Electronic transmission through AB-BA domain boundary in bilayer graphene

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We study the electron transmission through the domain boundary on bilayer graphene separating AB and BA stacking regions. Using the effective continuum model, we calculate the electron transmission probability as a function of the electron energy and the incident angle, for several specific boundary structures. The transmission strongly depends on the crystallographic direction of the boundary and also on the atomic configuration inside. At the low energy, the boundary is either insulating or highly transparent depending on the structure. In insulating cases, the transmission sharply rises when the Fermi energy is increased to a certain level, suggesting that the electric current through the boundary can be controlled by the field effect. The boundary parallel to the zigzag direction generally have different transmission properties between the two different valleys, and this enables to generate the valley polarized current in a certain configuration. We show that those characteristic features can be qualitatively explained by the transverse momentum conservation in the position-dependent band structure in the intermediate region.

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I. INTRODUCTION

In multilayer graphenes, the weak interlayer interaction allows various different stacking configurations, and there often appear the domain structures consisting of different stacking regions. Recent experiment found a novel type of domain boundary in bilayer graphene which connects two equivalent, but distinct Bernal-stacking structures referred to AB and BA, which are shown in Fig. 1(a) and (b), respectively. On the boundary, the AB structure is continuously deformed to the BA structure with in-plane distortion. Theoretically, the electronic band structure of the AB-BA domain boundary was recently calculated in presence of the interlayer asymmetric potential and it was shown that the boundary-localized states emerge inside the asymmetry-induced energy gap.

In two-dimensional crystal, a domain boundary significantly influences the electronic transport. There are several theoretical studies investigating the electron transmission through the graphene-based domain structures, such as the grain boundary on polycrystalline graphene and graphene monolayer-bilayer boundary. In this paper, we calculate the electronic transmission properties across AB-BA domain boundaries in bilayer graphene with no interlayer asymmetry. We consider several specific atomic configurations illustrated in Fig. 2. They are classified into armchair boundary [Figs. 2 (a) and (b)] and zigzag boundary [Figs. 2 (c) and (d)] depending on the orientation of the boundary relative to the honeycomb lattice. Each case is divided into AA type [Figs. 2 (a) and (c)] and SP type [Figs. 2 (b) and (d)], depending on whether the stacking structure in the intermediate region approximates AA stacking or SP stacking, shown in Fig. 1(c) and (d), respectively.

For each case, we calculate the transmission probability as a function of the incident angle and the electron energy using the effective continuum model. We find that the transmission strongly depends on the boundary structure. Particularly, we show that a low-energy electron easily passes through armchair SP [Figs. 2 (b)], and zigzag AA [Figs. 2 (c)], whereas it is almost completely reflected in armchair AA [Figs. 2 (a)], and zigzag SP [Figs. 2 (d)]. For the latter two cases, the transmission probability sharply rises when the Fermi energy is increased to a certain level. The zigzag boundaries generally have different transmission probability between the two different valleys, offering a possibility to generate the valley polarized current. We show that those characteristic features can be qualitatively understood by considering the local band structure in the intermediate region.

FIG. 1: Various stacking structures of bilayer graphene. (a) AB, (b) BA, (c) AA, and (d) SP stacking.
II. FORMULATION

A. Atomic structure

We consider the AB-BA domain boundaries on bilayer graphene defined by Figures 2 (a)-(d). In each case, the boundary divides the system into the AB region at left and the BA region at right. We set the $x$ axis perpendicularly to the boundary, and $y$ axis in parallel to the boundary. We also define the coordinates $x'$ and $y'$ fixed to the honeycomb lattice, along the zigzag and armchair directions, respectively. The relation between the two frames is given by $(x, y) = (x', y')$ for the armchair boundary [Figs. 2 (a) and (b)], and $(x, y) = (y', -x')$ for the zigzag boundary [Figs. 2 (c) and (d)]. We define $a_1 = a e_{x'}$ and $a_2 = (1/2) a e_{x'} + (\sqrt{3}/2) a e_{y'}$ as the lattice vectors of graphene, where $e_{x'}$ and $e_{y'}$ are the unit vectors along $x'$ and $y'$, respectively, and $a \approx 0.246$ nm is the lattice constant. We also define $\tau_i (i = 1, 2, 3)$ as the vectors from B site to the nearest A sites as in Fig. 2 (a). We also use $a_0 = a/\sqrt{3} \approx 0.142$ nm is the distance between the nearest carbon atoms in graphene.

