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Epitaxial Growth Of As Ilicene Sheet on Close-Packed Silver Surface

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ABSTRACT
Usingatomicresolvedscanningtunnelingmicrocppy,wepresentheretheexperimental evidence of a silicene sheet (graphene like structure) epitaxially grownonaclose-packedsilversurface(Ag(111)).Thishasbeenachievedviadirectcondensation of a silicon atomic flux onto the single-crystal substrate in ultra-highvacuum conditions. A highly ordered silicon structure, arranged within a honeycomblattice is synthesized and presenting two silicon sub-lattices occupying positions atdifferentheights (0.02nm)indicatingpossiblesp^2-sp^3 hybridizations.
Keywords:Silicon,Silicene,Ag,STM,epitaxy,2Dstructure

Silicenepresentsahoneycombstructuresimil artothatofgraphene,whichhasdemonstrated applications in nanotechnology and is currently the most investigated materialin physics and nanoscience[1]. The synthesis of this silicon-based crystalline material opens theway for studies of its physical/chemical properties – some of which have been predicted fromtheory to be similar to those of graphene – that have potential applications in nanotechnologywiththeaddedadvantageofbeingcom patiblewithexistingsemi-conductordevices.

Silicene has recently attracted strong theoretical attention[2-4]. For example, Cahangirovet al[4],using density functional theory, have shown that a silicon quasi 2-dimensional structure isstable (without of any imaginary vibrational frequency) only if a low buckling (LB), 0.044nm, is allowed. They also reportthatfor thisLBstructure, the Si-Sinearest-neighbourdistance is reduced to 0.225 nm from that of the bulk, and that the electronic density of statesindicates the system is ambipolar. Their calculated band structures exhibit a crossing at K andK' points (reflecting the semi-metallic character of silicene) and a linear dependency near thecrossing (reflecting a mass-less Dirac fermion character). The same authors find that silicenenano-ribbons (NRs) exhibit electronic and magnetic properties likewise very similar to thoseof graphene. From an experimental point of view, however, silicene sheets have not beensynthesized until now, although single-wall[5] and multi-wall[6] silicon nano-tubes have beenproduced, and monolayers of silicon have been synthesized by exfoliation[7] (though no 2Dcharacterhas been detected).

Our group began studying silicon adsorption on silver surfaces several years ago. OnAg(001) we observed super-structures that we eventually came to characterize as deformedhexagonal structures[8]. Subsequently, extensive investigations of Si sub-monolayer growth onAg(110) revealed self-assembled nanoribbons (NRs) 1.6 nm in width and several hundred nmin length[9-11]. These NRs show strong resistance to oxidation on their edges[12], an intriguingchemicalpropertygiventhestrongpropensit yofsiliconsurfacestooxidize.FortheseNRs,atomicall yresolvedscanningtunnelingmicroscopy(STM)imag esrevealedahoneycomb structure[11,13] that ab initio calculations[14] indicated to be composed of archedsilicene NRs. Recently, using angle-resolved photoemission spectroscopy (ARPES), we haveinferred that, as with that of graphene, the band dispersion along the direction of these NRsexhibitsDiraccones[15].

Thequestionthusaroseastowhetheracontinu ousfilmofsuchhoneycombstructures– namelysilicene– could beachieved.

Very recently we have succeeded in growing a silicene sheet on a Ag(111) surface, in ultra-high vacuum conditions, that we believe is the first evidence of silicene sheet synthesis. Theapparatus in which the experiments have been performed is equipped with the standard toolsfor surface preparation and characterization: an ion gun for surface cleaning, Low EnergyElectron Diffraction (LEED) instrument, an Auger Electron Spectrometer (AES) for chemicalsurface analysis and Scanning Tunneling Microscope (STM) for surface characterization atthe atomic scale. The STM experiments were performed at RT with a commercial OmicronSTM. The Ag(111) sample was cleaned by several cycles of sputtering (600 eVAr^+ ions, P ~10^{-5}Torr) followed by annealing at 400°C until a sharp p(1□ 1) pattern was obtained. Silicon,evaporated by direct current heating of a

piece of Si wafer, was deposited onto the Ag(111)surface held at ~ 250°C. The silver substrate temperature was controlled by a thermocouplelocatedcloseto thesample.

The experimental conditions for producing this silicon structure are quite stringentsince the temperature of the substrate must be kept between 220 and 250°C andthe rate ofdepositionof siliconmustbe lower than0.1monolayer perminute.Finally,extreme caremust be taken that exactly the amount of silicon required to produce a single monolayer isapplied.Underthesecondition,weproduced the silicenesheets inthreeexperiments.

As displayed in Fig. 1a, the atomically resolved STM image shows a highly ordered siliconmonolayer, arranged within a honeycomb lattice that covers the entire scanned area of thesubstrate (several hundred nm^2), while Fig. 1b presents an STM image showing that thesilicene film covers the surface steps like graphene grown on metals [16,17]. A detailed scrutinyof the STM images revealed that this structure is actually formed by two silicon sub-latticesoccupying positions at different heights (Fig. 2a). Analysis of several line-scan profiles – anexample of which is shown in Fig. 2b – yields a height difference of 0.02 nm. This smallobservedcorrugation(indicatingpossiblesp^2-sp^3hybridizations)isinlinewiththetheoreticallypredictedone[4].

These line-scan profiles contain several pieces of structural information which can be used toderive the Si-Si nearest-neighbours distance in silicene. A peak-to-peak analysis provides adirect measure of this distance, which is turns out to be between 0.19 and 0.2 nm, while avalley-to-valleyanalysisindicatesaSi-Sidistanceofabout0.18to0.19nm.Thatthisdistance (0.19±0.01 nm) is about 17% shorter than that for Si bulk (0.235 nm) suggests thatthe Ag substrate may play acatalyst role in the formation and stabilization of the silicenesheet . That the low energy electron diffraction (LEED) of the epitaxially grown film shows a$(2\sqrt{3}x2\sqrt{3})R30°$ superstructure confirms the existence of a long-range order. In addition thesuperstructureobservedintheLEEDpatternisnotvisibleintheSTMimagesprobablyduetoaweakelectroniccouplingbetween thesilicenesheet andtheAgsubstrate.

Combiningatomichigh-resolutionSTMimagesrecordedonthesamesamplebeforeandafter the silicon deposition without any rotation (shown in Fig. 3a and 3b, respectively) inconformity with the observed $(2\sqrt{3}x2\sqrt{3})R30°$ LEED pattern, we propose a model of silicenesheetadsorbedonaAg(111)surface(Fig.3c).Understandingthegrowthmechanismsandthe stability of the silicene sheet will allow us to assess the viability of silicene as a materialwithperspectivesforpotentialapplicationsin nanotechnology.Atomistic(abinitioandtight binding) calculations are in progress to unravel the mechanisms by which such a structure isformed. The ARPES measurements are also being programmed in order to reveal the silicenebanddispersion and to test theexistenceofDiraccones.

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