Electronic structure of the 4 × 4 silicene monolayer on semi-infinite Ag(111)

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Abstract

The electronic structure of the 4 × 4 silicene monolayer on a semi-infinite Ag(111) substrate is calculated within density functional theory by using the embedded Green’s function technique. The present calculation confirms the conclusion of previous studies that the two-dimensional (2D) Dirac bands do not exist on this surface as a result of the symmetry breaking and strong orbital hybridizations between the Si π and Ag sp states. In addition, by making use of the advantage of the semi-infinite calculation in which the energy continuum of the bulk Ag bands is fully reproduced, we investigate details of the silicene-induced electronic states, including not only their energy dispersion with 2D wave vector k but also their spectral shape as a function of energy at each k.

1. Introduction

Currently, considerable efforts are made to synthesize silicene, a two-dimensional (2D) honeycomb lattice made out of Si, on solid substrates. That the 2D crystal of Si prefers lightly-buckled honeycomb lattice, in which neighboring Si atoms are displaced alternately in the vertical direction, was originally predicted by density functional theory (DFT) calculations [1–3]. These calculations also revealed that freestanding lightly-buckled silicene sustains massless 2D Dirac bands with their crossing points located at the Fermi energy (E_F). This similarity in the electronic structure between graphene and silicene has raised much attention to silicene as a promising material for nanoelectronics. Furthermore, it was theoretically suggested that spin–orbit (SO) coupling in silicene, which is much larger than that in graphene, can be made use of to realize novel topological quantum phases in silicene monolayers, for example, by applying external fields [4–6].

So far, silicene was synthesized either by deposition of Si on Ag(111) [7–14] and on Ir(111) [16] or through surface segregation on ZrB2(0001) [15]. Among others, the stable 4 × 4 superstructure on Ag(111) was extensively studied. Its atomic configuration was investigated by scanning tunneling microscopy (STM) and low-energy electron diffraction experiments in combination with DFT calculations [9, 10]. It was revealed that the 4 × 4 unit cell of the Ag(111) surface is commensurate with the 3 × 3 unit cell of the single layer of a distorted honeycomb lattice of Si. An earlier angle-resolved photoemission spectroscopy (ARPES) measurement [11] suggested that 2D Dirac bands having a linear energy dispersion with 2D wave vector k persist on the 4 × 4 silicene/Ag(111) surface. However, the absence of Landau levels in a recent STM measurement under high magnetic field by Lin et al. indicated that 2D Dirac fermions do not exist on this surface [13]. Instead, their DFT calculation demonstrated that the band structure of silicene is strongly modified via the symmetry lowering and orbital hybridizations with the substrate Ag states. Similarly, a recent ARPES study of Mahatha et al. [14] revealed that a spectral feature, which was earlier interpreted as an evidence of the existence of 2D Dirac cones [12], is actually a saddle point of the free-electron-like Ag band. They also performed a DFT calculation by using a thick
(15-layer) Ag(111) slab, and the resultant dispersion curves of the surface bands were similar to those of a Ag sp free-electron-like state folded in the surface Brillouin zone (SBZ) of the 4 × 4 unit cell. These results reconfirm that no 2D Dirac bands exist on the 4 × 4 silicene/Ag(111) surface due to strong Ag–Si orbital hybridizations.

Consequently, the main focus in the study of silicene has moved to finding a substrate that interacts only weakly with silicene overlayers. Among the candidates are hexagonal BN, H-terminated Si, and solid Ar [17, 18]. Instead of pursuing this direction, in the present work we aim at completing our understanding of the electronic structure of the 4 × 4 silicene on Ag(111). Specifically, we present a first-principles DFT calculation of this surface by adopting a truly semi-infinite Ag(111) substrate instead of the slab approximation. As is well known, the clean Ag(111) surface has a projected bulk band gap straddling $E_F$ over a small part of SBZ surrounding the $\Gamma$ point, and a localized Shockley state (L-gap surface state) having a 2D free-electron-like energy dispersion appears within the projected band gap [19]. On the other hand, in the case of the 4 × 4 superstructure, no projected bulk band gap appears near $E_F$ because the bulk Ag bands are folded into a much smaller SBZ. As a result, essentially, all the localized surface states become resonant levels whose finite energy widths are determined by how strongly they interact with the substrate Ag bands.

