

Synthesis and properties of Silicene layers on metallic substrates

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Abstract

For the past three years many groups around the world work intensively to achieve the synthesis of silicene which is a new crystalline form of silicon i.e. a single atomic layer of silicon with a honeycomb atomic structure like graphene. Many theoretical calculations using ab initio or tight binding approach have shown that this new allotropic form of silicon (flat or weakly buckled) has an intrinsic stability with electronic properties almost identical to those graphene. In particular, π^* and π bands of the band structure form a Dirac cone at the K points of the Brillouin zone. Compared to graphene, the low overlap between the pz orbital makes silicene probably less stable but more reactive to the surface adsorption of foreign chemical species and therefore, all applications currently envisaged with graphene, could be shifted to this new material with the advantage of being easily transferable to the electronics industry which is essentially based on silicon [1]. From an experimental point of view, the first work showing a silicon layer with a 2D honeycomb structure suggesting a possible formation of silicene were made in Marseille (CNRS-CINAM) by thermal silicon deposition on (110) (100) and (111) Ag surfaces. Today despite the number of publications in the field, the atomic structure of silicene grown on this substrate is still under debate because none of these works have defined exactly its intrinsic structure.

For **Si/Ag(110)**, the first steps (<1ML) of silicon growth at room temperature (RT) reveal the formation of silicon nano-ribbons (NRs) [2], all parallel along the [-110] direction of silver, with perfect order. At slightly higher temperatures these unique 1D silicon NRs self-assemble to form a grating with a periodicity of 2.03 nm covering the entire substrate surface and giving rise to a (5x2) superstructure [3] (Figure 1a). STM images reveal a honeycomb arrangement (Figure 1b)[4] which have been confirmed within DFT-GGA calculation. The NR's may consist in slightly arch-shaped graphene-like stripes formed by a honeycomb structure, as seen in figure 1c [5]. All these results seems to show that silicon NRs grown on Ag(110) present a graphite-like structure which could be true silicene. Unfortunately, the knowledge of the Si-Si bond distance, which would definitively confirm the atomic structure, is still missing. At higher coverage (> 1 ML) one observes the formation of nano-ribbons with a pyramidal shape which could be a stack of silicene layers (Figure 1d) [6].

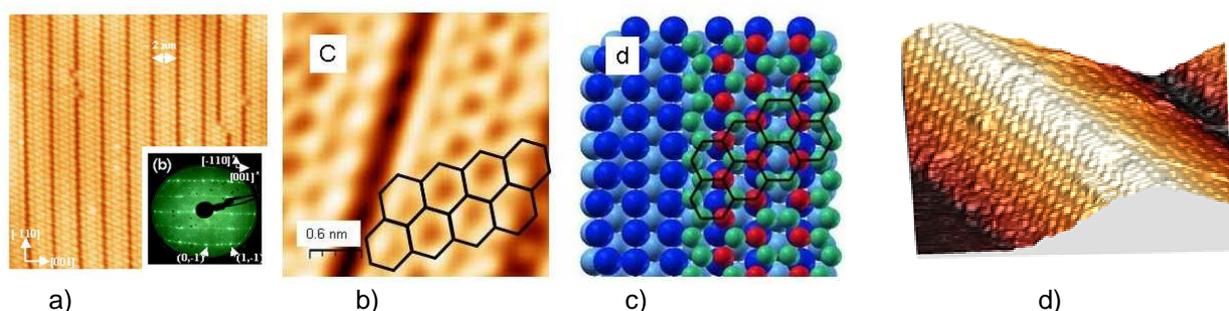


Figure 1 : a) Filled states STM image $(24 \text{ nm})^2$ of the surface at full coverage showing silicon nano-ribbons on Ag(110) surface and the corresponding (5x2) LEED pattern, b) Filled states high resolution STM image; c) corresponding ball model of the calculated atomic structure, d) stack of silicene nano-ribbons.

On **Ag(111)** face, the deposition of one monolayer gives rise to different superstructures (4×4) , $(\sqrt{13} \times \sqrt{13})R13.9^\circ$, $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ and $(\sqrt{7} \times \sqrt{7})R19.1^\circ$ which are strongly correlated to the growth conditions (substrate temperature and deposition rate)[7]. All these superstructures (and the corresponding STM images) can be explained by the same silicon mono layer (silicene ?) only rotated relative to the silver substrate (Figure 2A). The STM image topographies can be explained by the relative position of silicon atoms in relation to the silver atoms (yellow atoms on the figure 2A). Shortly after this observation, all these superstructures have been more or less confirmed by different groups [8,9] but with other structural models [8]. Note that there is still a large controversy concerning the $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ superstructure since it is not always observed [10,11]. Finally like on the (110) face, at

higher coverages one observes by LEED and by STM (Figure 2B), a new super-structure which could be the signature of the growth of a second silicene layer

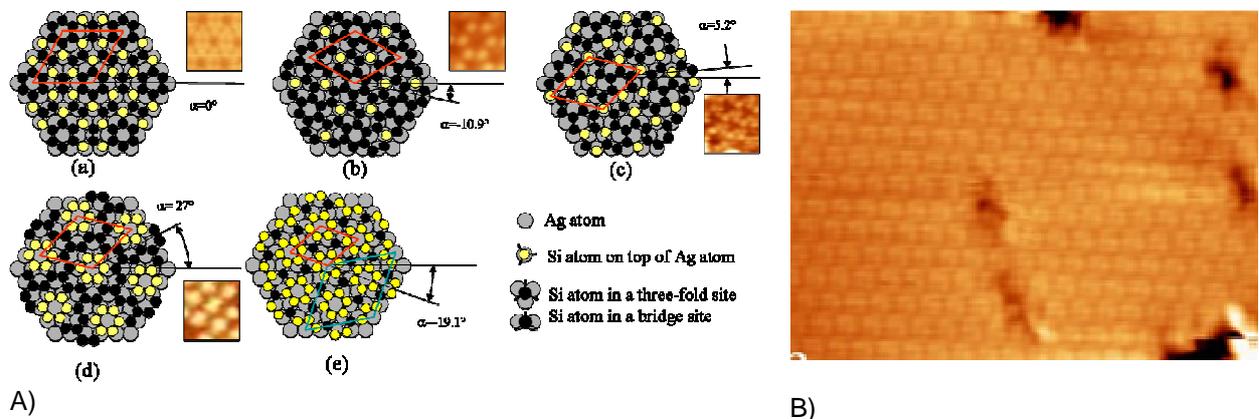


Figure 2: A) Ball models of one silicon monolayer on top of a Ag(111) surface (inserted are the corresponding STM images). α is the angle of rotation of the silicon layer relatively to silver. a) (4×4) superstructure; b) $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ superstructure; c) $(\sqrt{13} \times \sqrt{13})R13.9^\circ$ superstructure type I; d) $(\sqrt{13} \times \sqrt{13})R13.9^\circ$ superstructure type II and e) $(\sqrt{7} \times \sqrt{7})R19.1^\circ$ superstructures (expected but not observed). B) Filled state STM image ($12 \times 9 \text{ nm}^2$) of the surface of the silicene second layer.

On this (111) face, as well as the (110) face the question of the atomic structure is still open and only an accurate measurement of the Si-Si distance could clarify the situation.

In this presentation after a recall of the main results obtained in this field we will present our recent measurements of the Si-Si interatomic distances obtained on both faces by EXAFS.

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