



Honeycomb silicon: a review of silicene

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Received: 13 July 2015 / Accepted: 14 August 2015
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Abstract Silicene, a new allotrope of silicon in a two-dimensional honeycomb structure, has attracted intensive research interest due to its novel physical and chemical properties. Unlike carbon atoms in graphene, silicon atoms prefer to adopt sp^2/sp^3 -hybridized state in silicene, enhancing chemical activity on the surface and allowing tunable electronic states by chemical functionalization. The silicene monolayers epitaxially grown on Ag(111) surfaces demonstrate various reconstructions with different electronic structures. In this article, the structure, phonon modes, electronic properties, and chemical properties of silicene are reviewed based on theoretical and experimental works in recent years.

Keywords Silicene · Electronic states · Chemical functionalization

1 Introduction

The discovery of graphene in 2004 by Novoselov et al. [1] demonstrated that, for the first time, stable and single-atom-thick two-dimensional (2D) materials could be exfoliated from van der Waals solids, and these materials possess unique and fascinating properties due to their exotic electronic structures [1–6]. Since then, graphene has been one of the most extensively studied materials due to the wealth of anomalous physical and chemical phenomena that occur when charge and heat transport is confined to a plane. The rapid and recent advances in this carbon-based

2D material have raised teasing questions on exploring new 2D materials with distinct and exotic properties. Such possibilities have promoted a completely new research field of 2D crystals. There are many 2D materials that have been explored, and they exhibit rich spectrum of properties. For example, hexagonal boron nitride (h-BN) with the closest structure to graphene is an insulator [7], while monolayers MoS_2 and WS_2 are semiconductors with direct band gap [8, 9]. The abundant variety of properties in 2D materials suggests the candidate potential for the device engineering and application in sensing, photonics and energy storing, etc. Great efforts have been made to incorporate 2D atomic layers into devices to exhibit exceptional performance. It has been extremely difficult so far, however, to develop reliable and durable applications, especially in electronics, based on 2D materials due to their incompatibility with current semiconductor-based electronic techniques. Moreover, it is extremely hard to obtain single crystal with large size for characterization and device fabrication. Searching for the novel 2D materials is therefore highly desirable, especially for next-generation low-cost super-performance electronic devices.

Silicene is similar to graphene in that it is single atom thick, and it has the same characteristic honeycomb structure. It is a big challenge, however, to synthesize silicene, despite the similarity of electronic configurations between carbon atoms and silicon atoms. Nevertheless, the sp^2 hybridization is more stable than sp^3 hybridization for carbon, but situation is reversed for silicon. Thus, silicon atoms are energetically not favorable to spontaneously form silicene, and this limits conventional chemical or physical methods to prepare silicene. Despite the difficulty in fabrication, many theoretical calculations have predicted an exciting and rich physics in silicene [10–12]. For instance, the Dirac fermion state was demonstrated in a

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linear dispersion band structure close to Fermi level by density functional theory (DFT) calculations [11]. The quantum spin Hall effect (QSHE) and quantum anomalous Hall effect (QAHE) were also predicted in silicene [13–15]. The electronic properties of the silicene could be modulated by effect of substrate [16], defect [17, 18], interlayer coupling [19], and metal interaction [20]. These theoretical works have paved the way of exploiting the anisotropic transport behavior and experimentally investigating exotic properties of silicene [21–31]. Moreover, silicene is derived from silicon—the precise substance that silicon chips are made of. As such, it is inherently compatible with current chip-production processes, which is advantageous in contrast to graphene. There is no doubt that silicene could be a material of the future. On the energy front, silicene is expected to make solar power more practical and efficient by improving the storage capacity and output speed of solar cells [6]. Silicene may also yield advances in medical sensors (which monitor heart rates and blood flow), sharpen X-ray imaging, and improve DNA sequencing [3–6]. In addition, it will make health-monitoring devices faster, cheaper, and even disposable. It can create more efficient batteries, paper-thin cell phones, and flexible screens.

