupy 2/3 of the atoms of one lattice and the central "chains" are aligned between the Ag atom rows. Recently, theoretical calculations indicate that electron transport occurs coherently via atoms of the same sub-lattice [31]. Also, the 1D nanoribbon confines the 2D electron gas giving rise to electron scattering at armchair edges with the formation of quantum interferences localized on the bonds [25]. These two related effects indicate that the electron density is channeled along the nanoribbons.

4. Conclusion

In conclusion, we have presented a detailed experimental study of the epitaxial growth of silicon on Ag(110), held at 230 °C. The STM images reveal a self-assembled compact array of silicene nanoribbons with a very low density of defects. The NRs are tens of nanometers in length with a uniform width of 1.6 nm, and commensurate with the Ag(110) surface giving a (2x5) periodicity in the LEED measurements at saturation (1ML). We propose an atomic model of silicene nanoribbon with arm-chair edges. Careful scrutiny of the atomically resolved STM images, taken at several imaging conditions, indicates that not all silicon atoms in the NRs are observed. This is explained by a substantial buckling of the NRs and an electronic contribution due to the quantum confinement of the electrons in the NRs.

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