We define the atomic structure starting from uniform and infinite AB-stacked bilayer graphene. We divide the system into the left ($x < 0$), intermediate ($0 < x < W$) and right regions ($W < x$), where $W$ defines the width of the intermediate region. We fix the AB stacking in the left region, and invert AB stacking in the right region to BA stacking by translating layer 1 and 2 by $\Delta y'$ and $-\Delta y'$, respectively, along $y'$ direction (armchair direction). The direction of the translation is thus parallel and perpendicular to the boundary in armchair and zigzag boundary, respectively, resulting in shear and tensile lattice distortion, respectively.

The shift $\Delta y'$ is defined as

$$\Delta y' = \begin{cases} a_0 & \text{(AA type boundary),} \\ -a_0/2 & \text{(SP type boundary).} \end{cases}$$

For the intermediate region, we assume the shift linearly scales in proportion to $x$. The system is translationally symmetric along $y$ direction.

The width of the intermediate region $W$ in the real system is estimated at about 10 nm, and much larger than the atomic scale. The local lattice structure near every single point then approximates a bilayer graphene with a uniform displacement. Let us define $\delta$ as the interlayer displacement vector of layer 2 with respect to layer 1 starting from AA stacking, as illustrated in inset of Fig. 3. In the present systems, $\delta$ is parallel to $y'$ and depend only on $x$, so that it is written as $\delta(r) = \delta(x)e_{y'}$. 

FIG. 2: Schematic structures of several types of AB-BA domain boundary: (a) Armchair AA, (b) armchair SP, (c) zigzag AA, and (d) zigzag SP. In (c) and (d), a narrow strip in the upper part represents the uniform AB stacking bilayer before the distortion.
Bilayer graphene with a displacement direction in AA type boundary and SP type boundary. (Inset) Bilayer graphene with a displacement $\delta$.

The interlayer displacement $\delta(x)$ along the armchair direction in AA type boundary and SP type boundary. (Inset)

\[ \delta(x) = \begin{cases} a_0 & (x < 0) \\ a_0(1 - 2x/W) & (0 < x < W) \\ -a_0 & (W < x) \end{cases} \]

(2)

and for the SP type boundary,

\[ \delta(x) = \begin{cases} a_0 & (x < 0) \\ a_0(1 + x/W) & (0 < x < W) \\ a_0 & (W < x) \end{cases} \]

(3)

which are plotted in Fig. 3. The AA type boundary has the AA-stacked region ($\delta = 0$) at $x = W/2$, where the two honeycomb lattices completely overlap. The SP boundary has the structure called SP (saddle point) stacking ($\delta = 3a_0/2$) at $x = W/2$, where $A_2$ is located at the midpoint between the nearest $A_1$ sites. Experimentally, SP type boundary is more stable than AA type boundary because AA stacking is energetically unfavorable.

B. Effective continuum model

We derive the effective continuum model for AB-BA boundary from the tight-binding model for $p_z$ atomic orbitals, using a similar approach developed for rotationally stacked bilayer graphene. The Hamiltonian for the tight-binding model is written as

\[ H = -\sum_{\langle i,j \rangle} t(R_i - R_j)|R_i\rangle\langle R_j| + H.c., \]

(4)

where $R_i$ and $|R_i\rangle$ represent the lattice point and the atomic state at site $i$, respectively, and $t(R_i - R_j)$ is the transfer integral between the sites $i$ and $j$. We adopt an approximation, $|\delta| < 3a_0/1.5$.

\[ t(d) = V_{pp\pi}(d) \left(1 - \left(\frac{d}{d_0}\right)^2\right) + V_{pp\sigma}(d) \left(\frac{d}{d_0}\right)^2, \]

\[ V_{pp\pi}(d) = V_{pp\pi}^0 \exp \left(-\frac{d}{d_0}\right), \]

\[ V_{pp\sigma}(d) = V_{pp\sigma}^0 \exp \left(-\frac{d}{d_0}\right), \]

(5)

where $V_{pp\pi}^0 \approx -2.7$ eV is the transfer integral between the nearest-neighbor atoms of monolayer graphene, $V_{pp\sigma}^0 \approx 0.48$ eV is that between vertically located atoms on the neighboring layers, and $d_0 \approx 0.335$ nm is the interlayer spacing. $r_0$ is the decay length of the transfer integral, and is chosen as 0.184a so that the next nearest intralayer coupling becomes 0.1V_{pp\sigma}^0. The transfer integral for $d > 4a_0$ is exponentially small and can be safely neglected.