The main focus of the present paper is the electronic states of the silicene overlayer. Without the Ag(111) substrate, the electronic states of silicene at a given 2D $k$ point are discrete energy levels. By introducing the interaction with the energy continuum of the substrate Ag, the overlayer states at a given 2D $k$ point become resonant states with a finite life time and a finite energy width. There are other sources of the broadening of overlayer electronic states such as electron–electron interactions and electron–phonon interactions. What we discuss in the present paper is the broadening of the overlayer states via the hybridization with the energy continuum in the Ag substrate. The energy width of the overlayer band arising from this interaction is typically of the order of 100 meV and by factor 10 larger than those arising from electron–electron interactions or electron–phonon interactions. This energy broadening cannot be described properly if the substrate is represented by a thin slab made out of only 10–20 atomic layers, since the level spacing of the Ag bands at a given 2D $k$ point must be much smaller than the energy broadening of the overlayer band in order to be able to describe the latter quantity as a function of $k$. Alongside the energy dispersion curves of the resonant levels with 2D wave vector $k$, the energy width of the resonant band as a function of $k$ constitutes an important information on the electronic band structure of the silicene overlayer. For example, this quantity plays an essential role in determining the charge and heat transport across the substrate–overlayer interface. This is the reason why we consider that the present semi-infinite calculation is important for the better understanding of the 4 × 4 silicene overlayer on Ag(111).

2. Method

We consider the stable silicene monolayer forming a 4 × 4 superstructure on the Ag(111) substrate. The surface atomic structure is determined by total-energy minimization within DFT. The calculation is made by using the VASP program [20, 21], an implementation of the projector augmented-wave method [22], within the generalized gradient approximation where the exchange-correlation functional of Perdew–Burke–Ernzerhof was used [23]. While there is a fundamental difference in the one-electron energy levels at a single $k$ point between the slab and semi-infinite calculations (discrete versus continuous), integrated quantities such as electron charge densities and the total energy within DFT converge very rapidly with slab thickness in the case of metal substrates, which allows efficient structure optimization of crystal surfaces by using a thin slab. Therefore, in the present work, the surface is modeled by a slab consisting of five Ag(111) lattice layers to represent the substrate and the silicene monolayer on top of the substrate. We take the $z$ axis as the surface normal pointing to the vacuum. All the atoms are allowed to relax to reach the lowest-energy geometry, except for those in the bottom Ag layer, which are fixed at the ideal bulk positions.

The surface geometry thus obtained is used as the structural input data for the subsequent semi-infinite surface calculation. We calculate the electronic structure of the 4 × 4 silicene monolayer on semi-infinite Ag (111) within the local density approximation in DFT by using the embedded Green’s function (EGF) technique of Inglesfield [24, 25]. The calculation consists of three steps: (i) one makes a bulk DFT calculation of the fcc Ag crystal to determine the one-electron potential in the interior of the semi-infinite substrate. (ii) For the (111) crystal orientation and for a set of $(k, \epsilon)$ points, one computes the complex embedding potential, which is a generalized logarithmic derivative of the Bloch and evanescent wave functions that propagate or decay into the interior of solid [26]. (iii) One performs a self-consistent-field surface calculation, in which one explicitly treats only the embedded region with a finite thickness containing only a few surface atomic layers, while the effects of the semi-infinite substrate and the vacuum are incorporated via the embedding potentials acting on two boundary surfaces on both sides of the embedded region.
The main quantity calculated in the EGF method is the Green’s function,

\[ G(\omega, r, r') = \int_{SBZ} \frac{dk}{(2\pi)^2} G(k, \omega, r, r'), \]

where \( \omega \) is a complex energy and the \( k \)-resolved Green’s function \( G(k, \omega, r, r') \) is given in the spectral representation as

\[ G(k, \omega, r, r') = \sum_\alpha \frac{\psi_{\alpha k}(r) \psi_{\alpha k}^*(r')}{\omega - \epsilon_{\alpha k}}, \]

