Inter-Layer Coupling Effects on Vertical Electron Transport in Multilayer Graphene Nanoribbons

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Abstract. We have performed nonequilibrium Green function simulations on the vertical transport characteristics in multilayer graphene nanoribbons sandwiched between two graphene contact layers with varying the inter-layer coupling strength $\beta$. We find that the integrated transmission function thorough the top (or bottom) layer is hardly affected by $\beta$ when the incident energy is close to the Dirac point. The $\beta$-insensitive energy window becomes narrower as the channel length increases.

1. Introduction
Graphene exhibits ultrahigh carrier mobility owing to the massless Dirac fermions and is expected to be used as a channel material of transistors [1–4]. In the transistor application, a multilayer graphene is more favorable for enhancing the magnitude of the ON current. However, a strong inter-layer coupling loses the linear band dispersion [5] and may cause a reduction of the carrier mobility. Recently, multilayer graphene with a turbostratic structure have been grown experimentally [6]. The transport properties are reported to be improved by the weak inter-layer coupling of the turbostratic structure. The mechanism of the improvement is, however, not well understood yet. Here we calculate vertical transport characteristics in multilayer graphene nanoribbons (GNRs) sandwiched between two graphene contact layers using the nonequilibrium Green function (NEGF) method with varying the inter-layer coupling strength $\beta$.

2. Calculation Method
We consider a device model whose schematic diagram is given in Fig. 1. The channel consists of AB-stacked $N$-layer GNRs structure of length $L$ along the $x$-direction and of infinite length along the $y$-direction. We assign an index $l$ for each layer ($l = 1, 2, \ldots, N$). Each layer is coupled to the neighboring layers with the inter-layer transfer integral $\beta$, which can be different from the intra-layer transfer integral $t_{\perp}$ of graphite. Semi-infinite graphene electrodes are connected to the bottom ($l = 1$) and top ($l = N$) GNR layers. Therefore, the set-up clearly comprises one or more GNRs sandwiched between two graphene contact layers.

We use the NEGF formalism [7–9] combined with a nearest-neighbor tight-binding approximation to calculate integrated transmission functions $\tau_{\text{TL}}(E)$ from the top-right electrode to the top-left electrode, $\tau_{\text{BL}}(E)$ to the bottom-left electrode, and $\tau_{\text{BR}}(E)$ to the bottom-right electrode under the ballistic condition (no scattering). Along the $y$-direction, we apply the periodic boundary condition and use the eigenstate representation labeled by $k_y$. For a channel
Figure 1. (a) Device model for the NEGF simulation. AB-stacked N-layer GNRs structure of length $L$ is connected to semi-infinite graphene electrodes at the both ends of the bottom and top layers. We assign an index $l$ for each layer ($l = 1, 2, \ldots, N$). Each layer is coupled to the neighboring layers with the inter-layer transfer integral $\beta$. (b) Top view of the multilayer GNR structure. The thick black rectangles define the unit cells. We assign an index $j$ for each unit cell ($j = 1, 2, \ldots, M$). These figures illustrate the case for $N = 3$ and $M = 3$ consisting of $M$ unit cells of the channel length $L = M \times \sqrt{3}a$ ($a$ is the lattice constant), the total device Hamiltonian matrix, whose size is $(4MN) \times (4MN)$, can be written as

$$\hat{H}_{\text{dev}} = \begin{bmatrix} H_1 & S \\ S^\dagger & H_2 & S \\ & \ddots & \ddots \\ & & & \ddots & S^\dagger \\ & & & & H_M \end{bmatrix}. \quad (1)$$

Here $H_j$ is the Hamiltonian matrix of the size $(4N) \times (4N)$ of an isolated unit cell $j$, and $S$ represents the transfer between the neighboring unit cells. $H_j$ and $S$ can be written as

$$H_j = \begin{bmatrix} h_1 & s_{12} \\ s_{12} & h_2 & s_{23} \\ & \ddots & \ddots \\ & & & s_{N-1,N} & h_N \end{bmatrix}, \quad S = \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_N \end{bmatrix}. \quad (2)$$

Here $h_l$ is the Hamiltonian matrix of the size $4 \times 4$ for the 4 atoms of the $l$-th layer in the $j$-th unit cell, and $s_{ll'}$ represents the inter-layer transfer between the layers $l$ and $l'$ in the $j$-th unit cell. $s_l$ describes the transfer between the neighboring unit cells in the layer $l$.

The effects of the electrodes are accounted for by self-energy matrices; $\hat{\Sigma}_{\text{TR}}(E)$ is the self-energy matrix of the size $(4MN) \times (4MN)$ for the top-right, $\hat{\Sigma}_{\text{TL}}(E)$ the top-left, $\hat{\Sigma}_{\text{BR}}(E)$ the bottom-right, and $\hat{\Sigma}_{\text{BL}}(E)$ the bottom-left electrode. They are given by

$$\hat{\Sigma}_{\text{pR}}(E) = \begin{bmatrix} 0 \\ & \ddots \\ & & 0 \\ & & & \Sigma_{\text{pR}}(E) \end{bmatrix}, \quad \hat{\Sigma}_{\text{pL}}(E) = \begin{bmatrix} \Sigma_{\text{pL}}(E) \\ 0 \\ & \ddots \\ & & 0 \end{bmatrix}, \quad (p = T, B), \quad (3)$$

where $\Sigma_{\text{pR}}(E)$ and $\Sigma_{\text{pL}}(E)$, whose sizes are $(4N) \times (4N)$, are given by