The low-energy spectrum of the monolayer graphene is given by effective Dirac cones centered at $K_+$ and $K_-$ points, which are plotted in Fig. 3. They are given by $K_{\pm} = (\pm 2\sqrt{3}/a)(2/3)e_{c'}$. We express the low-energy states of the system in terms of the monolayer's bases in the vicinity of $K_{\pm}$ points. It is written as $|\Psi\rangle = \sum_i \psi(R_i)|R_i\rangle$ and

\[ \psi(R_{A_l}) = e^{iK_{\pm}R_{A_l}F_{A_l}^{K_{\pm}}(R_{A_l})} + e^{iK_{\pm}R_{A_l}F_{A_l}^{K_{\mp}}(R_{A_l})}, \]

\[ \psi(R_{B_l}) = e^{iK_{\pm}R_{B_l}F_{B_l}^{K_{\pm}}(R_{B_l})} + e^{iK_{\pm}R_{B_l}F_{B_l}^{K_{\mp}}(R_{B_l})}, \]

(6)

where $l = 1, 2$ is the layer index. Here $F_{A_l}^{K_{\pm}}$ and $F_{B_l}^{K_{\pm}}$ are envelope functions, which are slowly varying in the atomic scale.

When $W$ is much larger than the lattice constant, the interaction between the two graphene layers is dominated by the long-wavelength components. Then the states near the valley $K_+$ and those near $K_-$ are not hybridized and we may consider two valleys separately in constructing the Hamiltonian. The effective Hamiltonian for $(F_{A_1}^{K_\pm}, F_{B_1}^{K_\pm}, F_{A_2}^{K_\pm}, F_{B_2}^{K_\pm})$ is written as

\[ H_{\text{eff}} = \left( \begin{array}{cc} H_0 + V & U^\dagger \\ U & H_0 - V \end{array} \right), \]

(7)

where

\[ H_0 = \hbar v \left( \begin{array}{cc} 0 & \hat{k}_{x'} + i\hat{k}_{y'} \\ \hat{k}_{x'} - i\hat{k}_{y'} & 0 \end{array} \right), \]  

\[ V = \left( \begin{array}{cc} 0 & w^* \\ w & 0 \end{array} \right), \]

\[ U = \left( \begin{array}{cc} U_{A_2A_1} & U_{A_2B_1} \\ U_{B_2A_1} & U_{B_2B_1} \end{array} \right) = \left( \begin{array}{cc} u(K_\xi, \delta) & u(K_\xi, \delta + \tau_1) \\ u(K_\xi, \delta - \tau_1) & u(K_\xi, \delta) \end{array} \right). \]

(8)

$H_0$ is the effective Hamiltonian of monolayer graphene, where $\hat{k} = -i\partial/\partial r$, $\xi = \pm$ is the valley index corresponding to $K_{\pm}$, and $v$ is the band velocity of the
Dirac cone, which is given in the present tight-binding parameterization as \[12\]

\[ v \approx \frac{\sqrt{3} a}{2} V_{p p} (1 - 2e^{-a_0/r_0}). \tag{9} \]

The function \(\delta\) describes the interlayer interaction in bilayer graphene shifted by a constant displacement \(\delta\). The function \(u(k, \delta)\) is defined by \[12\]

\[ u(k, \delta) = \sum_{n_1, n_2} -t(n_1a_1 + n_2a_2 + d_0e_z + \delta) \]
\[ \times \exp[-i(k \cdot (n_1a_1 + n_2a_2 + \delta))], \tag{10} \]

where \(e_z\) is the unit vector perpendicular to graphene. In the effective Hamiltonian, we substitute \(K_\xi\) for \(k\) in \(u(k, \delta)\), i.e., neglect the \(k\)-dependent terms in the interlayer coupling. In \(A\) \((B)\) (Bernal) stacked graphene, this simplification corresponds to neglecting the trigonal warping and the electron hole asymmetry, corresponding to the band parameters called \(\gamma_1\) and \(\gamma_4\). \[23, 24\]

