Electronic transport through a silicene bilayer barrier

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Abstract. We investigate the electronic transport properties of a finite-size silicene bilayer barrier. We got the boundary conditions at the interface of monolayer and bilayer silicene using the tight-binding model. By matching the wavefunctions, we got the transmission probability as a function of incident angle for several lengths of bilayer barrier and incident energies. We found that a clear resonant tunneling appears because of evanescent modes in bilayer silicene. We also calculate the conductance in a overlap configuration which displays an oscillatory behavior as increase of either incident energy or length of bilayer barrier.

1. Introduction
Now, 2D materials are particularly important in materials science. By far, graphene, silicene, hBN, MoS₂ and black phosphorus, etc., have been extensively investigated for their fascinating properties. As a counterpart of graphene for silicon atoms, silicene [1] have been synthesized on some substrates by molecular beam epitaxy (MBE), such as Ag (111)[2-6], ZrB₂ (0001)[7], Ir (111)[8], and MoS₂[9]. Compared with graphene, electrons in silicene obey a similar Dirac equation around the $K(K')$ point of the Brillouin zone (BZ)[10,11]. Meanwhile, silicene has a larger spin–orbit coupling (SOC) which leads to the buckled structure between two sublattices, so the electronic structure is controllable by an external electric field. Many properties of silicene have been studied, such as electric tunable band structure[12], topological transition[13,14], the effects of impurity adsorption[15], and the spin/valley-dependent transport in ferromagnetic silicene junctions[16-18]. However, compared with the extensive studies on monolayer silicene, the investigation of nano-structures based on few-layer silicene is rare, such as interferometric optical effects which depend on polarization in multilayer nanostructures are reported[19], which is meaningful to the design of electronic devices based on silicene[20-31].

The experimental evidence of multilayer silicene has been reported[22]. Furthermore, researchers have identified the monolayer silicene have been observed by a experimental group on the Ag(111) surface as the bilayer silicene actually[28]. Different stacking orders can occur in bilayer silicene. Research indicates that AB (Bernal) stacking is stable and the energetically favored one as shown in Figure 1.[30] The vertical bond length between the upper silicene layer and lower layer is 2.53 Å, while the two sublattices (A and B) within one layer couple with a bond length 2.32 Å. TB parameters fitted for the bilayer silicene in comparison with those of the bilayer graphene [32] are given below[30]: $\gamma_0$, $\gamma_1$ and $\Delta$ are 1.13 (3.12), 2.025 (0.377) and -0.0691 (-0.0366) eV, respectively, where $\gamma_0$, $\gamma_1$ denote the hopping integrals for intralayer and interlayer nearest neighbor coupling, $\Delta$ is the onsite potential difference between AB sublattice in a layer. We can see the interlayer hopping plays an more important role in bilayer silicene than that in bilayer graphene.
In the paper, we investigated electronic transport properties through a finite-size silicene bilayer barrier (SBB) with monolayer leads. There are two possible geometries we address as island and overlap configurations, respectively. In the tight-binding model, the amplitudes of wavefunction obey the lattice Schrödinger equation at the interface, we got the boundary conditions at interface between monolayer and bilayer silicene. By matching the wavefunctions, we calculate the transmission probability as a function of incident angle for several lengths of bilayer barrier and incident energies. We found that a clear resonant tunneling appears because of evanescent modes in bilayer silicene. We also calculate the conductance in a overlap configuration which displays an oscillatory behavior as increase of either incident energy or length of bilayer barrier.

2. Theoretical description of the interface

Figure 1 shows atomic structure near the boundary between monolayer and bilayer silicene with Bernal stacking, where parameters $a = 2.53\text{Å}$, $\gamma_0 = 1.13\text{eV}$ and $\gamma_1 = 2.205\text{eV}$ are the bond length and hopping integrals for intralayer and interlayer nearest neighbor coupling, respectively. As shown, the zigzag type boundary is arranged along the $y$ axis. Sites belonging to the two sublattices in monolayer silicene are indicated by A and B. For the bilayer structure, top layer is denoted as 1 while bottom layer denoted as 2. The unit cell contains two silicon atoms denoted by A1 and B1 in layer 1, and A2 and B2 in layer 2. And B1 is vertically on the top of A2. The monolayer silicene connects with the bottom layer of bilayer region at the interface.