where \( \psi_{\alpha k} \) denotes the wave function of a one-electron state with energy \( \epsilon_{\alpha k} \) and the summation over index \( \alpha \) is understood to include both the localized surface states and Bloch states incident on the surface with 2D wavevector \( k \). In the above equations, we omitted the electron spin index as we do not consider SO coupling in the present work. Various quantities can be calculated from the Green’s function. For example, the \( k \)-resolved local density of states (DOS) can be obtained as

\[ \rho(k, \epsilon, r) = \sum_\alpha \delta(\epsilon - \epsilon_{\alpha k}) |\psi_{\alpha k}(r)|^2 = -\frac{1}{\pi} \text{Im} G(k, \epsilon + i\gamma, r, r), \]

where \( \gamma \) is a positive infinitesimal. We use the computer code that combines the EGF technique and the full-potential linearized augmented plane-wave (LAPW) method [27] as described in [28]. The plane-wave cutoff for the LAPW basis in the interstitial region is chosen as 10.24 Ry, while radial orbitals with angular momentum \( l \leq 5 \) are used for the LAPW basis inside muffin-tin spheres surrounding Ag and Si atoms. We use 16 independent \( k \) points in the SBZ of the 4×4 superstructure for the self-consistent charge density calculation.

3. Results and discussion

In figures 1(a) and (b) we show the optimized atomic structure of the 4×4 silicene monolayer on Ag(111) determined by the present DFT calculation. The surface structure is essentially identical with those reported by Lin et al [13] and Arafune et al [10]. In contrast to freestanding lightly-buckled silicene monolayer, in which...
neighboring Si atoms are alternately displaced in the vertical direction, the 18 Si atoms in the 4 × 4 unit are buckled irregularly, and only 6 Si atoms are largely relaxed toward the vacuum.

In figure 1(c) we show the band structure of the distorted silicene monolayer, which is obtained by removing the Ag substrate from the silicene/Ag(111) while keeping the atomic configuration of the silicene the same as those in panels (a) and (b). Here, energy \( \epsilon \) is measured relative to the Fermi level \( (E_F) \) and the energy bands are plotted along the \( M_2 - \Gamma - K_2 \) line in the SBZ of the 4 × 4 unit cell depicted in figure 1(d). In the same panel, we also show the SBZ of the 1 × 1 Ag(111) surface and that of the 1 × 1 honeycomb lattice of silicene. It is seen that \( K_1 \) and the other corner points of the SBZ of the 1 × 1 silicene, at which the band structure of freestanding lightly-buckled silicene exhibits linear band crossing at \( E_F \), coincide with \( \Gamma \) when folded into the SBZ of the 4 × 4 unit cell. Because of the symmetry lowering, the band structure of the distorted silicene in figure 1(c) exhibits no massless 2D Dirac bands crossing at \( \Gamma \). Instead, it possesses a direct energy gap at \( \Gamma \) between the occupied and unoccupied energy bands.

We now present results of our EGF calculation, which was made by including the silicene overlayer and the two outermost Ag(111) lattice layers in the embedded surface region. As the surface structure, we use the atomic coordinates obtained by the above-mentioned structural optimization, except for the bottom Ag layer, for which we took average over the slightly irregular \( z \) coordinates of the 16 atoms within the layer and replaced them by their mean value. To check the convergence with respect to the number of lattice layers, we also made an EGF calculation by including only the first Ag layer in the embedded region. The results obtained were practically identical with those with two Ag layers in the embedded region. This means that the one-electron potential in the Ag substrate converges very rapidly to the bulk one with distance from the surface by virtue of an efficient metallic screening.