The function \(u(K_\xi, \delta)\) is smoothly varying function in \(\delta\), and it is approximately written in terms of a few Fourier components as

\[ u(K_\xi, \delta) \approx \frac{\gamma_1}{3} \left( 1 + e^{-i\delta a^*_1 \cdot \delta} + e^{-i\delta a^*_2 \cdot \delta} \right), \]

\[ \gamma_1 \equiv u(K_\xi, 0) = t(0) - 3t(a) + 6t(\sqrt{3}a) + \cdots, \tag{11} \]

where \(a^*_i\) is the reciprocal lattice vector satisfying \(a_i \cdot a^*_j = 2\pi \delta_{ij}\) and \(t(x) \equiv t(x, 0, d_0)\). In the present choice of the tight-binding parameters, we have \(\gamma_1 \approx 0.32\) eV. In the following calculation, we scale the energy in units of \(\gamma_1\), and the wavenumber in units of \(\gamma_1/(\hbar v)\), so that the result does not depend on the values of \(v\) and \(\gamma_1\). When \(\delta = \delta e_y\), in particular, Eq. (11) becomes

\[ U_{A_2A_1} = U_{B_2B_1} = \frac{\gamma_1}{3} \left[ 1 + 2 \cos \frac{2\pi}{3} \delta \left( \frac{\delta}{a_0} + 1 \right) \right], \]
\[ U_{A_2B_1} = \frac{\gamma_1}{3} \left[ 1 + 2 \cos \frac{2\pi}{3} \delta \left( \frac{\delta}{a_0} - 1 \right) \right], \]
\[ U_{B_2A_1} = \frac{\gamma_1}{3} \left[ 1 + 2 \cos \frac{2\pi}{3} \delta \left( \frac{\delta}{a_0} + 1 \right) \right], \tag{12} \]

which are plotted against \(\delta\) in Fig. 4 (a). The shifts \(\delta = 0, a_0, 3a_0/2\) and \(2a_0\) correspond to AA, AB, SP and BA stacking, respectively, where \((U_{A_2A_1}, U_{A_2B_1}, U_{B_2A_1}) = (\gamma_1, 0, 0), (0, 0, \gamma_1), (\gamma_1, 1/3, 2/3, 2/3), (0, \gamma_1, 0)\), respectively.

The matrix \(V\) in Eq. (1) describes the effect of the lattice distortion \[25\]. Here \(w\) is given for \(0 < x < W\) by

\[ w = \begin{cases} (-i\lambda)\hbar v k_0 & \text{(armchair boundary)} \\ \hbar v k_0 & \text{(zigzag boundary)} \end{cases} \]

\[ k_0 = \frac{1}{r_0} \Delta y'/W, \tag{13} \]

and \(w = 0\) otherwise, where \(\Delta y'\) is defined in Eq. (1). \(k_0\) represents the shift of Dirac point in the wave space.

The direction of the shift is opposite between the two layers, and it is always parallel to the domain boundary \((y\) direction). As \(W\) increases, the effect of \(V\) becomes relatively unimportant compared to the interlayer interaction \(U\), since \(\hbar v k_0\) in \(V\) decreases as \(\propto 1/W\) while \(U\) is always of the order of \(\gamma_1\). At \(W = 5\hbar v/\gamma_1 \approx 10\) nm, for example, \(\hbar v k_0\) is of the order of 0.1\(\gamma_1\) so that the electronic property is primarily determined by \(U\).

C. Electron transmission

The electron transmission through the boundary can be obtained by using the transfer matrix. \[26, 27\] The effective Hamiltonian in Eq. (7) can be written as

\[ H_{\text{eff}} = P \frac{\partial}{\partial x} + Q(x). \tag{14} \]

with certain matrices \(P\) and \(Q\), where \(Q = Q(x)\) may depend on the position \(x\) and \(P\) is a constant matrix. Since the system is translationally symmetric along \(y\) direction, \(k_y = -i\partial/\partial y\) is replaced with the quantum number \(k_y\). The Schrödinger equation, \((\varepsilon - H_{\text{eff}}) \Psi = 0\), is transformed as a one-dimensional differential equation,

\[ \frac{\partial}{\partial x} F(x) = L(x) F(x), \tag{15} \]

where \(F = (F_{A_1}, F_{B_1}, F_{A_2}, F_{B_2})\) is the four-component wavefunction, and

\[ L(x) = P^{-1}(\varepsilon - Q(x)). \tag{16} \]

The transfer matrix is defined by

\[ F(x) = T(x, x') F(x'). \tag{17} \]

Using Eqs. (15) and (17), the differential equation for the transfer matrix is given by

\[ \frac{\partial}{\partial x} T(x, x') = L(x) T(x, x'). \tag{18} \]

We obtain the transfer matrix \(T(W, 0)\) connecting the left region and the right region by numerically integrating Eq. (15).

