Valley polarization in transmission through boundary between mono- and bi-layer graphene

Takeshi Nakanishi* and Tsuneya Ando†

*Nanotube Research Center, AIST, 1–1–1 Higashi, Tsukuba 305-8565, Japan
†Department of Physics, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8551, Japan

Abstract. The electron transmission between monolayer and bilayer graphene is theoretically studied within an effective-mass scheme. The transmission through the boundary is strongly dependent on the incident angle and the dependence is opposite between the K and K’ points, leading to valley polarization of transmitted wave.

Keywords: graphite, graphene, boundary condition, transmission, valley polarization

PACS: 73.63.-b, 72.10.-d, 73.21.Ac

Graphene consists of a two-dimensional hexagonal crystal of carbon atoms, in which electron dynamics is governed by the Dirac equation [1]. Transport properties in a monolayer graphene are quite intriguing, and the conductivity in the absence and presence of a magnetic field [2, 3], dynamical conductivity [4], and quantum corrections to the conductivity [5] were theoretically investigated prior to experiments. Bilayer graphene composed of a pair of graphene layers has a zero-gap structure with quadratic dispersion different from a linear dispersion in a monolayer graphene [6, 7]. The purpose of this paper is to study the boundary between monolayer and bilayer graphenes and show a valley polarization in transmission probability through the boundary.

In graphenes, states associated with K and K’ points, sometimes called valleys, are degenerate. In a graphene sheet with a finite width, localized edge states are formed, when the boundary is in a certain specific direction, and only a single right- and left-going wave can carry current at each of the K and K’ points [8]. A way to make valley filtering has been proposed with the explicit use of the fact [9]. Recently, edge states in bilayer graphene were studied [10].

A left half in Fig. 1 (a) shows the structure of monolayer graphene. A unit cell contains two carbon atoms denoted by A and B. We consider the coordinate system (x’,y’) fixed on the graphene and (x,y) rotated around the origin by η such that the y axis is always along the boundary of the bilayer graphene.

Electronic states in monolayer graphene are described in an effective-mass scheme. For states in the vicinity of the K point, the Schrödinger equation is given by

\[ \gamma(\hat{\sigma} \cdot \hat{k}) F^K(r) = \varepsilon F^K(r), \quad F^K(r) = \left( \begin{array}{c} F^K_A(r) \\ F^K_B(r) \end{array} \right), \]  

(1)

where \( \gamma \) is the band parameter, \( \hat{k} = (\hat{k}_x, \hat{k}_y) = -i\nabla \) is a wave vector operator, and \( \sigma_x \) and \( \sigma_y \) are the Pauli matrices [1]. Here, \( F^K_A \) and \( F^K_B \) are slowly-varying envelope functions describing amplitudes at A and B sites.

A bilayer graphene is arranged in the AB (Bernal) stacking, as shown on a right half in Fig. 1 (a). The bottom layer is denoted as 1 and the top layer denoted as 2. The unit cell contains two carbon atoms denoted by A1 and B1 in layer 1, and A2 and B2 in layer 2. For the inter-layer coupling, we include coupling \( \gamma \) between vertically neighboring atoms B1 and A2. The Schrödinger equation becomes

\[ \left( \gamma(\hat{\sigma} \cdot \hat{k}) + \frac{i}{2} \gamma \sigma_y \right) F^K(r) = \varepsilon F^K(r), \]  

(2)

with \( \sigma_\pm = \sigma_x \pm i\sigma_y \). \( F^K(r) \) is a four component vector consisting of \( F^K_A, F^K_B, F^K_{A1}, \) and \( F^K_{B2} \). For the K’ point the Schrödinger equations are obtained by replacing \( \hat{k}_y \) with \( -\hat{k}_y \) and therefore the wave functions by replacing \( k_y \) with \( -k_y \) in both monolayer and bilayer graphenes.