In order to analyze the spatial and energy distribution of the silicene-induced electronic states at each \( \mathbf{k} \) point, we calculate the \( k \)-resolved DOS of a surface atom defined by

\[
\rho_{\mathbf{k}}(\mathbf{k},\epsilon) = \frac{-1}{\pi} \int_R d\mathbf{r} \text{Im} \ G(\mathbf{k},\epsilon + i\gamma, \mathbf{r}, \mathbf{r}),
\]

where the integral is performed within a muffin-tin sphere with radius \( R \) centered at the atomic nucleus. Further, we define the \( k \)-resolved layer DOS, \( \bar{\rho}_{\mathbf{k}}(\mathbf{k},\epsilon) \), by the average of \( \rho_{\mathbf{k}}(\mathbf{k},\epsilon) \) over all the atoms within the same layer. In figure 2 we show a waterfall plot of \( \bar{\rho}_{\mathbf{k}}(\mathbf{k},\epsilon) \) of the silicene overlayer (average of \( \rho_{\mathbf{k}}(\mathbf{k},\epsilon) \) over 18 Si atoms) along the \( \Gamma - K_2 \) line in an energy range near \( E_F \). The calculated spectral density exhibits no projected bulk band gap, since the bulk Ag sp bands are projected into the small SBZ of the 4 × 4 superstructure. Consequently, the Si valence states (dominantly Si π as discussed later) hybridized with the sp bands of the substrate Ag make a nearly energy-independent background contribution to the calculated DOS in the whole energy range. It is to be noted that the bulk Ag 4d bands are located below \(-2.8 \text{ eV} \) relative to \( E_F \) and are not seen in figure 2. As is seen, about ten peaks appear within the energy range at each \( \mathbf{k} \). They are silicene-induced surface electronic states with different orbital characters and distinguishable energy dispersions with \( \mathbf{k} \). Their energy width, which is determined by the coupling strength with the Ag sp bands, is seen to vary considerably: some peaks are as sharp as \( \sim 0.1 \text{ eV} \), while others are wider than \( 0.5 \text{ eV} \).

To grasp the energy dispersion of the silicene-induced states with \( \mathbf{k} \) with more clarity, we show in figure 3(a) an intensity plot of \( \bar{\rho}_{\mathbf{k}}(\mathbf{k},\epsilon) \) of the silicene overlayer along \( M_2 - \Gamma - K_2 \). Here, white and dark-blue colors correspond to large and small values of DOS, respectively, and color mapping is adjusted such that the...
dispersion curves of the silicene-induced states become easily visible (see the figure caption for details). Compared to the band structures calculated with the slab approximation [13, 17, 29], the silicene-induced bands appear much more clearly, indicating the advantage of the present method based on the EGF technique. The contributions from different orbitals can be obtained by further decomposing $\rho_\sigma(k, \varepsilon)$. Figures 3(b) and (c) show the contributions of the Si $\sigma$ (3s + 3p$_{xy}$) and $\pi$ (3p$_z$) orbitals to $\rho_\sigma(k, \varepsilon)$, respectively. Concerning the Si $\pi$ states, they have relatively small spectral weight in the vicinity of $E_F$, and their spectral density is mainly distributed at lower and higher energy regions on both sides of $E_F$. As is seen, rather dispersionless resonant bands with large spectral amplitude appear in an energy range between −3 and −2 eV relative to $E_F$. They are mainly made out of Si 3p$_x$ and 3p$_z$ orbitals. As for the unoccupied part, one observes the energy bands with parabolic energy dispersions in an energy range between 1.0 and 2.5 eV above $E_F$. These bands are contributed by both Si 3s and 3p$_{xy}$.

On the other hand, the $k$-resolved spectral density of the Si $\pi$ state shown in figure 3(c) consists of a nearly energy-independent background part and several resonant bands with rather small energy widths (less than a few tenths of an eV). The former contribution is hardly seen in figure 3(c), since the DOS less than 10 a.u. is colored dark-blue in this figure. Instead, the featureless background DOS of the Si $\pi$ state extended in a wide energy range is unambiguously seen in figure 2 as mentioned before. Concerning the latter contribution, one observes several bands which exhibit asymmetric energy dispersions along the two symmetry directions. While no bands cross $E_F$ along $\Gamma - M_2$, two bands cross $E_F$ along $\Gamma - K_2$. At the $\Gamma$ point, two sharp resonant peaks with Si $\pi$ character appear at −1.1 and −0.4 eV below $E_F$. As seen from figure 3(b), the peak at −1.1 eV is contributed not only by Si $\pi$ but also by Si 3p$_{xy}$ states to a considerable extent. The peak at −0.4 eV may be related with the observed photoemission signal at −0.35 ± 0.05 eV below $E_F$ [12, 14], since $\Gamma$ is equivalent to the M point in the SBZ of $1 \times 1$ Ag(111). Evidently, in figure 3(c), one finds no energy dispersion curves reminiscent of the 2D Dirac cones. Thus, the present semi-infinite calculation reconfirms the conclusion of the previous studies [13, 14] that 2D Dirac bands are destroyed in the 4 × 4 silicene monolayer on Ag(111). The energy dispersion curves of the interface states as discussed above are in agreement with those calculated by Mahatha et al [14] by using a 15-layer Ag substrate, except that their dispersion curves exhibit small energy discontinuities arising from the slab approximation. On the other hand, there is some discrepancy between their results and the present ones concerning the spatial distribution of the interface states, which will be discussed in the following.