In the AB-stacked region in \(x < 0\) and the BA-stacked region in \(x > W\), the system is uniform and \(L(x)\) becomes independent of \(x\). In each region, the solution of Eq. (15) can be written as a linear combination of \(u_j \exp(\lambda_j x)\), where \(\lambda_j\) and \(u_j\) \((j = 1, 2, 3, 4)\) are the eigen values and eigen vectors of the matrix \(L\), respectively. The four eigen values are identical in AB and BA regions and written as

\[ \lambda = \pm i \frac{\hbar v}{\hbar v} \sqrt{\varepsilon^2 \pm \gamma_1 \varepsilon - (\hbar v k_y)^2}, \tag{19} \]

where two plus-minus signs give four possible combinations. The corresponding eigen state is a traveling mode when \(\lambda\) is purely imaginary, while it is an evanescent
mode otherwise. The four eigen values consist of two right-going modes and two left-going modes, where a right-going mode can be a traveling mode with velocity in the positive $x$ direction, or an evanescent mode decaying in the positive $x$ direction.

Let $\lambda_{+ i}$ ($i = 1, 2$) the right-going modes and $\lambda_{- i}$ ($i = 1, 2$) the left-going modes. The wavefunction at $x = 0$ is written as

$$ F(0) = (u_{+, 1}^{(L)}, u_{+, 2}^{(L)}, u_{-, 1}^{(L)}, u_{-, 2}^{(L)}) ^T,$$

where $u_{+, i}^{(L)}$ is the eigenvector in the AB-region corresponding to $\lambda_{+ i}$, and $C_{\pm, i}^{(L)}$ is the amplitude. Similarly, the wavefunction at $x = W$ is written as

$$ F(W) = U^{(R)} C^{(R)},$$

where $U^{(R)} = (u_{+, 1}^{(R)}, u_{+, 2}^{(R)}, u_{-, 1}^{(R)}, u_{-, 2}^{(R)})$ is the eigenvectors in the BA-region. The scripts (L) and (R) represent the left (AB) region and the right (BA) region, respectively. The matrices $U^{(L)}$ and $U^{(R)}$ are not unitary in general when they include evanescent modes.

Using Eqs. (17), (20) and (21), we obtain an equation connecting the left and right wave amplitudes,

$$ C^{(R)} = \tilde{T} C^{(L)},$$

where $\tilde{T} = [U^{(R)}]^{-1}T(W, 0)U^{(L)}$. We write this in the form,

$$ \begin{pmatrix} C_{+}^{(R)} \\ C_{-}^{(R)} \end{pmatrix} = \begin{pmatrix} \tilde{T}_{11} & \tilde{T}_{12} \\ \tilde{T}_{21} & \tilde{T}_{22} \end{pmatrix} \begin{pmatrix} C_{+}^{(L)} \\ C_{-}^{(L)} \end{pmatrix},$$

where $C_{+}^{(R)} = (C_{+1}^{(R)}, C_{+2}^{(R)})$ etc., and $\tilde{T}_{ij}$'s are 2 × 2 block matrices. By sorting the wave amplitudes into in-coming modes, $C_{+}^{(L)}$ and $C_{-}^{(L)}$, and out-going modes, $C_{+}^{(R)}$ and $C_{-}^{(R)}$, we obtain

$$ \begin{pmatrix} C_{+}^{(L)} \\ C_{-}^{(L)} \end{pmatrix} = S \begin{pmatrix} C_{+}^{(R)} \\ C_{-}^{(R)} \end{pmatrix},$$

where

$$ S = \begin{pmatrix} -\tilde{T}_{21}^{-1} \tilde{T}_{22} & \tilde{T}_{21}^{-1} \tilde{T}_{22}^{-1} \\ \tilde{T}_{11} - \tilde{T}_{12} \tilde{T}_{22}^{-1} \tilde{T}_{21} & \tilde{T}_{12} \tilde{T}_{22}^{-1} \tilde{T}_{21} \end{pmatrix}.$$

$|S_{ij}|^2$ describes the transmission probability from the in-coming channel $i$ to out-going channel $j$.

