Modeling of Temperature and Field-Dependent Electron Mobility in a Single-Layer Graphene Sheet

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***Abstract*— In this paper, we address a physics-based analytical model of electric-field-dependent electron mobility (μ) in a single-layer graphene sheet using the formulation of Landauer and Mc Kelvey's carrier flux approach under finite temperature and quasi-ballistic regime. The energy-dependent, near-elastic scattering rate of in-plane and out-of-plane (flexural) phonons with the electrons are considered to estimate μ over a wide range of temperature. We also demonstrate the variation of μ with carrier concentration as well as the longitudinal electric field. We find that at high electric field ($>10^6$ $\mathrm{Vm^{-1}}$), the mobility falls sharply, exhibiting the scattering between the electrons and flexural phonons. We also note here that under quasi-ballistic transport, the mobility tends to a constant value at low temperature, rather than in between T^{-2} and T^{-1} in strongly diffusive regime. Our analytical results agree well with the available experimental data, while the methodologies are put forward to estimate the other carrier-transmission-dependent transport properties.**

***Index Terms*— Flexural phonons, graphene, mobility.**

I. Introduction

GRAPHENE exhibits remarkable room temperature (RT) mobility of the order of 20 000–200 000 $\mathrm{cm^2V^{-1}s^{-1}}$, which is explained through several theoretical and simulative works [1]–[5]. Initially, it is reported that the mobility in single-layer graphene (SLG) sheet is mainly dominated by the in-plane phonon and electron interactions [2]. However, from recent reports, it appears that the involvement of out-of-plane (known as flexural) phonons also play a substantial role in determining the magnitude and variation of μ with temperature, in case the sheet relaxes between the contacts at the two ends [6]. The motivation of this paper lies in the demonstration of the flexural phonon dominated μ under the application of a longitudinal static electric field. This is extremely useful in performance analysis of graphene-based devices and interconnects, where self-consistency in electric field is mostly required [7].

In this paper, we develop Landauer's field-dependent transmission coefficient under quasi-ballistic regime at isothermal condition to derive the electron mobility in an SLG sheet. This is evaluated through the derivation of average electron energy, number of transmission channels, backscattering mean free path λ and carrier flux in the presence of a constant longitudinal electric field ε directed from the right-to-left contact. Apart from the determination of μ, the proposed model is also used to analyze the electrical conductivity and the current–voltage characteristics in an SLG-based field-effect transistor when the longitudinal electric field surpasses the transverse electric field.

II. Model Development

In the absence of any external perturbation, the Dirac-cone-type energy band structure in SLG sheet is written as

$$E = \hbar v_F k \tag{1}$$

where $\bar{h}$, v_F ($= 10^6$ $\mathrm{ms^{-1}}$), and k are the reduced Planck's constant, Fermi velocity, and electron wave vector, respectively. Using this and the 2-D density-of-states

$$N_{2D}(E) = \frac{2}{\pi}\frac{E}{(\hbar v_F)^2} \tag{2}$$

the average electron energy can be written as

$$\langle E_{2D}\rangle = 2k_BT\left[\frac{F_2(\eta)}{F_1(\eta)}\right] \tag{3}$$

where k_B is the Boltzmann's constant, T the temperature, $F_j(\eta)$ the Fermi-Dirac integral of order j, $\eta = E_F/k_BT$, and E_F is the Fermi energy with respect to the conduction band minimum which can be written as $E_F = \hbar v_F\sqrt{n_{2D}\pi}$ in which n_{2D} is the 2-D electron density.

Because of the distribution of carrier velocity along both the longitudinal as well as lateral direction of the sheet, we consider the net average electron velocity along $+x$ direction, which is

$$\langle v_{x_+}\rangle = v_F\frac{\int_{-\pi/2}^{+\pi/2} cos\theta d\theta}{\pi} = \frac{2}{\pi}v_F \tag{4}$$

in which θ is the back-scattering angle measured from $+x$ to $-x$ direction. This gives the number of channels as $M(E) = 2WE/\pi\hbar v_F$, where W is the width of the sheet.