To study the spatial distribution of the silicene-induced electronic states, we compare in figure 4 the $k$-resolved layer DOS of the two outermost Ag lattice layers with the corresponding one of the silicene overlayer. Regarding the Si $\pi$ state, the energy bands dispersing asymmetrically along the two symmetry directions as discussed above are clearly seen in $\rho_\pi(k, \varepsilon)$ of both the Ag layers. This indicates that these resonant bands should be identified as the interface state involving strong orbital hybridizations between the Si $\pi$ and Ag sp states. Mahatha et al [14] described this interface state as being mainly localized in the first Ag layer and to a much smaller extent in the second Ag layer. However, as stated above, its wave function has an appreciable amplitude also on the second Ag layer. For more quantitative discussion, we show in figure 5 $\rho_\pi(k, \varepsilon)$ of the three layers at
the Γ point, at which the Si π state forms a sharp DOS peak at −0.4 eV relative to \( E_F \). As seen from figure 5(b), the DOS peak associated with this state for the second Ag layer is only slightly smaller than the corresponding one for the first Ag layer. Even after subtracting the contribution of the widely spread background DOS, the integrated weight of this DOS peak for the second Ag layer is as large as \( \sim 40\% \) of that for the first Ag layer. Hence, the interface state made out of the Si π and Ag sp states is not so strongly localized in the first Ag layer.

Secondly, Mahatha \textit{et al} \cite{14} noted that the main structure of the σ bands of the freestanding silicene monolayer is retained apart from their slight shifts toward higher binding energies even in the presence of the Ag substrate. This might give an impression that the Si σ bands are only weakly coupled with the Ag sp states. In reality, as seen from figure 4(b), the interface states with strong σ character within the silicene overlayer (especially the rather dispersionless σ bands below \( E_F \)) make a considerable contribution to the one-electron spectral density of the first Ag layer. A more quantitative evidence for the strong hybridization between the Si σ and Ag sp states is provided in figure 5, where the DOS peaks of the Si σ states (blue and green lines) shown in panel (a) appear as large peaks in the DOS spectrum of the first Ag layer. On the other hands, the wave functions of the Si σ bands decay more rapidly with distance from the surface than the Si π state, and the DOS peaks associated with the σ bands become much smaller in \( \rho_\sigma (\epsilon, \mathbf{k}) \) of the second Ag layer shown in figures 4(c) and 5(b).

Here, we like to discuss shortly the possible origin of the interface state made out of the Si π and Ag sp states. According to Mahatha \textit{et al} \cite{14}, this state can be described as a free-electron-like Ag state localized at the interface via the Si–Ag interaction. However, it was not argued why such a 2D free-electron-like band can

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**Figure 4.** Intensity plot of \( \rho_\sigma (\epsilon, \mathbf{k}) \) of (a) silicene overlayer, (b) first Ag layer, and (c) second Ag layer for the 4 × 4 silicene/Ag(111) surface along \( M_2 - \Gamma - K_2 \). The same color mapping is used as that in figure 5. Panel (a), which is the same as figure 3(a), is shown again for a better comparison of DOS between layers.

