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Carrier Mobility Study in Zinc doped Armchair Graphene Nanoribbon via Phonon Interactions

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Abstract:

Electron mobility which is one of the important electron transport parameters is calculated for zinc doped armchair graphene nanoribbon (aGNR) via electron acoustical phonon interactions on the basis of acoustical deformation potential (ADP) coupling mechanism. The lower doping concentration (x = 1%) is considered in this study. Moreover, the impact of magnetic field is studied on electron mobility. It has been observed that the acoustical deformation potential contributed electron mobility decreases as the strength of magnetic field increases. In addition to this we have also observe that the scattering rate of electrons traversing through the nanoribbon rises with increasing strength of magnetic field which is due to the fact that the electron effective mass increases with increasing strength of magnetic field.

Keywords

Graphene nanoribbon, Magnetotransport parameters, Electron mobility

1. Introduction

Graphene is considered as a unique and wonder an atom thick two dimensional material by a scientific society and is single atomic layer of carbon organized to form honeycomb lattice. Entire society of scientists and engineers attracted towards graphene and its allotropes because of its unique physicochemical properties such as high thermal conductivity (5000 W m^{-1} K^{-1}), excellent electrical conductivity (10^8 S m^{-1}), high Young's modulus (1.1-1.8 TPa) [1-4]. Researchers find unlimited potential for the application of graphene in many fields, including electronics [5], energy storage [6-8], bioelectronics sensors [9]. The narrow strip or ribbon of graphene sheet is known as graphene nanoribbon (GNR). Although graphene is zero band gap material, the GNR possess energy band gap which increases with the reduction of width of the ribbon [10]. In the similar fashion as pristine and doped graphene, its allotrope graphene nanoribbon in its pristine and doped form also attracts researchers because of its novel properties such as inclusion of energy band gap in it. Hence, interest also builds up towards the transition metals (e.g. Zn, Mn, etc) doped graphene nanoribbon [11-13]. It is observed that with low doping concentration of transition metals, novel magnetic [14] behavior reveled in doped form which leads many potential applications for nanoelectronics and spintronic devices. The doping of transition metals in to GNR converts it in to ferromagnetic semiconductor which is considered as building block for future spintronic devices such as spin transistors consuming very less power for its operation. Moreover, the preservation of ferromagnetism more than the room temperature by the minute concentration of doping of transition metals in graphene is considered as one of the important technological frontiers [15] because the Curie temperature (T_C) is observed inversely proportional to the third power of the crystal host lattice parameter [16]. As graphene possesses comparatively smaller lattice parameters, in present work we study the electron mobility for zinc (a transition metal), doped armchair graphene nanoribbon (aGNR) at quite below to quite above room temperature regime under the effect of both electric and magnetic fields. The present work centers more on the constraints that limit the high electron mobility with doping of zinc. We consider the acoustical deformation potential (ADP) scattering mechanism to calculate electron scattering rate and electron mobility. The calculations are carried out for below and beyond room temperature because at this temperature scale, the acoustical phonon scattering is dominant under the impact of magnetic field. The content of the present work is as follows: the computational approach together with parameters used in calculations are included in section 2. We discuss our results of present study with proper justification with the help of electronic and vibrational properties of armchair graphene nanoribbon (aGNR) along with the doping of Zn in it in section 3. Finally, section 4 presents the conclusion of the present study.

2. Methodology

In general, for the solids, the energy band structure is determined by the crystal potential. The conduction and valance bands may vary if the lattice constants vary even in minute fraction. These variations lead strain in the material which generates the change in lattice spacing (u) which in turn generates the acoustical waves (phonons). For acoustical phonons,

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the interaction potential offered to conduction electrons is given as follows:

$$U_{ap}(x,t) = D_a \, {\partial u}/{\partial x} \quad (1)$$

Here, D_a is acoustical deformation potential. For the electron phonon interaction, scattering the interaction potential is given as $U_s = k_\beta u_\beta$ wherein k_β is the wave vector and u_β is the lattice vibration Fourier component mathematically defined as

$$u_\beta = A_\beta e^{i(\beta z - \omega t)} + A_\beta^* e^{-i(\beta z - \omega t)} \quad (2)$$