In the presence of a constant electric field (ε) along $-x$ direction, the electron gains energy by an amount $q\varepsilon x$ in

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addition to $\langle E_{2D}\rangle$. Hence in such a case, the 2-D isotropic backscattering mean free path is written as

$$\lambda_{2D}(x) = \frac{\pi}{2} v_F \left[\frac{\langle E_{2D}\rangle + q\varepsilon x}{D + C\left(\langle E_{2D}\rangle + q\varepsilon x\right)^2}\right] \tag{5}$$

where the quasi-elastic electron–phonon (e–p) scattering rate is given by

$$\frac{1}{\tau_{e-p}} = \frac{1}{\tau_{\text{in-plane}}} + \frac{1}{\tau_{\text{flex}}} \tag{6}$$

in which

$$\frac{1}{\tau_{\text{in-plane}}} = C\langle E_{2D}\rangle \tag{7}$$

and

$$\frac{1}{\tau_{\text{flex}}} = \frac{D}{\langle E_{2D}\rangle} \tag{8}$$

are the in-plane and flexural phonon scattering rates with the electrons respectively [8] where,

$$C = \left[\frac{g^2}{2v_L^2} + \frac{\hbar^2 v_F^2 \beta^2}{4a^2}\left(\frac{1}{v_L^2} + \frac{1}{v_T^2}\right)\right]\frac{k_B T}{2\rho\hbar^3 v_F^2} \tag{9}$$

and

$$D = \left(\frac{g^2}{2} + \frac{\hbar^2 v_F^2 \beta^2}{4a^2}\right)\frac{(k_B T)^2}{64\pi\hbar\varsigma^2}\ln\left(\frac{k_B T}{\hbar\omega_c}\right) \tag{10}$$

in which a, the distance between the nearest carbon atoms is 0.14 nm, the mass density being $\rho = 7.6\times10^{-6}$ kgm^{-2}. Using the membrane physics [9], the longitudinal and transverse sound velocity for SLG sheet can be written as $v_L = \sqrt{\frac{\bar{\lambda}+2\bar{\mu}}{\rho}} = 2.1\times10^4$ ms^{-1} and $v_T = \sqrt{\frac{\bar{\mu}}{\rho}} = 2.1\times10^4$ ms^{-1}, in which $\bar{\lambda}$ and $\bar{\mu}$ are the Lame coefficients with $\bar{\mu} \sim 3\bar{\lambda} \sim 9$ eVÅ^{-2} for SLG [8], [10]–[12]. The bending rigidity being $\varsigma = 1$ eV, which gives the flexural phonon diffusivity as $\alpha = \sqrt{\frac{\varsigma}{\rho}} = 4.6\times10^{-7}$ m^{2}s^{-1} [8]. The parameter g is the screened electron–phonon coupling parameter g. However, it should be noted that the unscreened deformation potential (g_0) is theoretically evaluated to be around 10–30 eV [2], which is also in the range of experimental reach [13]. Particularly, this g_0 is used for lightly doped graphene sheet. For doped system, it should be the Thomas–Fermi screening deformation potential [14]. Now following [8], the Fermi energy weighted screened scalar deformation potential is written as $g(k_F) = g_0/\epsilon(k_F)$ in which $g_0 \sim 25$ eV and $\epsilon(k_F)$ is the band structure-dependent Thomas–Fermi dielectric function at the Fermi level, which is written as $\epsilon(k_F) = 1 + q^2 N_{2D}(k_F)/2\epsilon_0 k_F$. This gives $g(k_F) \sim 3$ eV. The cutoff ZA phonon wave vector q_c which defines the bending rigidity in graphene membrane is evaluated from the height–height correlation function at the condition when this function changes its behavior from harmonic to nonharmonic. Using the self-consistent screening approximation, this is found to be 0.1 Å^{-1} [15]. This set the harmonic cut-off frequency $\omega_c = \alpha q_c^2 = 0.46$ THz. This can be compared with the upper limit of the ZA phonon branch cut-off frequency from the dispersion relation [16], [17].

With the determination of relaxation rates and backscattering mean free path, the carrier transmission factor is evaluated from Mc Kelvey's 1-D directed flux theory [18]. The main assumptions behind this theoretical development are as follows.

1) The system is assumed to be under near equilibrium so that the transmission factor $\top_{+-}(E) = \top_{-+}(E) = \top(E)$, where the symbols + and − represents the left and right contacts.
2) The contact − is a perfectly absorbing contact, so that there is no carrier from contact − that comes in.
3) Average velocity of the right and left moving carriers are the same.
4) There is no carrier recombination or generation.
5) Vertical transmission is neglected.

