Evaluation of Mobility in Graphene Nanoribbons Including Line Edge Roughness Scattering

Lang Zeng, Xiao Yan Liu*, Gang Du, Jin Feng Kang, and Ru Qi Han
Key Laboratory of Microelectronic Devices and Circuits, Institute of Microelectronics, Peking University, 100871, P. R. China
*E-mail address: xyliu@ime.pku.edu.cn

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 $\varepsilon(k_n,k_y)=\hbar v_F\sqrt{k_n^2+k_y^2}$ which employs the hard-wall boundary conditions at the edges, where v_F =10^8 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 $n=\pm1,\pm2,\pm4,\pm5,\pm7,\pm8,\ldots$ [5]. This leads to a bandgap of $\varepsilon_g\sim1.38/W\ eV$, with W expressed in nanometer [9].

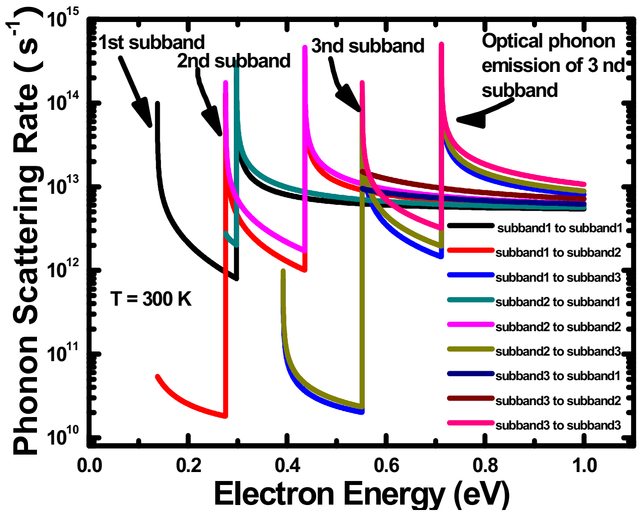

Fig. 1 The phonon scattering rate between different subbands. The energy of carriers is measured with respect to the Dirac point. Three peaks are onset of each subband and the other three are onset of optical phonon emission in each subband. The lowest three subbands are considered in this work.

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} =1.4×10^9 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

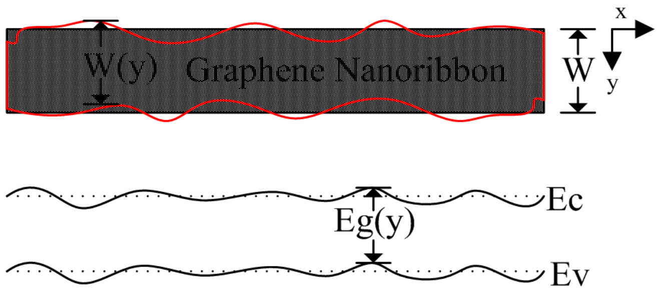

Fig. 2 The schematic demonstration of GNRs Line Edge Roughness and the fluctuation of band edge potential which cause the scattering of carriers. The perturbation potential for the nth subband is expressed as following:

$$V_{LER}(y) = -\frac{\delta W(y)}{W}\varepsilon_n$$

by $W(y) = W + \delta W(y)$, where $\delta W(y)$ describes the roughness and W is the spatially averaged width as shown in Fig. 2 [5]. There edge roughness $\delta W(y)$ is described as $\langle \delta W(y)\delta W(y+\Delta y)\rangle = H^2 e^{-|\Delta y|/\Lambda}$, where H is the amplitude and Λ is the correlation length of the roughness. The LER scattering rate can be expressed as

$$S_{LER}(\varepsilon) = \frac{\pi\varepsilon_n^2}{\hbar}\frac{H^2}{W^2}\frac{\Lambda}{1+4k_y^2\Lambda^2}\rho(\varepsilon)(1+\cos\theta_{kk'}) \qquad [5],$$