$$\Sigma_{\text{Tq}}(E) = \begin{bmatrix} 0 \\ & \ddots \\ & & 0 \\ & & & \sigma_{\text{Tq}}(E) \end{bmatrix}, \quad \Sigma_{\text{Bq}}(E) = \begin{bmatrix} \sigma_{\text{Bq}}(E) \\ 0 \\ & \ddots \\ & & 0 \end{bmatrix}, \quad (q = R, L). \quad (4)$$
Here $\sigma_{TR}(E)$ is the self-energy matrix of the size $4 \times 4$ for the top-right, $\sigma_{TL}(E)$ the top-left, $\sigma_{BR}(E)$ the bottom-right, and $\sigma_{BL}(E)$ the bottom-left electrode. These self-energies are calculated using the method of Ref. 10.

In the ballistic limit, the integrated transmission functions from the top-right electrode can be written as

$$\tau_m(E) = \frac{1}{2\pi} \int \text{trace}[\Gamma_m(E)G(E)\Gamma_{TR}(E)G^\dagger(E)]dk_y, \ (m = TL, BR, BL). \quad (5)$$

with $G(E) = [E - \hat{H}_{dev} - \hat{\Sigma}_{TR}(E) - \hat{\Sigma}_{TL}(E) - \hat{\Sigma}_{BR}(E) - \hat{\Sigma}_{BL}(E)]^{-1}, \ \Gamma_m(E) = i[\hat{\Sigma}_m(E) - \hat{\Sigma}_m^\dagger(E)]$ ($m = TR, TL, BR, BL$). We adopt the recursive Green function algorithm [11] for calculating the Green function $G(E)$.

To investigate the inter-layer coupling effects on the vertical transport characteristics, we calculate the integrated transmission functions with varying the inter-layer transfer integral, $\beta$, from 0 to $t_\perp$ ($= 0.39 \text{ eV}$) of graphite [3].

3. Results and Discussion

Figure 2 shows $\tau_{TL}(E)$ and $\tau_{BL}(E)$ of a multilayer GNR with $N = 3$ and $L = 10 \text{ nm}$ for $\beta = 0, 0.05, 0.1,$ and $0.3 \text{ eV}$. $\tau_{BR}(E)$ (not shown in Fig. 2) exhibits similar behavior to $\tau_{BL}(E)$. $\tau_{TL}(E)$ for a monolayer graphene ($\beta = 0$) have a linear relation near the Dirac point as shown by dashed lines in Fig. 2. As $\beta$ increases $\tau_{TL}(E)$ decreases except for an energy region close to the Dirac point, where $\tau_{TL}(E)$ are found to be hardly affected by $\beta$. This is because the GNR layers sandwiched between the bottom and top graphene layers open a bandgap, which prevents vertical electrons’ flow between the top and bottom layers near the Dirac point. Figure 3 shows $\tau_{TL}(E)$ of a multilayer GNR with $L = 10 \text{ nm}$ and $\beta = 0.05 \text{ eV}$ for $N = 2, 3, 4,$ and $5$. We see the $\beta$-insensitive energy window near the Dirac point regardless of $N$ except for $N = 2$ where $\beta$ affects the transmission even close to the Dirac point. This is due to the absence of nanoribbon layers for $N = 2$.

Figure 4 shows $\tau_{TL}(E)$ of a multilayer GNR with $N = 3$ and $\beta = 0.05 \text{ eV}$ for $L = 10, 15,$ and $20 \text{ nm}$. We find that the $\beta$-insensitive energy window becomes narrower as the channel length, $L$, increases. We introduce the critical inter-layer coupling, $\beta_c$, which is defined by $\beta$ for which $\tau_{TL}(k_B T) (T = 300 \text{ K})$ becomes 95% of that for $\beta = 0$ (see dotted line in Fig. 4). Figure 5 shows

![Figure 2](image1.png)

**Figure 2.** $\tau_{TL}(E)$ and $\tau_{BL}(E)$ for $\beta = 0, 0.05, 0.1,$ and $0.3 \text{ eV}$. Red dash straight lines are $\tau_{TL}(E)$ for a monolayer graphene.

![Figure 3](image2.png)

**Figure 3.** $\tau_{TL}(E)$ for $N = 2, 3, 4,$ and $5$. Red dash straight lines are $\tau_{TL}(E)$ for a monolayer graphene.
Figure 4. $\tau_{TL}(E)$ of $L = 10, 15, \text{ and } 20\ \text{nm}$ for $\beta = 0.05\ \text{eV}$. Red dashed lines show $\tau_{TL}(E)$ for a monolayer graphene. Blue dotted line represents the thermal energy at 300K.

Figure 5. Channel length, $L$, dependence of critical inter-layer coupling strength $\beta_c$. Red arrow indicates $\beta = t_{\perp}$ of graphite.

channel length, $L$, dependence of $\beta_c$. For a smaller $\beta$, the channel length can be increased while keeping the $\beta$-insensitive energy window.

4. Conclusion
We have calculated vertical transport characteristics in multilayer GNRs sandwiched between two graphene contact layers by using NEGF method combined with a tight-binding approximation with varying the inter-layer coupling strength $\beta$. We find that the integrated transmission function thorough the top (or bottom) layer of the multilayer GNR is hardly affected by the inter-layer coupling strength when the incident energy is close to the Dirac point. The $\beta$-insensitive energy window becomes narrower as the channel length increases.

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