### III. BILAYER GRAPHENE WITH CONSTANT DISPLACEMENT

In the large $W$ limit where $\delta$ is slowly varying in position, the local electronic structure at every single point can be approximately described by the electronic spectrum of uniform bilayer graphene with constant $\delta$. The $\delta$-dependent band structure intuitively explains the transmission properties of AB-BA boundary as shown later. In the literature, the effect of interlayer sliding on the band structure was studied for the cases in the vicinity of AB stacking. For the present purposes, we consider the band structure in all the range of the displacement along $y'$ to cover AB, AA and SP. Fig. 4 (b)-(f) show the band dispersion near $K_-$ point for several $\delta$'s along AA-AB-SP line, obtained from Eq. (7) with constant $\delta$ and $V = 0$. In each figure, the left panel shows the surface plot of the energy band in $k_{y'} > 0$, and the right panel the contour plot at several energies. The spectrum of $K_+$ are obtained by replacing $k_{x'}$ with $-k_{x'}$.

At $\delta = 0$ [AA stacking, Fig. 4 (b)] [30, 32], the energy spectrum consists of four bands expressed by

$$ \varepsilon_{s_{1} s_{2}}^{AA}(k) = s_{1} \gamma_{1} + s_{2} \hbar v k,$$

where $s_{1} = \pm$, $s_{2} = \pm$, and $k = (k_{x}^2 + k_{y}'^2)^{1/2}$. This represents two pairs of Dirac cones shifted by $\pm \gamma_{1}$ in energy, which intersect at $E = 0$ with a Fermi circle of radius $\gamma_{1}/(\hbar v)$. When $\delta$ is increased from 0, the band anticrossing occurs at the intersection, while a pair of band touching point remains on $k_{y'}$ axis on the zero energy plane. For $0 < \delta < a_{0}$, the touching position is given by

$$ k_{x'} = 0, \quad k_{y'} = \pm \gamma_{1} \hbar v \sqrt{\frac{1}{3} + \frac{2}{3} \cos \left( \frac{2 \pi \delta}{3 a_{0}} \right)}.$$

At $\delta = a_{0}$ [AB stacking, Fig. 4 (d)], the split Dirac points merge at the origin, giving the hyperbolic dispersion expressed by, [23, 24]

$$ \varepsilon_{s_{1} s_{2}}^{AB}(k) = s_{1} \left\{ \frac{\gamma_{1}}{2} + s_{2} \sqrt{\left( \frac{\gamma_{1}}{2} \right)^{2} + (\hbar v k)^{2}} \right\}.$$

When $\delta$ exceeds 1, the band touching point again split but now along $k_{x'}$ axis, and also shift in energy as shown in $\delta = 1.25a_{0}$ [Fig. 4(e)]. At $\delta = 1.5a_{0}$ [SP stacking, Fig. 4(f)], the spectrum is separated into two Dirac cones shifted in $k_{x'}$ axis and energy axis, which are given by

$$ \varepsilon_{s_{1} s_{2}}^{SP}(k) = s_{1} \left\{ \frac{\gamma_{1}}{3} + s_{2} \sqrt{\left( \hbar v k_{x} + s_{1} \frac{2 \gamma_{1}}{3} \right)^{2} + (\hbar v k_{y})^{2}} \right\}.$$

The spectrum of $\delta$ is equivalent to that of $3a_{0} - \delta$ while the roles of $A$ and $B$ sublattices are swapped, and thus the spectra from $\delta = 1.5a_{0}$ to $3a_{0}$ is identical those from $\delta = 1.5a_{0}$ to 0. The band structure is periodic in $\delta$ with period of $3a_{0}$.

The conduction band and the valence band are never separated by an energy gap in any value of $\delta$, and this is because both the spatial inversion symmetry and the time-reversal symmetry remain unbroken in $\delta$. The robustness of the band touching point in presence of the two
symmetries was discussed for several graphene-based systems [33], and it can also be explained for general systems using the Berry phase argument, as shown in Appendix A.

IV. RESULTS AND DISCUSSION

We calculate the electron transmission probability for the AB-BA boundaries of Figure 2(a)-(d). For the width of the boundary, we assume $W = 5\hbar v/\gamma_1 \sim 10\text{nm}$ to simulate the experimental situation [4], and this is about ten times larger than the schematic diagram in Fig. 2. We consider the electron energy range $0 < \varepsilon < \gamma_1$, where we have a single Fermi circle of the radius $k(\varepsilon) = \sqrt{\varepsilon^2 + \gamma_1 \varepsilon}/(\hbar v)$ in the left and right regions. We assume that an electron enters the intermediate region from the left with energy $\varepsilon$ and angle $\theta (-\pi/2 < \theta < \pi/2)$, with the initial wavevector $k(\varepsilon)(\cos \theta, \sin \theta)$. Since the transverse wavevector $k_y$ is preserved throughout the scattering process, the electron transmits to the right region with the same angle $\theta$ with the probability $P(\theta)$, which reflects back to the left region with the angle $\pi - \theta$ with the probability $1 - P(\theta)$.

