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Silicene-Like Domains on $IrSi_3$ Crystallites

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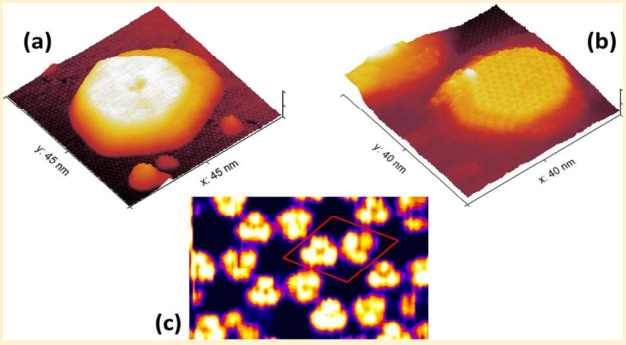
ABSTRACT: Recently, silicene, the graphene equivalent of silicon, has attracted a lot of attention because of its compatibility with Si-based electronics. So far, silicene has been epitaxially grown on various crystalline surfaces such as Ag(110), Ag(111), Ir(111), ZrB_2(0001), and Au(110) substrates. Here, we present a new method to grow silicene via high-temperature surface reconstruction of hexagonal $IrSi_3$ nanocrystals. The h-$IrSi_3$ nanocrystals are formed by annealing thin Ir layers on the Si(111) surface. A detailed analysis of the scanning tunneling microscopy images shows the formation of silicene-like domains on the surface of some of the $IrSi_3$ crystallites. We studied both morphology and electronic properties of these domains by using both scanning tunneling microscopy/spectroscopy and first-principles calculation methods.



INTRODUCTION

Graphene has attracted a lot of attention for its unique properties, which include excellent electrical/thermal conductivity and strong mechanical strength.[1,2] The immediate alternatives for graphene are from the other group IV elements in the periodic table with the similar electron configuration, that is, silicon (Si) and germanium (Ge).[3] Although all three elements have four electrons in their outermost s- and p-orbitals, energetically, the most favorable crystal structure of Si and Ge is the diamond structure.[4] Therefore, for Si and Ge, graphite-like allotropes (hereafter referred as silicene and germanene) do not exist in nature. Hence, silicene and germanene have to be synthesized. The term "silicene" was introduced by Guzmán-Verri and Lew Yan Voon in 2007 to refer to the two-dimensional structure of silicon atoms in a honeycomb arrangement.[5] Takeda and Shiraishi were the first to predict the possibility of a stable single sheet of Si.[6] In that paper, the authors predicted that silicene will not be flat but puckered. Further, theoretical calculations on free-standing silicene showed that this two-dimensional system can be stable with properties similar to graphene such as linear dispersion with the Dirac cone at the corner of the Brillouin zone.[7−9] Theoretical studies also showed that the spin−orbit coupling strength is much larger in silicene than that in graphene which can make the quantum spin Hall effect detectable experimentally.[10]

Silicene's novel properties predicted by theorists and its relatively easy integration into the current semiconductor technology motivated some experimental groups to start working on growing silicene. The very first silicene was grown on Ag(110) and Ag(111) surfaces.[11−20] Recently, it has been shown that silicene can be grown on Ir(111),[21] ZrB_2(0001), and[22] Au(110)[23] substrates. One of the most studied silicene systems is silicene/Ag(111). Owing to the interaction between silicene and the substrate, the bucking pattern of Si atoms is rearranged resulting in various superstructures such as (4×4), $(\sqrt{13} \times \sqrt{13})R13.9°$, and $(2\sqrt{3} \times 2\sqrt{3})$, [with respect to the Ag(111) surface lattice] and (3×3) [with respect to silicene (1×1)].[24−26] All these superstructures show slightly different honeycomb configurations. ARPES measurements on 4×4-silicene along the Ag $\overline{\Gamma}-\overline{K}$ direction through the silicene $\overline{K}$ point show a downward dispersing branch of the honeycomb silicene bands. The dispersion is similar to the dispersion of graphene around the $\overline{K}$ point, indicating that electrons behave as massless Dirac fermions.[27] ARPES measurements on $\sqrt{3} \times \sqrt{3}$-silicene exhibit Λ- and V-shaped linear π and π^* silicene bands at the $\overline{\Gamma}_0$ point along the $\overline{\Gamma}-\overline{K}$ silicene direction.[28]

Another method to grow silicene or germanene is to use high-temperature surface reconstruction of metal silicides/germanides.[29,30] In this paper, we show that the deposition of a few monolayers of Ir on Si(111) followed by annealing at 750 °C leads to the formation of $IrSi_3$ nanocrystals. Scanning tunneling microscopy (STM) images of these crystallites show a surface reconstruction with a buckled honeycomb structure that resembles previously reported silicene-like regions on $MoSi_2$ crystallites supported on Si(001).

EXPERIMENT

The Si(111) samples used in the STM experiments were cut from nominally flat 76.2 mm by 0.38 mm, single side-polished n-type (phosphorous doped) wafers. The samples were mounted on molybdenum holders, and the contact of the

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