First, we consider a zigzag boundary ZZ1 with \( \eta = -\pi/6 \) as illustrated in Fig. 1 (a). We can derive the boundary condition for the envelope functions using their
relation to the amplitude of the wave function in a tight-binding model [1]. The results are [11]

\[ F_{A}^{0}(0, y) = F_{B}^{0}(0, y), \quad F_{B}^{0}(0, y) = 0, \quad (\nu = K, K'). \]  

(3)

These conditions do not cause mixing between the K and K' points, leading to the absence of inter-valley transmission through the boundary.

We consider transmission of electron wave injected from the K valley in the monolayer side at the Fermi level with wave vector \( (k_x, k_y) = k(\cos \theta, \sin \theta) \) in the case that electron concentration is the same in a monolayer and bilayer graphene. The transmission of electron wave through the boundary can explicitly be calculated by considering right- and left-going traveling modes in monolayer graphene and a right-going traveling mode and an evanescent mode decaying in the positive x direction in the bilayer graphene.

In the energy region close to the Dirac point \( \gamma k/\gamma_1 \to 0 \), an analytical expression can be obtained for the transmission probability \( T^K \) [11]. The transmission vanishes for \( k = 0 \) and increases in proportion to \( k \). It takes a maximum at \( \theta = \theta_0 \), with \( \theta_0 = \sin^{-1}(1/\sqrt{3}) \approx 0.196\pi \), where \( s \) denote the sign of \( \varepsilon \). For the K' point the transmission probability \( T_{K'} \) is obtained by replacing \( \theta \) with \(-\theta\). The valley polarization [9] of the transmitted wave becomes

\[ P = \frac{T_{K'} - T_{K}}{T_{K'} + T_{K'}} = s \frac{2 \sin \theta \sqrt{1 + \sin^2 \theta}}{1 + 2 \sin^2 \theta}. \]  

(4)

The valley polarization increases with the incident angle \( \theta \), up to \( P = \pm 2/3 \approx \pm 0.94 \) at \( \theta = \pm \pi/2 \).

Figure 2 shows an example of calculated transmission probability as a function of incident angle \( \theta \). The electron density is specified by \( k \) corresponding to the Fermi energy in the monolayer and the results in the low-density regime \( \gamma k/\gamma_1 \leq \sqrt{2} \) are shown. The transmission probability varies strongly as a function of the incident angle and its maximum appears at an angle deviating from the vertical direction. At the bottom of the first excited conduction band, i.e., \( k\gamma/\gamma_1 = \sqrt{2} \), it completely vanishes in the region \( \theta \leq 0 \). This is closely related to the presence of a perfectly reflecting state, which emerges only for the ZZ1 boundary [11]. This asymmetry is opposite between the K and K' points, showing that strong valley polarization, can be induced across the interface of monolayer and bilayer graphenes.

For a ZZ2 boundary depicted in Fig. 1 (b), the boundary conditions in layer 1 are the same as for ZZ1 and \( F_{A2}^{0}(0, y) = 0 \) in layer 2. Boundary conditions are derived also for the armchair boundary (\( \eta = 0 \), showing that inter-valley mixing occurs in contrast to the zigzag boundaries. The inter-valley transmission and reflection probabilities are much smaller than the intra-valley probabilities when the electron density is sufficiently small. In spite of the difference in the boundary conditions, the calculated valley polarization is similar for different boundaries, except in the high-concentration region \( \gamma k/\gamma_1 \approx \sqrt{2} \).

In conclusion, boundary conditions between monolayer and bilayer graphene have been obtained within an effective-mass scheme. The transmission probability can be quite different between K and K' states for waves incident in oblique directions, resulting in significant valley polarization of waves transmitted through the boundary. This work was supported in part by Grant-in-Aid for Scientific Research on Priority Area “Carbon Nanotube Nanoelectronics,” by Grant-in-Aid for Scientific Research, and by GCOE Program at Tokyo Tech “Nanoscience and Quantum Physics” from Ministry of Education, Culture, Sports, Science and Technology Japan.

REFERENCES