Figs. 5(a)-(d) show the transmission probability $P(\theta)$ through the domain boundaries of Figs. 2(a)-(d), respectively, for $K_-$ electron with several different energies. In the armchair boundaries [Fig. 5(a),(b)], $P(\theta)$ is symmetric with respect to $\theta = 0$ due to the $C_2$ rotation symmetry about $x$ axis (zigzag direction), and $P(\theta)$ becomes identical in $K_+$ and $K_-$. In the zigzag boundary [Fig. 5(c),(d)], $P(\theta)$ is generally asymmetric, and $P(\theta)$ at $K_+$ is equal to $P(-\theta)$ at $K_-$. This is because the zigzag boundary is symmetric with respect to the reflection about $x$ axis (armchair direction), which interchanges $K_+$ and $K_-$. The transmission strongly depends on the boundary structure. In the low energy $\varepsilon/\gamma_1 = 0.05$, an electron
FIG. 5: Electron transmission probability $P(\theta)$ through the domain boundaries in Figs. 2, calculated for $K_-$ electron with several different energies. Lower panel shows the local electronic band structure in the intermediate regions as a function of $\delta$.

Electron well passes in armchair SP [Fig. 5(b)] and zigzag AA [Fig. 5(c)], while it is almost completely reflected in armchair AA [Fig. 5(a)] and zigzag SP [Fig. 5(d)]. These features can be roughly understood by considering the local electronic band structure of fixed $\delta$ discussed in Sec. III, which is presented in the lower panel in each of Figs. 5(a)-(d). In the armchair AA, the low-energy Fermi circle splits along $k_y$ direction and it prevents the electron transmission because there are no intermediate $k_y$ matching the initial $k_y$. In the armchair SP, on the other hand, the electron well transmits because the Fermi circle splits in $k_x$ direction in this case, so that the electron can travel keeping the initial $k_y$. In the zigzag boundaries [Fig. 5(c),(d)], the direction of the Fermi surface splitting...
is rotated by 90° so that the properties of the AA type and SP type are interchanged.

The transmission sensitively depends on the electron energy in accordance with the change of the Fermi surface. In the armchair AA, the transmission is suddenly switched on when the energy is increased to as large as $\varepsilon/\gamma_1 = 0.4$. In the band structure, correspondingly, the Fermi circles in the intermediate region begin to overlap with the initial Fermi circle in the AB region. In the zigzag SP [Fig. 5 (d)], similarly, $P(\theta)$ rises in increasing energy as the Fermi circle overlap becomes significant. The transmission probability remains small around $\theta = 0$, and this corresponds to the absence of electronic states near $k_y = 0$ in the intermediate region due to the Fermi circle splitting. The correspondence between the transmission and the band structure at fixed $\delta$ is intuitive but only approximate, because the local band structure is not well-defined in a finite $W$, and also the lattice distortion gives some shift of the Dirac cone.

These characteristic features of the AB-BA boundary can be exploited to control the electronic transport. Particularly, the armchair AA [Fig. 5(a)] and zigzag SP [Fig. 5 (d)] have a striking property that the electron transmission is almost zero near the charge neutral point, and it sharply rises when the Fermi energy is increased to a certain level. This suggests that the electric current through the AB-BA boundary can be controlled by the field effect through a single gate electrode.

The zigzag boundaries generally have different transmission probability between $K_+$ and $K_-$ valleys, and it is possible in principle to generate the valley polarized current. Similar valley-selective mechanism was previously proposed for the graphene monolayer-bilayer junction [3], and also for bilayer graphene with spatially modulated gate-electric field [34]. Now, the transmission probability of $K_-$ and that of $K_+$ through a zigzag boundary have opposite angle dependence, $P(\theta)$ and $P(-\theta)$, respectively. In the zigzag AA [Fig. 5(c)], $P(\theta)$ at $\varepsilon/\gamma_1 = 0.4$ is significant only in $\theta > 0$, so that transmitted electrons are nearly polarized to $K_-$ in $\theta > 0$, and to $K_+$ in $\theta < 0$. The valley polarized current can be generated by an electronic channel obliquely crossing the boundary, as illustrated in Fig. 5(a). The polarization should be enhanced by in multiple boundaries as in shown Fig. 5(b). There the transmission probability from BA to AB is identical to that form AB to BA, because they are just related by interchanging the top and the bottom layers.

