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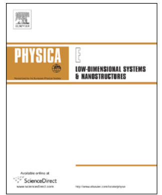

Low-field carrier transport properties in biased bilayer graphene

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ABSTRACT

Based on a semiclassical Boltzmann transport equation in random phase approximation, we develop a theoretical model to understand low-field carrier transport in biased bilayer graphene, which takes into account the charged impurity scattering, acoustic phonon scattering, and surface polar phonon scattering as three main scattering mechanisms. The surface polar optical phonon scattering of carriers in supported bilayer graphene is thoroughly studied using the Rode iteration method. By considering the metal–BLG contact resistance as the only one free fitting parameter, we find that the carrier density dependence of the calculated total conductivity agrees well with that observed in experiment under different temperatures. The conductivity results also suggest that in high carrier density range, the metal–BLG contact resistance can be a significant factor in determining the BLG conductivity at low temperature, and both acoustic phonon scattering and surface polar phonon scattering play important roles at higher temperature, especially for BLG samples with a low doping concentration, which can compete with charged impurity scattering.

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1. Introduction

Bilayer graphene (BLG) has attracted tremendous attention in the last few years due to its tunable band gap [1–4]. Currently, one of the central issues in BLG research is to develop strategies for improving carrier mobility, therefore it is crucial to understand the distinct scattering mechanisms in biased bilayer graphene from a scientific point of view and for achieving practical applications.

Different experiments and theories in the low-field regime have revealed that carrier transport in graphene can be significantly influenced by many factors including Coulomb scattering [5,6], short-range (defect) scattering [7], in-plane acoustic phonon scattering [8], substrate surface polar phonon scattering [9–11], and contact resistance [12,13]. However, the origin of short-range scattering in exfoliated graphene supported on SiO_2 remains controversial. Similar to monolayer graphene, Coulomb scattering and short-range scattering in doped and biased BLG supported on SiO_2 are commonly considered as the dominant scattering mechanisms to explain the experimental data observed by different groups [14,15], but much less is known about the effect of distinct phonon scattering on low-field carrier conductivity. Moreover, recent experimental studies have revealed that the measured conductivity of relatively high doped BLG [16] or dual-gated BLG [17] shows an anomalous increase with decreasing temperature in all carrier density regime, which is different from that observed in previous study [14]. On the other hand, the metal–BLG Schottky barrier height considered to estimate the on/off ratio in gapped BLG [18], which leads to the contact resistance, also increases as the temperature decreases, suggesting that the contact resistance should have a significant contribution in determining the BLG conductivity. Despite the extensive research efforts already made, a comprehensive understanding of low-field carrier transport properties in biased BLG is still lacking and theoretical study on this issue is in urgent need.

In this work, we have developed a detailed microscopic transport theory for doped and biased BLG at finite temperature by taking into account the charged impurity scattering, acoustic phonon scattering, and surface polar phonon scattering as three main scattering mechanisms. In addition, both voltage gate and charged impurity induced perpendicular electric field and the metal–BLG contact resistance have been included in the conductivity model.

2. Theoretical model

We consider a doped and biased Bernal-stacking BLG transistor supported on the SiO_2 substrate, as depicted in Fig. 1. The effective low-energy two-band Hamiltonian can be well approximated

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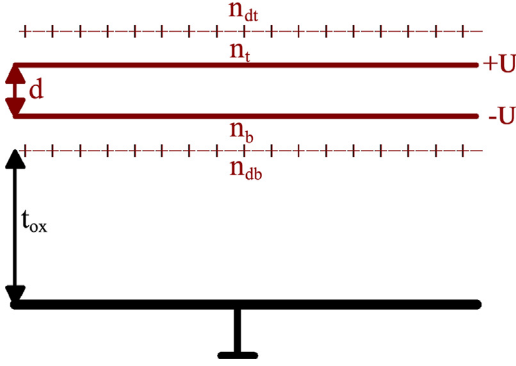

Fig. 1. Schematic of the AB-stacked BLG on SiO_2. Cross section shows compensated charged impurity n_{dt} (n_{db}) on the top (bottom) layer of the BLG.