![Atomic structure near the boundary between monolayer and bilayer silicene](image)

**Figure 1.** Atomic structure near the boundary between monolayer and bilayer silicene. The shaded circles at $x=-a$ denote fictitious atoms extrapolated from the top layer.

In the vicinity of the $K/K'$ point, the effective low-energy Hamiltonian of monolayer silicene in the basis $\left(\psi_A^{K/K'}, \psi_B^{K/K'}\right)$ is given by[6,7]

$$H_{\rho\rho} = \begin{pmatrix}
-\eta \sigma\lambda_{SO} & \upsilon \pi_{\eta} \\
\upsilon \pi_{\eta}^* & \eta \sigma\lambda_{SO}
\end{pmatrix}$$

(1)
where \( \eta = \pm 1 \) correspond to the \( K \) and \( K' \) valleys, \( \sigma = \pm 1 \) denote the spin indices, \( \lambda_{SO} = 3.9 \) meV is the strength of SOC, \( \nu = 3/2a\gamma_0 \), \( \pi_\eta = k_x + i\eta k_y \) with \( (k_x, k_y) \) is the wave vector. The corresponding eigenvalue and eigenvector can be obtained

\[
E = \pm \sqrt{(\eta \sigma \lambda_{SO})^2 + \nu^2 k^2},
\]

and

\[
\psi_{\text{mono}}(r) = \left( \frac{\nu \tau_\eta}{E + \eta \sigma \lambda_{SO}} \right) e^{ikr}.
\]

The effective Hamiltonian in the basis \( (\psi_K^{1K'}, \psi_K^{2K'}, \psi_A^{1}, \psi_A^{2}, \psi_B^{1}, \psi_B^{2}) \) for bilayer silicene can be written as[19]

\[
H_{\eta \sigma} = \begin{pmatrix}
-\eta \sigma \lambda_{SO} + \Delta & \nu \pi_\eta & 0 & 0 \\
\nu \pi_\eta^* & \eta \sigma \lambda_{SO} + \gamma_1 & 0 & 0 \\
0 & \gamma_1 & -\eta \sigma \lambda_{SO} + \nu \pi_\eta & 0 \\
0 & 0 & \nu \pi_\eta^* & \eta \sigma \lambda_{SO} + \Delta
\end{pmatrix}
\]

where \( \Delta = -0.0691 \) eV is the onsite potential difference between AB sublattice. The dispersion relation satisfies the following equation

\[
(E^2 - \lambda_{SO}^2 - \gamma_1^2)\left[(\Delta - E)^2 - \lambda_{SO}^2 \right] + 2\nu^2 k^2 \left[-E^2 + \lambda_{SO}^2 + \Delta E\right] + \nu^2 k^4 = 0
\]

for which a approximate solution can be given properly

\[
E \approx s \left( \frac{\gamma_1 \pm \sqrt{\nu^2 k^2 + \gamma_1^2}}{2} \right)^2 + \lambda_{SO}^2 + \Delta
\]

with \( s = \pm 1 \). In the energy range \( \lambda_{SO} + \Delta < E < \gamma_1 + \Delta \), we have a traveling mode

\[
\psi_{\text{bilayer}}(r) = \begin{pmatrix}
\gamma_1 (\eta \sigma \lambda_{SO} - \Delta + E) (k_x - i\eta k_y) \\
\gamma_1 (\eta \sigma \lambda_{SO} - \Delta + E) (k_y - i\eta k_x) \\
\gamma_1 \nu (k_x - i\eta k_y) \\
\gamma_1 \nu (k_y - i\eta k_x) \\
\nu (k_x - i\eta k_y) \\
\nu (k_y - i\eta k_x)
\end{pmatrix} e^{ikr}
\]

apart from a normalization constant. It's worth noting that we also have evanescent modes decaying or growing exponentially. The decaying mode in the positive \( x \) direction can be written as