where $\rho(\varepsilon)$ is the DOS of nth subband, $\varepsilon_n = \hbar v_F |k_n|$ is the conduction band energy of the nth subband and $\theta_{\kappa\kappa'}$ is the angle between state κ and κ'. 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 Λ, 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 (ε_g~1.38/W eV , with W expressed in nanometer) [9]. Fig. 4 illustrates the dependence of the LER scattering rate on roughness amplitude H and correlation length Λ with GNRs width of 5 nm. The scattering rate increases with bigger roughness amplitude H while it decreases with bigger correlation length Λ. Also it can be found that roughness amplitude H has more impact on LER scattering rate than that of correlation length Λ, which indicates that roughness amplitude H affect mobility more than correlation length Λ.

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

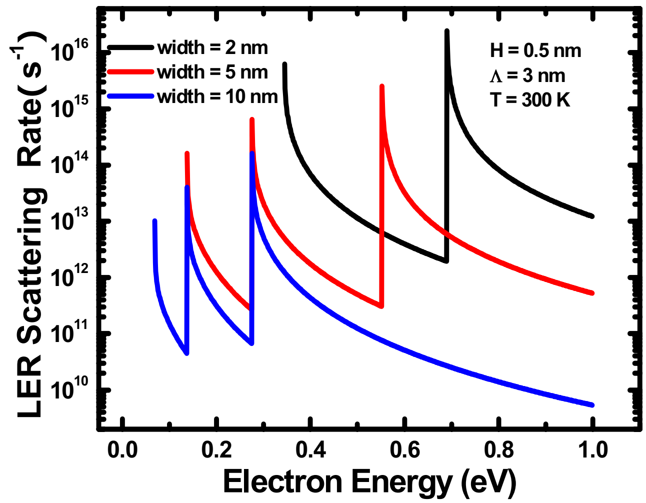

Fig. 3 The LER scattering rate dependence on GNRs width with typical roughness amplitude H of 0.5 nm and correlation length Λ of 3 nm. The energy of electrons is measured with respect to the Dirac point. The LER scattering rate is higher with small GNRs width.

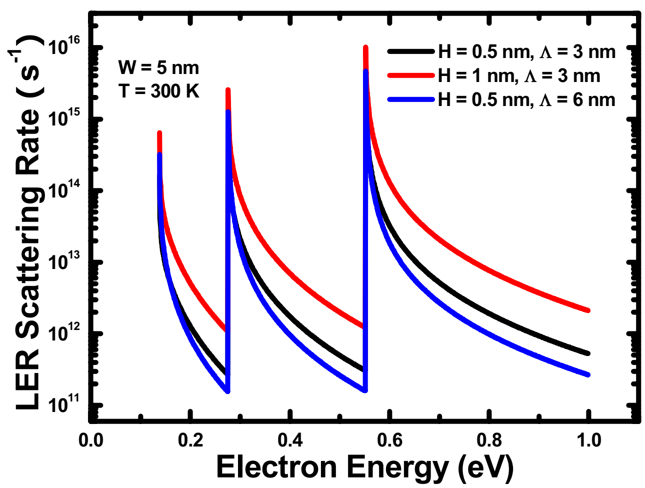

Fig. 4 The LER scattering rate dependence on roughness amplitude H and correlation length Λ with GNRs width of 5 nm. The energy of carriers is measured with respect to the Dirac point. The LER scattering rate increases with large roughness amplitude H and small correlation length Λ.

