Evaluation of Mobility in Graphene Nanoribbons Including Line Edge Roughness Scattering
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Abstract—This work employs single particle Monte Carlo method to calculation the electron mobility in Graphene Nanoribbons including phonon scattering (acoustic and optical) and Line Edge Roughness scattering. Mobility as high as 2×10^4 cm^2/Vs is obtained and when the GNRs width is 2 nm, the mobility reduces to only about 200 cm^2/Vs. These results agree well with experiment results. Also the effect of roughness parameters on mobility is analyzed.

Keywords—Graphene Nanoribbons; Monte Carlo; scattering; mobility.

I. Introduction
Graphene has attracted much attention since its first isolation in 2004 [1]. However, since two-dimensional (2D) graphene sheet is a gapless material, there has been substantial interest in patterning them into graphene nanoribbons (GNRs) [2]. Graphene as thin as 3 nm will open a gap of 0.3-0.4 eV [3, 4], but the measured carrier mobilities in the first ultrathin GNRs are reported to be much lower than in corresponding 2D graphene sheets [3, 4]. It is essential to identify the effect of various carrier scattering mechanisms on mobility to improve the transport properties of GNRs. In this work, a comprehensive analysis of various carrier scattering mechanisms that affect electron mobilities including acoustic phonon scattering, optical phonon scattering (absorption and emission) and line edge roughness (LER) scattering [5] is presented using single particle Monte Carlo method [6, 7]. The obtained mobilities are as high as 2×10^4 cm^2/Vs while it decreases with the increase of electrical field. The results reveal that LER scattering can deteriorate the mobilities. The thinner GNRs have lower mobilities since LER scattering is more severe with smaller GNRs width. It is also revealed that roughness amplitude H affects mobilities most.

II. Scattering Mechanisms and Monte Carlo Methodology
Semiconducting armchair GNRs with lengths L along the y directions are considered, the band structure is described as \( \varepsilon(k_y, k_n) = \hbar v_F \sqrt{k_n^2 + k_y^2} \) which employs the hard-wall boundary conditions at the edges, where \( v_F = 10^6 \) cm/s is the Fermi velocity [5]. The allowed transverse wave vectors \( k_n \) for semiconducting armchair GNRs are quantized to values \( k_n = \pm n\pi / 3W \), depending on the width \( W \); here \( n = \pm 1, \pm 2, \pm 4, \pm 5, \pm 7, \pm 8, ... \) [5]. This leads to a bandgap of \( \varepsilon_g \sim 1.38 / W \) eV \( \), with \( W \) expressed in nanometer [9].

For acoustic phonon scattering, we use Fermi’s golden rule and the deformation potential approximation. The deformation potential for acoustic phonons \( D_{ac} \) is 16 eV [5] and the phonon dispersion curves are determined using zone folded graphene phonon spectra [8]. Here we only consider the longitudinal mode since this mode induces higher deformation potential than the out of plane and flexural modes [6, 10]. For optical phonon scattering, we consider the zone boundary phonon of energy \( \hbar \omega_{LO} = 160 \) meV, with an optical deformation potential \( D_{op} = 1.4 \times 10^9 \) eV/cm [5]. In this work, the lowest three subband and both intrasubband and intersubband phonon scattering (acoustic and optical) between the three subbands are considered. In Fig. 1 it is plotted phonon scattering rate between different subbands and is observed six peaks, of which three are onset of each subband and three are onset of optical phonon emission in each subband.

In the very thin GNRs, Line Edge Roughness (LER) scattering sometimes is the dominating scattering mechanism. To describe the effect of LER scattering on charge transport, the width of GNRs is assumed as a function of the longitudinal axis y. The GNRs width is given as a Gaussian function of roughness amplitude H.
Wy = Wy(δ) + W, where Wy(δ) describes the roughness and W is the spatially averaged width as shown in Fig. 2 [5]. There edge roughness Wy(δ) is described as

\[ \langle \delta W(y) \delta W(y + \Delta y) \rangle = H^2 e^{-|y|/\Lambda} \]

where H is the amplitude and \( \Lambda \) is the correlation length of the roughness. The LER scattering rate can be expressed as

\[ S_{LER}(\epsilon) = \frac{\pi e^2}{\hbar} \frac{H^2}{W^2} \frac{\Lambda}{1 + 4k_F^2\Lambda^2} \rho(\epsilon)(1 + \cos \theta_{\kappa\kappa'}) \]  