\[
\phi_{\text{bilayer}}(r) = \begin{pmatrix}
\gamma_1 (\eta \sigma \lambda_{SO} - \Delta + E) (k_x - i\eta k_y) \\
\gamma_1 (\eta \sigma \lambda_{SO} - \Delta + E) (k_y - i\eta k_x) \\
i \gamma_1 \nu (k_x - i\eta k_y) \\
i \gamma_1 \nu (k_y - i\eta k_x) \\
\nu (k_x - i\eta k_y) \\
\nu (k_y - i\eta k_x)
\end{pmatrix} e^{-k_x x + i\eta y}
with \( \kappa_s = \sqrt{k_s^2 - \frac{(E - \Delta)^2 - \lambda_{SO}^2 - \gamma_1 \sqrt{(E - \Delta)^2 - \lambda_{SO}^2}}{\Delta}} \). Compared with bilayer graphene, the first excited conduction band is higher, evanescent modes will exist in a wider energy range.

At the interface of monolayer and bilayer silicene, a boundary condition should be constructed for wavefunction matching. In the tight-binding model, the amplitudes of wavefunction obey the lattice Schrödinger equation at the interface, we can obtain the following set of equations:

\[
\begin{align*}
E\psi_{0}^{A2} &= -\gamma_0\psi_{0}^{B1} - 2\gamma_0 \cos \frac{\sqrt{3}k\alpha}{2}\psi_{0}^{B2} \\
E\psi_{-\frac{\Delta}{2}}^{B1} &= -\gamma_0\psi_{-\frac{\Delta}{2}}^{A0} - 2\gamma_0 \cos \frac{\sqrt{3}k\alpha}{2}\psi_{-\frac{\Delta}{2}}^{A0} \\
E\psi_{0}^{B1} &= -\gamma_0\psi_{0}^{A2} - 2\gamma_0 \cos \frac{\sqrt{3}k\alpha}{2}\psi_{0}^{A0}
\end{align*}
\]

where the subscripts show the distances from the interface. Here we introduced three columns of fictitious amplitudes \( \psi_{-\frac{\Delta}{2}}^{B2}, \psi_{0}^{A0} \) and \( \psi_{-\frac{\Delta}{2}}^{A1} \), which are extrapolated from the other region for wavefunction matching at the interface. Then, we can obtain the boundary condition at the interface as

\[
\psi_{-\frac{\Delta}{2}}^{B2} = \psi_{0}^{A1}, \quad \psi_{0}^{A0} = \psi_{-\frac{\Delta}{2}}^{A2}, \quad \psi_{-\frac{\Delta}{2}}^{A0} = 0.
\]

Using the boundary condition, we can consider more complex scattering conveniently, such as a monolayer-bilayer-monolayer (MBM) junction.

3. Silicene bilayer barrier with monolayer leads

There are two possible geometries for a finite-size silicene bilayer barrier with two contacts as shown in Figure 2. First, we can put a flake on the top of an infinite monolayer, so that the monolayer part of the system plays the role of leads. Second, the finite-size bilayer can be formed by the overlap of two semi-infinite layers. We will refer to them as island and overlap configurations, respectively. In both cases, the length of the bilayer region is \( L \).

**Figure 2.** Schematic view of two possible geometries of the silicene bilayer barrier. The left panels correspond to island configuration, and the other correspond to overlap configuration. The upper panels are the top views, while the lower ones are the side views.
Figure 2(a) shows the island configuration with two different zigzag interfaces at $x=0$ and $x=L$, where $L=(3N+1)a/2$ is the length of bilayer barrier with an integer $N$. As follows in section 1, we can get the boundary conditions at $x=0$ and $x=L$ using extrapolated wavefunctions, respectively.

$$\psi_{x}^{B_{2}} = \psi_{x}^{B_{2}}, \quad \psi_{0}^{A} = \psi_{0}^{A}, \quad \psi_{-d}^{A} = 0,$$

$$\psi_{L+d}^{B_{2}} = \psi_{L+d}^{B}, \quad \psi_{L-a}^{A} = \psi_{L-a}^{A}, \quad \psi_{L-a}^{B_{1}} = 0.$$ (11)