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

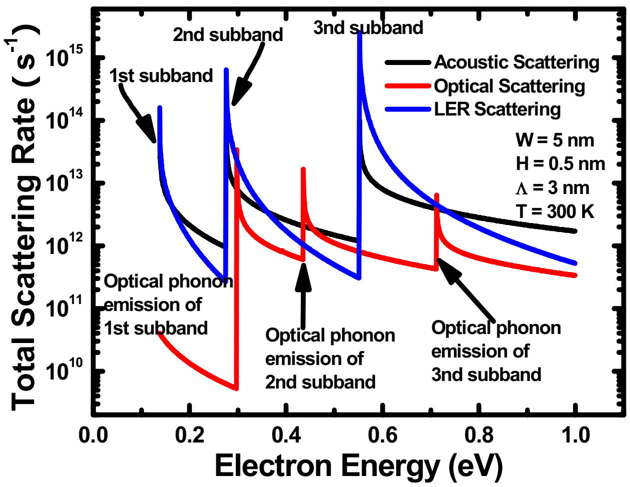

Fig. 5 The three total scattering rates. The energy of carriers is measured with respect to the Dirac point. At each onset of subband the LER scattering rate is highest while it decreases more sharply than acoustic phonon scattering rate. The optical phonon scattering takes effect at high energy region.

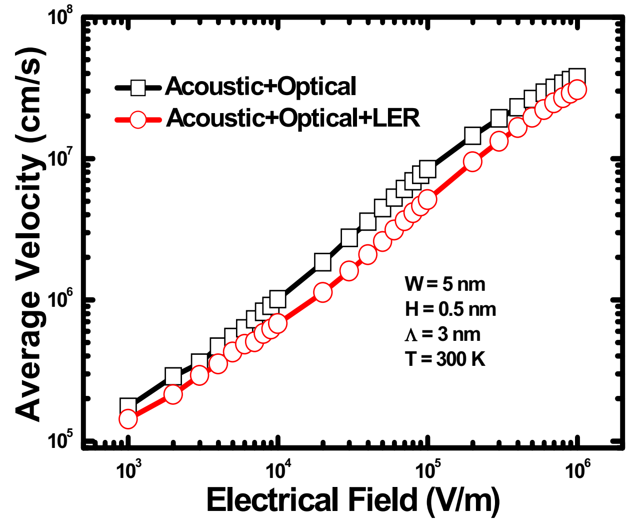

Fig. 6 The average velocity of electrons in GNRs under various electrical fields with and without LER scattering. The average velocity increases with electrical field. With LER scattering taken into account the average velocity is lower.

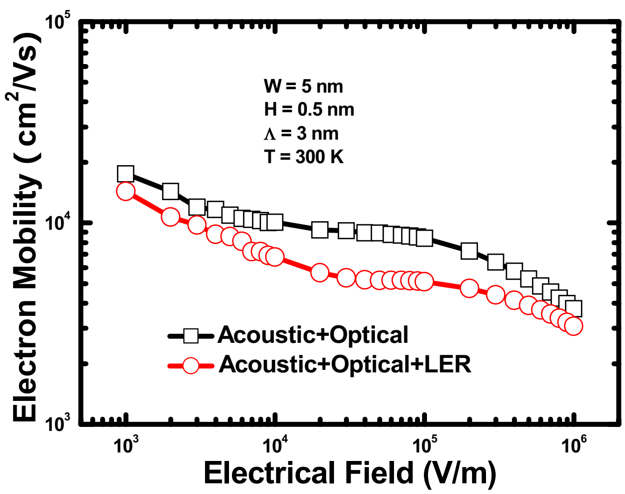

Fig. 7 The mobilities of electrons in GNRs under various electrical fields with and without LER scattering. The LER scattering can deteriorate electron mobilities and the electron mobilities decrease with increasing electrical field.

for the saving of memory usage while the energy is measured with respect to the Dirac point. For electron energy that is larger than 1 eV, the scattering rate is calculated on-line. The lowest three subbands are considered in this work. First the total scattering rate is used to calculate the free flight time of electrons, and then the scattering rates of each kind of scattering mechanism which can be intrasubband or intersubband are used to determine the type of scattering occurring. When the scattering mechanism is chosen, it is used to determine the final state of electron, which comprises of electron energy, momentum and subband index. Since we treat acoustic phonon scattering as elastic scattering it need to perform much more scattering events (1×10^8 times) to reach approximately constant velocities, contrasting to which in Ref. [6] after only 1×10^6 scattering events the constant velocity is achieved since in that reference the acoustic phonon scattering is treated as inelastic scattering.

