

Short Term Mobility 2011 Report :

Silicite: Multilayers of Silicene nano-ribbons

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A strong interest for silicene, that is a one-atom thick silicon sheet arranged in a honeycomb lattice [1], has been recently developed. Theory predicted free-standing silicene sheets and ribbons to be stable either in a flat or in a low puckered configuration. In both cases they would present basically the same electronic properties of graphene [1-3]. The predicted electronic structure of silicene presents π and π^* bands, which form so-called Dirac cones at the Brillouin zone corners. Consequently, as in graphene, the charge carriers in silicene would behave as massless relativistic particles. Therefore all graphene expectations [4], such as high-speed electronic nanometric devices based on ballistic transport at room temperature, could be transferred to this innovative material with the crucial advantage of easily fitting into the silicon-based electronics industry.

Recently, we reported on the electronic properties of straight, 1.6 nm wide, silicene nano-ribbons on Ag(110), arranged in a one-dimensional grating with a pitch of 2 nm, whose high-resolution scanning tunneling microscopy images reveal a honeycomb geometry [5-11]. Angle-resolved photoemission (ARPES) shows quantum confined electronic states of one-dimensional character [12]. The silicon band dispersion along the direction of the nano-ribbons suggests behaviour analogous to the Dirac cones of graphene on different substrates [12].

Here, we report a preliminary results on the realization and study of multilayers of silicene nano-ribbons on Ag(110), coined “silicite”, studied by reflection high energy electron diffraction (RHEED) and scanning tunneling microscopy (STM), during the short term mobility stage of last November 2011 at National Institute for Materials Science (NIMS) Laboratory of Tsukuba (Japan). This study is extremely interesting and confirms the results obtained by ARPES, where the presence of π and π^* bands of the Dirac cones at the Brillouin zone corners, in analogy to what newly discovered for silicene, points out to a findings of a new Silicon material, the analogous of graphite. We observed the growth of silicite by RHEED and STM, and the closing of the gap of the $\pi\pi^*$ states of SiNRs vs the breakaway of the last silicene layer from the Ag substrate by ARPES [P. De Padova, paper in preparation].

STM/STS and RHEED observations were carried out at the Nano Functionality Integration Group, International Center for Materials Nanoarchitectonics, NIMS in Tsukuba (Japan). The Ag(110) substrate was cleaned in the UHV chamber (base pressure: $7.5 \cdot 10^{-11}$ mbar) by repeatedly sputtering with Ar^+ ions and annealing the substrate at 750 K, while keeping the pressure below $2 \cdot 10^{-10}$ mbar during heating. An infrared pyrometer was used to measure the sample temperature. Si was evaporated at a rate of ~ 0.03 ML/min from a Si source, up to 4 monolayer (ML), while the Ag substrate was kept at $T \sim 470$ K to produce the multilayers of array of SiNRs. The STM images were recorded at RT in constant-current mode at a bias voltage from ± 0.1 to ± 3 V and a tunneling current from 1 to 10 nA. Two STM probes resistance measurements on silicite are still in progress at NIMS laboratory.

The growth of *silicite* was investigated. The RHEED of Fig. 1 (a) and 1 (b) are the pattern corresponding to the 1×1 of the clean Ag(110) surface. Below 1ML of Si coverage the SiNRs show a 5×2 symmetry (not shown), indeed at the completion of the first layer or more, as displayed in Figure 1(b) and 1(c), the RHEED exhibit a 5×4 symmetry. This symmetry is preserved for several silicene layers, as showed in Figure 2 (d) and 2(e) for about 4 ML of silicene, where the RHEED exhibit a perfect $\times 4$ along the $[100]^*$ and a $\times 5$ along the $[1-11]^*$ direction. Here, we can see the V-shape typical of a 3D growth, which points out to the achieving the multilayer of silicene NRs (silicite). It is worth

noting that this 3D growth is localized only along the $[1-10]^*$ direction furnishing a set of silicene layers, which maintain the $\times 4$ along the $[100]$ direction. Theoretical calculations within local-density approximation on Si multilayers arranged in honeycomb-like structure were found energetically possible [13].