Figure 2(b) shows the overlap configuration with two similar zigzag interfaces at $x=0$ and $x=L$. We can also write the boundary conditions at $x=0$ and $x=L$ as follows

$$\psi_{-d}^{B} = \psi_{-d}^{B_{2}}, \quad \psi_{0}^{A} = \psi_{0}^{A}, \quad \psi_{-d}^{B_{1}} = 0,$$

$$\psi_{L}^{B} = \psi_{L}^{B_{2}}, \quad \psi_{L-a}^{A} = \psi_{L-a}^{A}, \quad \psi_{L-a}^{B_{2}} = 0.$$ (12)

By the wavefunction matching at the interface, we can calculate the transmission probability. Further, by setting $k_{x} = k \cos \theta$ and $k_{y} = k \sin \theta$ with incident angle $\theta$, we can get the ballistic conductance at zero temperature according to Landauer-Büttiker formula[33,34]

$$G = G_{0} \int_{\pi/2}^{\pi/2} T_{qe} \cos k d\theta$$

where $G_{0} = e^{2}L_{y} \sqrt{E^{2} - \lambda_{SO}^{2}} / \pi^{2} \hbar$ is taken as the conductance unit with the transverse length $L_{y}$, $T_{qe}$ is the transmission probability.

4. Results and discussion

In what follows, we present some numerical examples of transmissions and conductances for the silicene bilayer barrier (SBB) with the variation of incident energy $E$ and the length of barrier $L$ according to equations (11)–(13). Here, we consider electron transmission between monolayer and bilayer silicene with a same electron concentration. This can be realized when the electron density is changed by a gate voltage.

![Figure 3](image_url)

Figure 3. (Color online) Transmissions in silicene bilayer barrier as a function of incident angle $\theta$ for several $L$ and $E$. (a) corresponds to the island configuration, (b), (c) and (d) correspond to the overlap configuration.
Substituting the incident, reflected and transmitted wavefunctions into the above boundary condition (11) and (12), respectively, we can get the scattering properties of SBB as shown in Figure 3. Figure 3(a) corresponds to the island configuration, (b), (c) and (d) correspond to the overlap configuration. It shows the calculated transmission for the two type bilayer barriers depends strongly on incident angle, and is suppressed when $N$ increases in both cases. By comparing the two panels (a) and (b), we found that the electronic transport is harder in the SBB with the overlap configuration at low energy region than with the island configuration. With the increase of $E$, the contribution of evanescent modes for $E < \gamma_1 + \Delta$ will appear. In order to understand this conjecture, we calculated the transmission in the overlap configuration for example, with $E = 0.1\gamma_1, 0.3\gamma_1, 0.5\gamma_1, 0.9\gamma_1$ and $N = 10$ as shown in Figure 3(c). It clearly shows that the number of resonant tunneling peaks tend to increase with the increase of incident energy. On the other hand, the number does not change basically for different lengths of bilayer barrier as shown in Figure 3(d).

**Figure 4.** The conductances as a function of the incident energy $E$ with $N = 10$ and length of silicene bilayer barrier $N$ with $E = 0.3\gamma_1$ in (a) and (b), respectively. Figure 4(a) and (b) display the conductances as a function of the incident energy $E$ and length of silicene bilayer barrier $N$ in overlap configuration, respectively. It clearly shows that conductance changes drastically and displays an oscillatory behavior as increase of $E$. At the energy range, there is only one transmission channel in the bilayer barrier region, we think the oscillatory behavior originates from the interference of reflect waves for interfaces existence. Meanwhile, the lowest points in the curve are increasing with incident energy because the tunneling enhances. As shown in Figure 4(b), the oscillatory behavior of conductance also appears with increase of the length of silicene bilayer barrier, like in graphene system[35-36]. These effects must be fully considered in electronic device design based on this system.

5. Conclusion
In summary, we have investigated the electronic transport properties in a silicene bilayer barrier. We got the boundary condition at the interface in the tight-binding model. By matching the wavefunctions, we got the transmissions in silicene bilayer barrier as a function of incident angle $\theta$ for several $L$ and $E$. It shows that a clear resonant tunneling at $E < \gamma_1 + \Delta$ appears because of evanescent modes. We also calculate the conductance in overlap configuration which displays an oscillatory behavior as increase of either $E$ or $N$. The results will provide physical models and theoretical validity in designing electronic devices based on bilayer silicene nanostructures.
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