While we concentrated on the boundaries parallel to the zigzag direction or the armchair direction in the present work, AB-BA boundary can occur along any crystallographic direction. Fig. 7 shows AB-BA island structures separated by (a) AA type boundary and SP type boundary, where we translate the layer 1 and 2 inside the inner circle by $\Delta y'$ and $-\Delta y'$ [defined in Eq. (4)], respectively, while keeping the AB structure outside the outer circle. In each case, we see that the armchair boundary continuously transforms into the zigzag boundary as moving along the circumference. For a boundary along the intermediate direction between armchair and zigzag, we can calculate the transmission probability in the same theoretical basis, by rotating the crystal axis $(x', y')$ with respect to $(x, y)$ in the effective Hamiltonian, Eq. (7). We expect the transmission probability continuously changes as a function of the boundary angle, to interpolate the armchair and zigzag results.

![FIG. 6: Electronic channel diagonally crossing AB-BA boundary: (a) single boundary and (b) multiple boundary case.](image)

V. CONCLUSION

We studied the electron transmission properties for AB-BA domain boundary in bilayer graphene. Assuming several specific boundary structures, we calculate the electron transmission probability as a function of the electron energy and the incident angle. We find that the transmission strongly depends on the boundary structure. In low-energy region, particularly, the boundary is almost insulating in armchair AA and zigzag SP while it is highly transparent in armchair SP and zigzag AA. In insulating cases, the transmission probability sharply rises when the Fermi energy is increased to a certain level. The zigzag boundaries generally have different transmission properties between $K_+$ and $K_-$ valleys due to the symmetrical reason, and this offers a possibility to generate the valley polarized current. The characteristic features of the electron transmission can be qualitatively understood by the intermediate local band structure which continuously changes across the boundary. In particular, the transport gap in armchair AA and zigzag SP is explained by the the wavenumber mismatch in the Fermi surface of the intermediate region.

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Appendix A: Robustness of Dirac points

Here we show that the band touching point never disappears in presence of the spatial inversion symmetry (SI) and the time-reversal symmetry (TR). We consider a general periodic system, and take a Bloch eigenstate $\psi_k(r) = e^{i\mathbf{k} \cdot \mathbf{r}} u_k(r)$. The Berry curvature is defined as

$$\mathcal{F}(\mathbf{k}) = \nabla_k \times \mathbf{A}(\mathbf{k}),$$  \hspace{1cm} (A1)

with a vector field in $k$-space,

$$\mathbf{A}(\mathbf{k}) = -i \langle u_k | \nabla_k | u_k \rangle.$$  \hspace{1cm} (A2)

In presence of TR symmetry and SI symmetry, we immediately find that $\mathcal{F}(\mathbf{k}) = 0$ at any non-degenerate points, because TR and SI require $\mathcal{F}(-\mathbf{k}) = -\mathcal{F}(\mathbf{k})$ and $\mathcal{F}(-\mathbf{k}) = \mathcal{F}(\mathbf{k})$, respectively [35, 36].

We define the Berry phase for a closed path $C$ on the $k$-space as,

$$\gamma_C = \oint_C d\mathbf{k} \cdot \mathbf{A}(\mathbf{k}).$$  \hspace{1cm} (A3)

By using the Stokes theorem, this is transformed as

$$\gamma_C = \int_S d^2k \cdot \mathcal{F}(\mathbf{k}),$$  \hspace{1cm} (A4)

where $S$ is the $k$-space area enclosed by $C$. In TR and SI symmetry, $\gamma_C$ can be non-zero only when $S$ includes a band degeneracy point inside, because otherwise $\mathcal{F}(\mathbf{k})$ vanishes everywhere on $S$. In a massless Dirac Hamiltonian, for example, $\gamma_C$ around the Dirac point is $\pi$.

If we have a single degenerate point around which $\gamma_C$ is non-zero, the band touching cannot be resolved in any perturbations which keep TR, SI, and the original translational symmetry (i.e., different $k$-points are not coupled). This is because, if an infinitesimal perturbation splits the band degeneracy, the nonzero Berry phase around this point should immediately jump to zero because there are no degeneracy points inside $S$ any more, but this is obviously impossible because the change of the wave function on the path $C$ is also infinitesimal. A band gap can open only when a pair of degeneracy points having opposite Berry phases $\gamma_C$ and $-\gamma_C$ meet and annihilate at a single $k$-point.
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