[5],

where \( \rho(\epsilon) \) is the DOS of \( n \)th subband, \( \epsilon_n = \hbar v_F |k_n| \) is the conduction band energy of the \( n \)th subband and \( \theta_{\kappa\kappa'} \) is the angle between state \( \kappa \) and \( \kappa' \). Since the scattering potential is only dependent on the longitudinal axis, the LER scattering is intrasubband. Fig. 3 shows the LER scattering rate as a function of GNRs width ranging from 2 nm to 10 nm. It is shown that with the same roughness parameters amplitude H and correlation length \( \Lambda \), the thinner the GNRs are the larger the LER scattering rate is. Also it can be observed that the band gap becomes large as the GNRs width decreases \( (\epsilon_g \approx 1.38/W \text{ eV}) \), with W expressed in nanometer) [9]. Fig. 4 illustrates the dependence of the LER scattering rate on roughness amplitude H and correlation length \( \Lambda \) with GNRs width of 5 nm. The scattering rate increases with bigger roughness amplitude H while it decreases with bigger correlation length \( \Lambda \). Also it can be found that roughness amplitude H has more impact on LER scattering rate than that of correlation length \( \Lambda \), which indicates that roughness amplitude H affect mobility more than correlation length \( \Lambda \).

These three kind of scattering mechanisms are together plotted in Fig. 5. It is shown that acoustic phonon scattering and LER scattering are the dominating scattering mechanisms while the optical phonon scattering can’t be neglected at high energy region. Also it is observed that the LER scattering curve goes down more sharply than the acoustic phonon scattering curve.

We employ single particle Monte Carlo method to obtain the electron average velocity in GNRs under various external electrical fields and for the acceleration of calculation we build scattering rate table in a very fine grid (0.01 meV). The energy range of scattering rate table is between 0 eV and 1 eV.
The calculated average electron velocities in GNRs under various electrical fields with and without LER scattering are plotted in Fig. 6 and the corresponding electron mobilities in GNRs under various electrical fields with and without LER scattering are shown in Fig. 7. It is revealed in these two figures that electrons in GNRs have mobilities as high as 2×10^4 cm^2/Vs under low electrical field when the edge is smooth. This result agrees well with experimental measurement and other theoretical calculation [5, 6, 11]. It is observed that the LER scattering can deteriorate the mobilities but when the GNRs width is 5 nm with roughness amplitude H of 0.5 nm and correlation length Λ of 3 nm it doesn’t lower the mobility much. It is also revealed that the mobilities are lower at high electrical field; this result also can be found in two-dimensional graphene sheet [6]. The explanation is that at higher electrical field the average energy of electron is higher thus the optical phonon scattering begin to have effect.

Fig. 8 shows the GNRs mobilities as a function of width W = 6 nm, 10 nm, 15 nm, 20 nm, and 25 nm for three different values of roughness amplitude H = 0.5 nm, 1 nm, and 2 nm with correlation length Λ = 2 nm, 3 nm, and 4 nm. The GNRs are at an ambient temperature T = 300 K. It is observed that the LER scattering can deteriorate the mobilities but when the GNRs width is 5 nm with roughness amplitude H of 0.5 nm and correlation length Λ of 3 nm it doesn’t lower the mobility much. It is also revealed that the mobilities are lower at high electrical field; this result also can be found in two-dimensional graphene sheet [6]. The explanation is that at higher electrical field the average energy of electron is higher thus the optical phonon scattering begin to have effect.
width ranging from 2 nm to 10 nm with various roughness amplitude $H$ and correlation length $\Lambda$ or smooth edge. It is shown that the mobilities decrease with GNRs width. The smooth GNRs have the highest mobilities while the large roughness amplitude $H$ leads to lowest mobilities.

In Fig. 9 it is shown the electron mobility dependence on roughness amplitude $H$ and correlation length $\Lambda$ with typical GNRs width of 5 nm. It is observed that the roughness amplitude $H$ can affect mobility severely while correlation length $\Lambda$ has only negligible effect on mobility.

**IV. Summary**

In this work it is presented a comprehensive analysis of GNRs mobilities by Monte Carlo method. The acoustic phonon scattering, optical phonon scattering (absorption and emission) and LER scattering are taken into account. Mobility as high as $2 \times 10^4$ cm$^2$/Vs is obtained while it decreases when electrical field increases. The mobilities are deteriorated by LER scattering and since LER scattering rate is higher with smaller GNRs width, the thinner GNRs have lower mobilities. Also it is revealed that roughness amplitude $H$ can affect mobilities much while correlation length $\Lambda$ has negligible effect on mobility.

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**Reference**