around the K point of the Brillouin zone [19]

$$H=\begin{pmatrix} U & \hbar^2(\hat{k}_x+i\hat{k}_y)^2/2m^* \\ \hbar^2(\hat{k}_x-i\hat{k}_y)^2/2m^* & -U \end{pmatrix} \tag{1}$$

where $\hat{\mathbf{k}}=(\hat{k}_x,\hat{k}_y)$ is a wave vector operator, the effective mass $m^*=\gamma/(2v_F^2)$, with γ=0.39 eV, and U is the interlayer asymmetry tunable by the perpendicular electric field. The wave functions of Eq. (1) can be written as

$$\Psi_{s\mathbf{k}}(\mathbf{r})=\frac{1}{L}F_{s\mathbf{k}}\exp(i\mathbf{k}\cdot\mathbf{r}) \tag{2}$$

with

$$F_{s\mathbf{k}}=\begin{cases}\begin{pmatrix}\cos(\alpha_{\mathbf{k}}/2)\\ -\sin(\alpha_{\mathbf{k}}/2)\exp(2i\theta_{\mathbf{k}})\end{pmatrix} & \text{if } s=1;\\ \begin{pmatrix}\sin(\alpha_{\mathbf{k}}/2)\\ \cos(\alpha_{\mathbf{k}}/2)\exp(2i\theta_{\mathbf{k}})\end{pmatrix} & \text{if } s=-1;\end{cases} \tag{3}$$

where L^2 is the area of the system, $\theta_{\mathbf{k}}=\arctan(k_y/k_x)$ is the polar angle of the wave vector $\mathbf{k}$, $\tan\alpha_k=\hbar^2k^2/(2m^*U)$ and $s=\pm1$ corresponds to the conduction and valence band, respectively. The corresponding energy dispersion $\varepsilon_{s,\mathbf{k}}=s\sqrt{(\hbar^2\mathbf{k}^2/(2m^*))^2+U^2}$, its finite band gap is $2|U|$, and density of state (DOS) per unit energy is $D(\varepsilon)=m^*g/(4\pi\hbar^2\sqrt{\varepsilon^2-U^2})$, where $g=g_sg_v$ is the total degeneracy ($g_s=2$, $g_v=2$ being the spin and valley degeneracy).

To illustrate the disorder-induced spatial charge inhomogeneity of BLG, we assume that the puddle surface potential V ranging from $-\Delta$ to Δ can be described approximately by an uniform distribution function, and an equivalent equilibrium distribution function can be obtained by

$$f_0(\varepsilon)=\frac{1}{2\Delta}\int_{-\Delta}^{\Delta}\frac{1}{\exp[\beta(\varepsilon-\mu-V)]+1}dV =\frac{1}{2\beta\Delta}\ln\left\{\frac{1+\exp[\beta(\Delta-\varepsilon+\mu)]}{1+\exp[-\beta(\Delta+\varepsilon-\mu)]}\right\} \tag{4}$$

where μ is the average Fermi level, and $\beta=1/kT$. Note that when $\Delta=0$, $f_0(\varepsilon)$ in Eq. (4) reduces to Fermi distribution function $f_0(\varepsilon)=\{1+\exp[\beta(\varepsilon-\mu)]\}^{-1}$.

According to the Gauss Law, the net carrier densities ($n_{t,b}$) on the layers and the interlayer asymmetry (U) depend on the external gate voltage (V_g) and charged impurity densities, which can be obtained by

$$n_t+n_b=C_{ox}/eV_{g0}$$
$$2U=e^2d/\varepsilon_0(n_t-n_{dt}) \tag{5}$$

where $n_t=n_t^e-n_t^h(n_b=n_b^e-n_b^h)$ is the net carrier density of the top (bottom) layer, C_{ox} is the gate capacitance per unit area, n_{dt} is the compensated charged impurity density of the top layer, and $V_{g0}=V_g-V_{NP}$ is the compensated gate voltage, with V_{NP} being the corresponding gate voltage of minimum conductivity. By considering the dominant Hartree term of the interaction but neglect exchange and correlation energies, the electron and hole densities $n_{t,b}^e, n_{t,b}^h$ on the individual layer are given by, respectively [20,21]

$$n_{t,b}^h=\frac{m^*g}{4\pi\hbar^2}\int_{-\infty}^{-|U|}\sqrt{\frac{\varepsilon\pm U}{\varepsilon\mp U}}(1-f_0(\varepsilon))\,d\varepsilon$$
$$n_{t,b}^e=n_{t,b}^c+n_{t,b}^v \tag{6}$$