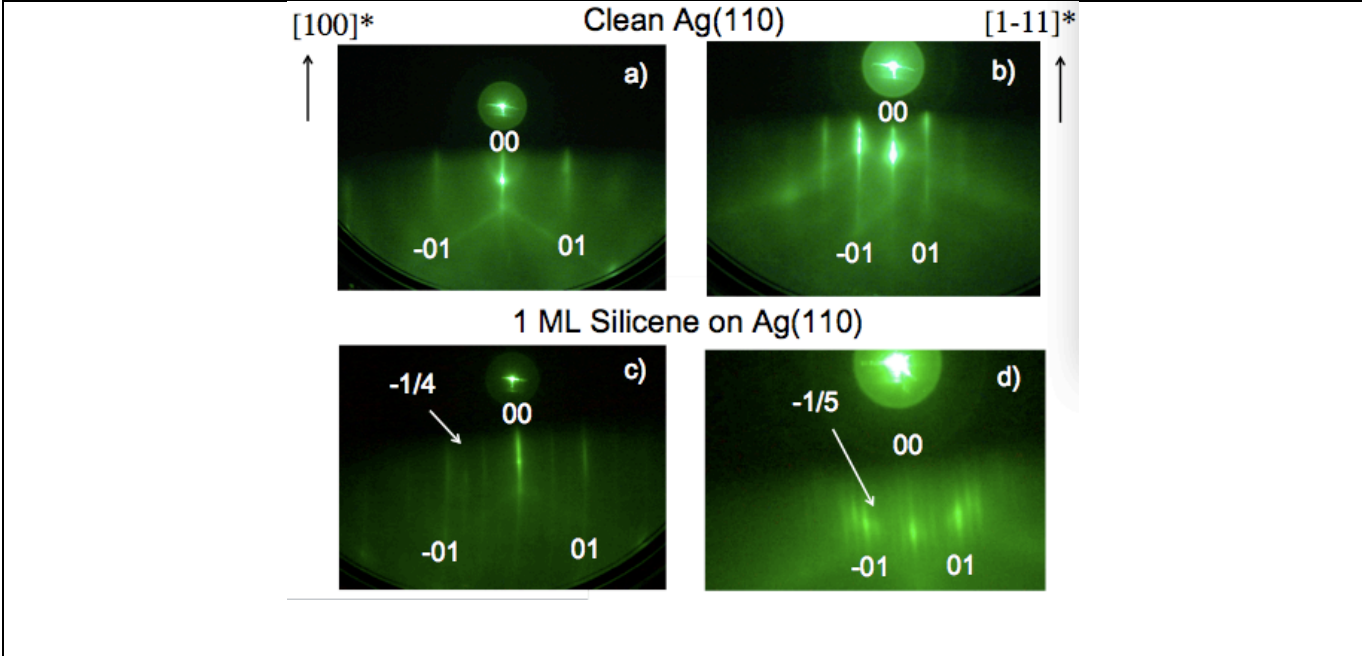


Fig. 1 RHEED patterns of clean Ag(110) (a) and (b) and after the growth of 1.5 ML of silicene (c) and (d).

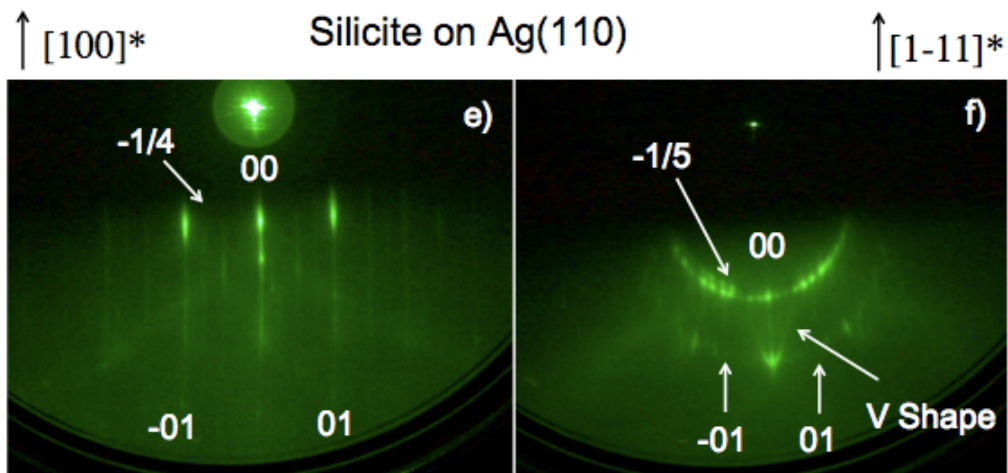


Fig. 2 RHEED patterns from 2 ML of silicene (e) and (f).