2 2D structure of silicene

Silicene, silicon-based graphene-like sheets, has been proposed recently by first-principle total-energy calculations [32]. However, different from the planar structure of graphene with sp^2 hybridization network, silicene is a low-buckled structure due to mix of sp^2 and sp^3 hybridization. Due to the competition between sp^2 hybridization and sp^3 hybridization, rich phases of silicene have been reported grown on various substrates, including Ag(111) [2, 10, 13, 28, 33, 34], Ag(110) [35], Au(110) [36], Ir(111) [3], and ZrB₂-covered Si(111) [4]. Here, we focus on the structure of silicene phases grown on Ag(111).

2.1 3×3 silicene

3×3 silicene is 4×4 reconstruction with respect to the Ag(111) substrate or 3×3 reconstruction with respect to 1×1 silicene [10]. Large-scale 3×3 silicene films can be easily prepared by keeping substrate temperature around 420 K during deposition. In 2012, three groups reported detailed structure models of 3×3 silicene by comparing scanning tunnel microscope (STM) results with theoretical calculation [2, 13, 20]. Figure 1a shows the phase exhibiting honeycomb structures (labeled H). The other phase consisting of close-packed protrusions (labeled T) is shown in Fig. 1b. These two phases coexist with each

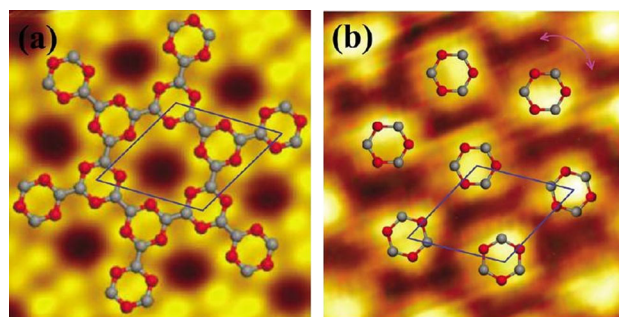


Fig. 1 (Color online) STM images and structure models of H phase silicene (a) and T phase silicene (b). Reprinted with permission from Ref. [2]. Copyright (2012) American Chemical Society

other, indicating similar formation energy and stability. However, phase T tends to form at a lower Si coverage and lower temperature compared to phase H. At higher Si coverage, phase T will disappear and be replaced by phase H. Thus, phase H is regarded as the stable phase of 3×3 silicene, and phase T is a precursor of phase H. Based on the structure in STM observation and first-principle calculation, a structure model of a low-buckled honeycomb structure with missing of a hexagonal silicon rings at the corner in each 3×3 cell is proposed, as shown in structure model in Fig. 1b. Although similar STM results have been represented by Liu et al. [20] and Vogt et al. [13], different structure models have been proposed, where the hole in STM image is attributed to six Si atoms buckled upward. The recent work of hydrogen absorption on 3×3 silicene reported by Qiu et al. [37] is helpful to clarify this controversy. It is found that absorption of hydrogen changes buckling structure of 3×3 silicene by detailed discussion on STM results and theoretical calculation; they proposed a structure model with intact honeycomb structure.

2.2 $\sqrt{7} \times \sqrt{7}$ silicene

With increasing substrate temperature to 480 K, a new phase of silicene named as $\sqrt{7} \times \sqrt{7}$ silicene emerges [2]. This phase usually manifests itself as a defective moiré pattern with a period about 3.8 nm, as shown in Fig. 2. Figure 2b shows that this moiré pattern consists of hexagonal rings at bright part and defective part between them. By first-principle calculation, they construct a structure model for $\sqrt{7} \times \sqrt{7}$ silicene (Fig. 2d, f). They attribute the bright parts of moiré pattern to the position deviation of silicon atoms from that of Ag(111). Thus, the strong interaction between silicene and Ag(111) substrate will make hexagonal rings stable and complete. In other parts of moiré pattern, because of larger deviation of position between silicon atoms and that of substrate, the interaction breaks these hexagonal rings.

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