Using the current continuity and the boundary conditions

$$\left[n_{2D}^+(x) - n_{2D}^-(x)\right]\langle v_x\rangle = \left[n_{2D}^+(0) - n_{2D}^-(0)\right]\langle v_0\rangle \tag{11}$$

and

$$n_{2D}^+(L)\langle v_{L_+}\rangle = \left[n_{2D}^+(0) - n_{2D}^-(0)\right]\langle v_0\rangle \tag{12}$$

respectively, the Landauer's transmission coefficient $\top(\langle E_{2D}\rangle)$ can be evaluated as

$$\top(\langle E_{2D}\rangle) = 1 - \frac{n_{2D}^-(0)}{n_{2D}^+(0)} = \frac{1}{1+\phi} \tag{13}$$

in which $n_{2D}^{\pm}(x)$ is the electron density along the $+x$ and $-x$ directions respectively and

$$\phi = \frac{2}{\pi v_F}\left\{\frac{D}{q\varepsilon} ln\left(1 + \frac{L}{L_{kT}}\right) + C\langle E_{2D}\rangle L\left(1 + \frac{L}{2L_{kT}}\right)\right\} \tag{14}$$

where $L_{kT} = \langle E_{2D}\rangle/q\varepsilon$, which is generally denoted as the distance to which the potential drops to a value $k_B T/q$ of its maximum at the source terminal [18]. For the present case, this value lies between $2k_B T/q\varepsilon \le L_{kT} \le 2E_F/3q\varepsilon$. Evidently in the low field limit, $L/L_{kT} \to 0$ which implies that $\phi \to 2/\pi v_F\left[\frac{D}{\langle E_{2D}\rangle} + C\langle E_{2D}\rangle\right]L$ and thus, $\top(\langle E_{2D}\rangle) \to \lambda_{2D}/\lambda_{2D} + L$ where $\lambda_{2D} = \pi/2v_F\tau(\langle E_{2D}\rangle)$. Thus, we see from (13) that the transmission is dependent on the band structure of the channel provided the backscattering mean free path length is energy-dependent via the scattering rates. The situation changes when the rates are energy-independent and no applied bias is involved. Using these aforementioned relations, the 2-D SLG field-dependent mobility can be expressed as

$$\mu = \frac{2q}{h}\frac{\top(\langle E_{2D}\rangle) M(E_F)}{n_{2D}}. \tag{15}$$

III. Results and Discussion

Using (1) and assuming a high n-type carrier degeneracy, the sheet mobility under uniform temperature distribution and longitudinal electric field is evaluated analytically from (15). We have taken the sheet dimensions to be $L = 1.2$ μm and $W = 2$ μm to compare our analytical model with the reported experimental results [8]. The variation of μ with T is exhibited in Fig. 1 for a sheet electron concentration of $n_{2D} = 10^{13}$ m^{-2}, which indicates that μ decreases with the increase in temperature >10 K from a value of ∼350 to 7 m^{2}V^{-1}s^{-1} at low

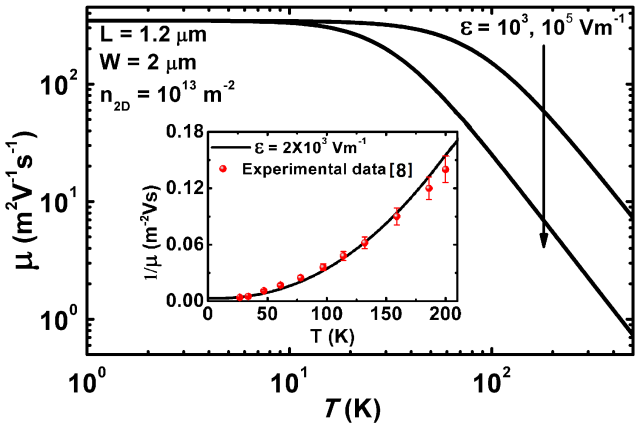

Fig. 1. μ as a function of temperature at different ε. The inset exhibits our analytical results at 10^3 Vm^{-1} compared to the experimental data [8].

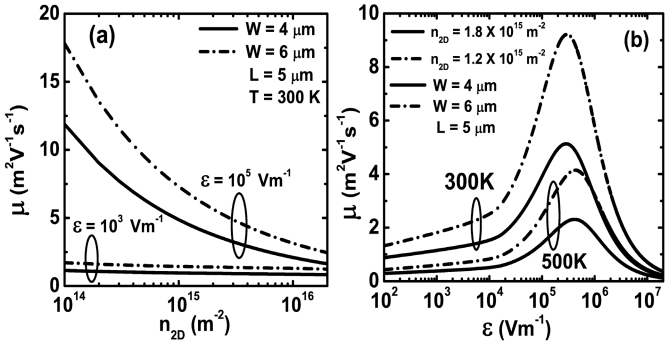

Fig. 2. (a) μ as a function of n_{2D} with varying ε at RT. (b) μ as a function of ε at different temperature.

electric field limit ($\varepsilon < 10^5$ Vm^{-1}). Also, we see that as the field magnitude increases from 10^3 to 10^5 Vm^{-1}, μ starts decreasing and converges to its saturation value at 0 Vm^{-1}.