III. Results and Discussions

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 GNRs

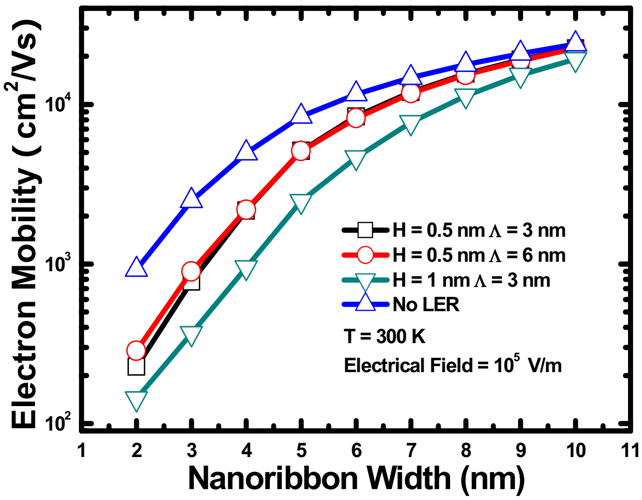

Fig. 8 The electron mobility dependence on GNRs width with various roughness amplitude H and correlation length Λ or smooth edge. It is shown that the mobilities decrease with GNRs width. The smooth GNRs have the highest mobilities while the large roughness amplitude H leads to lowest mobilities.

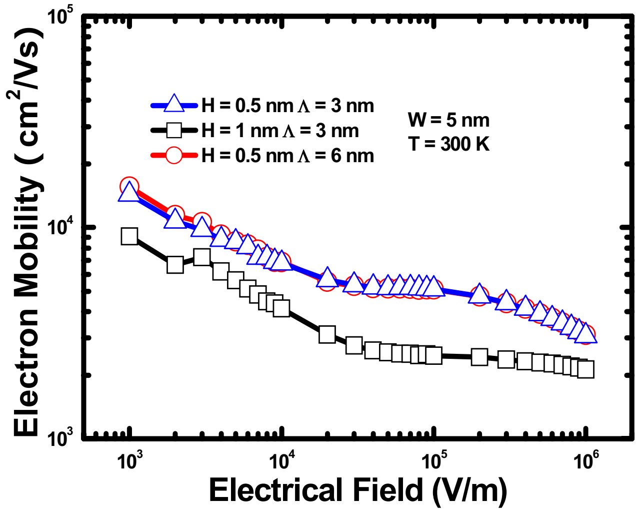

Fig. 9 The electron mobility dependence on roughness amplitude H and correlation length Λ with typical GNRs width of 5 nm. It is observed that the roughness amplitude H can affect mobility severely while correlation length Λ has only negligible effect on mobility.

width ranging from 2 nm to 10 nm with various roughness amplitude H and correlation length Λ or smooth edge. It is shown that the mobility of 2 nm width GNRs is two magnitudes lower than that of 10 nm width GNRs. The mobility of 2 nm width GNRs is only 100~200 cm^2/Vs. In a recently reported experimental work by Dai' group [3, 4], they successfully got sub-10 nm GNRs by chemical method and the analysis based on electrostatic simulations of gate capacitances led to an estimated hole mobility which is symmetrical with electron mobility in the width ≤ 10 nm ribbons of ~100 to 200 cm^2/Vs. When the roughness amplitude (0.5 nm) can be comparable to GNRs width (2 nm), the LER scattering is very severe thus leads to a quite low mobility. It is also observed that the smooth edge GNRs have the highest mobilities while 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 Λ with typical GNRs width of 5 nm. It is observed that the roughness amplitude H can affect mobility serious since it can affect LER scattering rate much as shown in Fig. 4 while correlation length Λ has negligible effect on mobility. For GNRs width of 5 nm, the mobility of roughness amplitude H of 0.5 nm is about two times of that of roughness amplitude H of 1 nm. When the GNRs widths reduces, the roughness parameters will affect the mobility more severely as indicating in Fig. 8 for different GNRs width.

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 2×10^4 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 Λ has negligible effect on mobility.

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