We display in fig. 3 a large-scale STM image evidencing the SiNRs having the 5×4 periodicity grown on the Ag(110) terraces. They are all aligned along the $[-110]_{\text{Ag}}$ direction, showing lengths of several nanometers. The Ag(110) surface is full covered by SiNRs, and on top of the first Si monolayer are observable brighter SiNRs structures, which are the onset of the growth of the second Si layer. As reported in previous works, the SiNRs possess a honeycomb-like arrangement, which continues to preserve at Si layer bigger than 1 ML. This evidences a new allotrope of silicon, coined silicite, i.e., more than one thick atomic graphene-like Si layer.

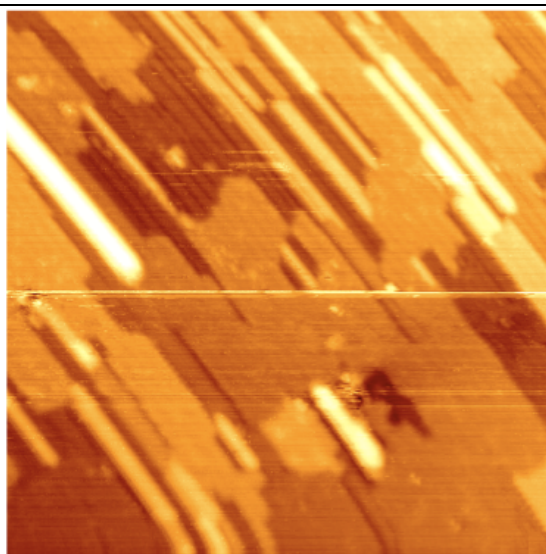


Figure 3 400 x 400 nm² image (V = - 0.19 V, I = 2.54 nA) high-resolution filled-states STM image from 1.5 ML of Si deposited on Ag(110).

To better evidence that, we report in Figure 4 a filled-state STM image from 4 MLs Si grown on Ag(110). The RHEED correspondent to this growth is showed in Figure 2, where the 3D Si structures are arranged only along the c-axis (perpendicular to the surface), being in the others direction formed by 2D layer of silicene NRs. The line profile taken perpendicularly to the silicite is reported in Figure 5.

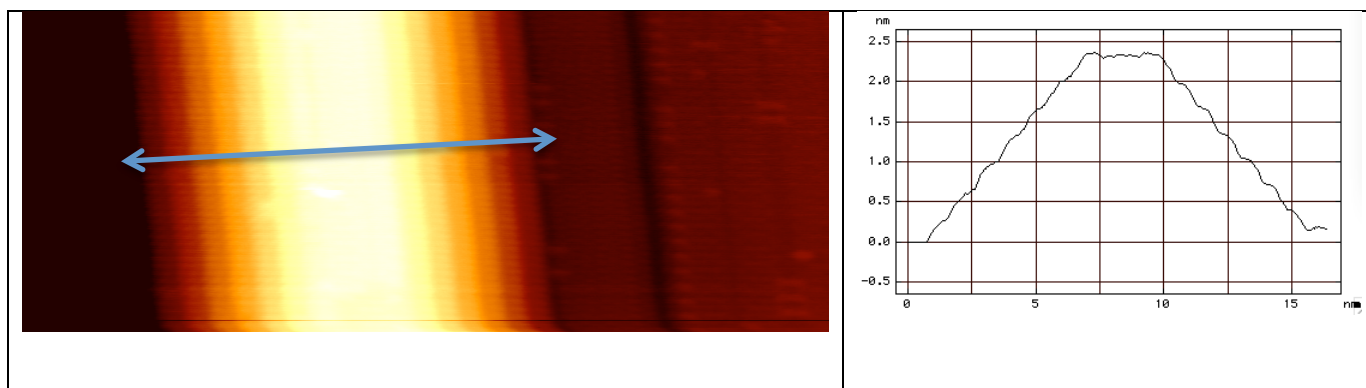


Figure 4 400 x 400 nm² image (V = - 0.19 V, I = 2.54 nA) high-resolution filled-states STM image from 1.5 ML of Si deposited on Ag(110).

Figure 5 Line profile of the silicite reported in Figure 4. The distance between two silicene layers is about 0.3 nm. The width of the silicite is about 15 nm.

The electronic properties of this array of multilayer of SiNRs, which consists of π and π^* bands forming projections of Dirac cones at the extremities of the 1D Brillouin zone, confirm their graphite nature of their Si-Si bonds exhibiting the sp^2 -like hybridization. This peculiar nature of silicite SiNRs confers to this new allotrope Si a remarkable interest for material science. The paper of these scientific results is in preparation.

Acknowledgements

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