It can be seen that under such conditions, a change in two decades of ε changes μ by almost one decade beyond RT. It also appears that μ at low temperature becomes almost constant because of vanishing electron interaction with the in-plane and flexural phonons, which makes $\phi \to 0$. The symbols in the inset shown the experimental results [8] of inverse μ as a function of T obtained by using back-gate electrostatic method. Although Castro *et al.* [8] did not particularly mention the value of the transverse field from their gate electrostatics, it has been noted that the application of transverse electric field changes the Fermi-level of graphene which under a known value of gate capacitance allows the estimation of Fermi energy, thus μ by varying the system cryostat temperature. In Fig. 1, we demonstrate an alternate mechanism to achieve the same variation of μ at a longitudinal electric field of 10^3 Vm^{-1} (which corresponds to 1.2 mV) by deriving an energy and field-dependent carrier flux relation.

At this point, it should be noted that the mobility model as presented in this paper is valid for the temperature range higher than the Bloch–Gruneisen range (T_{BG}) for both the electron interaction with in-plane and flexural phonons. Particularly, T_{BG} for SLG is calculated to $57\sqrt{n_{2D}}$ K, $38\sqrt{n_{2D}}$ K, and $0.1n_{2D}$ K for electron interaction with the longitudinal, transverse, and flexural phonons, respectively, in which n_{2D} is in the order of 10^{16} m^{-2} [2, 8, 13]. Because the degree of carrier degeneracy involved in our model ranges from 10^{13}–10^{15} m^{-2}, T is always higher than T_{BG}, and thus our model remains valid for $T \gg T_{BG}$. However, if one increases the carrier degeneracy, T_{BG} increases and the crossover conditions of the mobility due to flexural and in-plane parts need to be reformulated [19]. Furthermore, the present model of mobility is determined for quasi-ballistic carrier transport ($\lambda \sim L$). Equation (13) with the allied definitions represents the transmission factor at $\lambda \sim L$ in the presence of an external electric field to estimate the mobility due to both the relaxation rates. This quasi-ballistic condition is the main reason for the resultant mobility tends to a constant value as the temperature decreased instead of the reported T^{-1} for strongly diffusive regime [19]. In such a case, $\lambda \gg L$ and, hence, one achieves back the relevant resistivity/mobility formulation from the linearized Boltzmann's solution as shown in details elsewhere [8].

Fig. 2(a) and (b) exhibits the variation of μ as a function of n_{2D} and ε, respectively, at different sheet dimensions and temperatures. For different values of n_{2D}, there is no much difference in μ but the rate of change of μ depends on the transmission coefficient dominated through the carrier Fermi energy.

It appears from Fig. 2(b) that μ rises and falls sharply at low temperatures $> \varepsilon = 10^4$ Vm^{-1} for a sheet dimension of 5×4 and 5×6 $\mu\mathrm{m}^2$. At carrier concentration of 1.8×10^{15} m^{-2}, average energy of the electron depends on the Fermi energy which increases the electron and in-plane phonon scattering rate, and, hence, reduces μ than that of the case when $n_{2D} = 1.2 \times 10^{15}$ m^{-2}. Higher field [as shown in Fig. 2(b)], exhibits the case when the infrared flexural phonon dominates and controls the decay.

Finally, we emphasize that the mobility limiting mechanisms in SLG sheet comes from various other defects. For example, if the surface is not ultraflat, electron–hole puddle densities emerge [20] which degrade the mobility. It is also found that the effect of unscreened acoustic phonon scattering limits the SLG mobility to vary as $T^{-1} > 100$ K [2]. For smaller dimensions, the effect of edge roughness scattering is found to dominate. However, this paper estimates the effect of electrons and flexural/in-plane phonon interactions to estimate the mobility.

IV. Conclusion

We presented a temperature and electric-field-dependent electron mobility in SLG sheet in the presence of both the in-plane and flexural phonon–electron interactions for the estimation of electron mobilities over a wide range of temperature. The variation of μ with carrier concentration as well as longitudinal electric field was demonstrated and found that at high electric field, the mobility fell sharply due to the scattering between the electrons, and flexural phonons. Using carrier flux method, we found that our methodologies were in good agreement with the available experimental data over a wide range of temperature.

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