with

$$n_{t,b}^c=\frac{m^*g}{4\pi\hbar^2}\int_{|U|}^{+\infty}\sqrt{\frac{\varepsilon\pm U}{\varepsilon\mp U}}f_0(\varepsilon)\,d\varepsilon$$
$$n_{t,b}^v=\mp\frac{m^*gU}{4\pi\hbar^2}\ln\frac{2\gamma_1}{|U|} \tag{7}$$

where the plus (minus) sign corresponds to the top (bottom) layer, $n_{t,b}^c$ and $n_{t,b}^v$ are the conduction and filled valence band electron density on the individual layers, respectively. Once a compensated gate voltage (V_{g0}) or net carrier density (n) is given, U and μ can be obtained by the solution of Eqs. (5)–(7) self-consistently, which will be used to calculate the carrier conductivity of doped and biased BLG in the following part.

In our Boltzmann theory, we consider three distinct scattering mechanisms that can be significant factors in determining the BLG conductivity, namely the charged impurity, substrate surface polar phonon, and in-plane acoustic phonon scattering processes. Given that the substrate surface polar phonon scattering is inelastic, the relaxation time approximation cannot be used since it is impossible to define a simple relaxation time that does not depend on the distribution function. For such cases, the actual distribution function under low-field condition can be derived by the Rode iterative method [22]. If we use the Legendre expansion for the distribution function and only keep terms that are linear in the field, we have

$$f(\mathbf{k})=f_0(\mathbf{k})+g(\mathbf{k})\cos\theta \tag{8}$$

where θ is the angle between the $\mathbf{k}$ vector and the applied electric field $\mathbf{F}$, $f_0(\mathbf{k})$ is the equilibrium distribution function, and $g(\mathbf{k})$ is a function of the $\mathbf{k}$ vector, which can be obtained by

$$g(\mathbf{k})=\frac{I_1(\mathbf{k})+eFv_{\mathbf{k}}\frac{\partial f_{\mathbf{k}}^0}{\partial\varepsilon}}{\frac{1}{\tau_m^{el}(\mathbf{k})}+I_0(\mathbf{k})} \tag{9}$$

with

$$I_1(\mathbf{k})=\sum_{\mathbf{k}'}g(\mathbf{k}')\cos\theta[S_{\mathbf{k}',\mathbf{k}}^{in}(1-f_{\mathbf{k}}^0)+S_{\mathbf{k},\mathbf{k}'}^{in}f_{\mathbf{k}}^0]$$
$$I_0(\mathbf{k})=\sum_{\mathbf{k}'}S_{\mathbf{k}',\mathbf{k}}^{in}f_{\mathbf{k}'}^0+S_{\mathbf{k},\mathbf{k}'}^{in}(1-f_{\mathbf{k}'}^0) \tag{10}$$

where $\tau_m^{el}(\mathbf{k})$ or $\tau_m^{el}(\varepsilon)$ is the energy-dependent momentum relaxation time in the elastic scattering processes, and $S_{\mathbf{k},\mathbf{k}'}^{in}$ is the scattering rate from the state $\mathbf{k}$ to the state $\mathbf{k}'$ in the inelastic scattering processes. They are derived by the Fermis golden rule, respectively

$$\frac{1}{\tau_m^{el}(\varepsilon)}=\frac{2\pi}{\hbar}\sum_{\mathbf{k}'}|M^{el}(\mathbf{k},\mathbf{k}')|^2(1-\cos\theta_{\mathbf{k}\mathbf{k}'})\delta(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}) \tag{11}$$

and

$$S_{\mathbf{k},\mathbf{k}'}^{in}=\frac{2\pi}{\hbar}|M^{in}(\mathbf{k},\mathbf{k}')|^2\delta(\varepsilon_{\mathbf{k}'}-\varepsilon_{\mathbf{k}}\pm\hbar\omega) \tag{12}$$

where $\theta_{\mathbf{k}\mathbf{k}'}$ is the scattering angle between the scattering in and out wave vectors $\mathbf{k}$ and $\mathbf{k}'$, $M^{el}(\mathbf{k},\mathbf{k}')$ and $M^{in}(\mathbf{k},\mathbf{k}')$ is the matrix

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