**Figure 5.** (a) \( k \)-resolved layer DOS, \( \rho_\sigma (\epsilon, \mathbf{k}) \), of the 4 × 4 silicene overlayer at Γ decomposed into three orbital components. (b) \( \rho_\sigma (\epsilon, \mathbf{k}) \) at \( \Gamma \) of the first and second Ag layers.
emerge on the surface of a 3D crystal in which the outermost Ag layer is fully coupled with the rest of the substrate. As a possible scenario, we suggest that such a localized state might be split off from the surface-projected bulk sp band of Ag. To explain this, we show in figure 6 the k-resolved DOS of a first-layer surface atom for the clean Ag surface along M−Γ−K of the 1×1 unit cell. At each k point, the projected bulk sp band of Ag exhibits a van Hove singularity since the band is a one-dimensional function of the wave number in the z direction, and thus, its DOS diverges as $|\epsilon - \epsilon_b|^{1/2}$ with $\epsilon_b$ denoting either the lower or upper boundary energy of the projected band. The DOS projected on surface atoms does not exhibit a true divergence since the amplitude of the wave function within the muffin-tin sphere of a surface atom is reduced as $\epsilon \to \epsilon_b$. However, as marked by red arrows in figure 6, the van Hove singularity manifests itself as a large enhancement of the k-resolved DOS for surface atoms at the lower edge of the projected bulk sp band. In contrast, an analogous enhancement of the DOS does not occur at the upper edge of the projected bulk sp band, since a part of the spectral density is transferred to the localized surface band split off from the band edge, which is known in the case of Ag(111) as the L-gap surface state[19]. It might happen that a localized surface state is split off from the lower band edge of the projected bulk sp band when the Ag–Si interaction is strong enough in a certain k region of SBZ. Eventually, such a localized state may become a resonant level with a finite width when k is folded into the small SBZ of the 4×4 unit cell. However, this energy width may be rather small as far as the majority of its charge density stays within the Ag layers, since the potential components associated with the 4×4 super structure decay rapidly in the interior of the Ag substrate.

Finally, we show in figure 7(a) the orbital-decomposed DOS of the silicene overlayer calculated by integrating each orbital component of $\rho_\epsilon(k, \epsilon)$ over the whole SBZ. The Si π state exhibits a rather featureless DOS in a wide energy range when integrated over the SBZ. It may be evident that there appears no linear DOS characteristic of the 2D Dirac bands. On the other hand, the DOS of the Si σ band takes the smallest value at around $E_F$ and its main spectral weight is divided into two energy regions below and above $E_F$. The sharp DOS

**Figure 6.** k-resolved DOS of a first-layer surface atom for the clean Ag(111) surface along M−Γ−K of the 1×1 unit cell. Red arrows indicate the lower boundary line of the projected bulk Ag sp band, where the k-resolved DOS of the surface atoms is enhanced.

**Figure 7.** Orbital-decomposed DOS of (a) the silicene overlayer and (b) the first substrate Ag layer calculated by integrating each orbital component of $\rho_\epsilon(k, \epsilon)$ over the whole SBZ.
peak of the Si3pₓₒ orbitals located between −3 and −2 eV relative to Eᵦ is associated with the rather dispersionless Si σ bands seen in figures 3 and 4. In figure 7(b) we show the corresponding orbital-decomposed DOS of the first Ag layer. As is seen, the DOS of the Ag sp states varies only weakly in a wide energy range. In this panel, one can also see the large DOS amplitude arising from the Ag 5d bands.

4. Conclusion

We investigated the electronic structure of the 4 × 4 silicene monolayer on a semi-infinite Ag(111) substrate within DFT. The surface structure was optimized by a slab calculation, and the structure thus obtained was used as input data for the subsequent semi-infinite surface calculation based on the embedded EGF formalism. Our calculation reconfirms the conclusion of previous studies that the 2D Dirac bands do not exist on this surface as a result of the symmetry breaking and strong orbital hybridizations between the Si σ and Ag sp states. Since the energy continuum of the projected bulk bands of Ag is non-vanishing over a wide energy range in the entire SBZ, the silicene-induced electronic states become surface resonances with a finite width rather than localized surface states. We have revealed not only the spacial distribution and the energy dispersion with 2D wave vector k of the silicene σ and π states, but also their continuous DOS spectrum at each k by exploiting the advantage of the present semi-infinite calculation. We also suggested a possible mechanism for the 2D free-electron-like band to emerge at the interface due to the strong Ag–Si interaction.

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