Therefore, the scattering potential may be expressed as

$$U_s = k_\beta A_\beta e^{i(\beta z - \omega t)} + k_\beta A_\beta^* e^{-i(\beta z - \omega t)} \quad (3)$$

The wave function for the plane wave restricted to a normalized length, $-{L}/{2} \le z \le {L}/{2}$ is given as

$$\psi(z) = \frac{1}{\sqrt{L}} e^{ikz} \quad (4)$$

The matrix element is given by

$$H_{k\cdot k} = \int_{-L/2}^{L/2} \psi(z) U_s \psi^*(z) dz$$

$$= k_\beta A_\beta \int_{-\frac{L}{2}}^{\frac{L}{2}} \left(\frac{1}{L}\right) \left[e^{i(k-k'\pm\beta)z}\right] dz \quad (5)$$

The electron scattering rate is given by Fermi's golden rule as follows:

$$S(k',k) = \frac{2\pi}{\hbar} |H_{k'k}|^2 \delta((E(k') - E(k) \pm \hbar\omega)$$

$$= \frac{2\pi}{\hbar^2 v\beta} |k_\beta|^2 |A_\beta|^2 \delta(\pm cos\theta + \frac{\hbar\beta}{2p} \pm \frac{\omega}{v\beta}) \quad (6)$$

Here $|A_\beta|^2$ is the square of the amplitude of quanta of lattice vibration and is expressed as

$$|A_\beta|^2 = \frac{\hbar}{2\rho\omega_{\beta\Omega}} (N_\beta + {1}/{2} \pm {1}/{2}) \text{ and}$$

$$|k_\beta|^2 = \beta^2 D_a^2 \quad (7)$$

From Eq. (7) and Eq. (6), the summation of *S (k', k)* in the momentum space gives the total electron momentum scattering rate, and hence the electron momentum scattering rate is given as [11,17]

$$\frac{1}{\tau(p)} = \frac{1}{\tau_m(p)} = \frac{\pi m^* D_a^2 k_B T_L}{\hbar^3 w C_l} \quad (8)$$

wherein, $m^*$is electron effective mass, *w* is a width of nanoribbon, C_l is the longitudinal elastic constant, k_B is Boltzmann constant and T_L is lattice temperature, D_a is the acoustical deformation potential (ADP) [18,19] which is given by

$$D_a = k_B T_l \sqrt{{M}/{m^*}} \quad (9)$$

where $m^* = {\hbar^2}/{(\partial^2 E/\partial k^2)}$ is electron effective mass and *M* is mass of atom, *T* is absolute temperature measured in Kelvin, and m_0 is electronic rest mass. Now, on applying electric field *F* to the any electronic device results in acceleration of the electrons and hence it increases the electron energy [20]. Hence, under this field, the acoustical deformation potential limited mobility is given by [21]

$$\mu_{dp} = \frac{3.17\times10^{-5} \, \rho v_s^2}{\left({m^*}/{m_0}\right)^{5/2} D_a^2 T^{3/2}} \quad (10)$$

where, ρ is nanoribbon mass density, v_s is the average phonon velocity in material. The impact of magnetic field on hot carrier scattering rate is given by [22]

$$\frac{1}{\tau_{mag}} = \frac{D_a^2 k_B T_L e B \sqrt{2m_e^*}}{2\pi\hbar^3 \rho v_d^2 \sqrt{E_k}} \quad (11)$$

where, E_k is electronic kinetic energy and v_d is the electron drift velocity, h is Planck's constant, D_a is acoustical deformation potential. Now, as the externally applied magnetic field affects the electronic resistivity, the acoustical phonon limited carrier resistivity (ρ_{mag}) under the impact of magnetic field is given by [23]

$$\rho_{mag} = \frac{D_a^2 \sqrt{m_e^* B^2}}{n(2\pi)^{3/2}\hbar^2 \rho v_s^2 \sqrt{k_B T_L}} \, ln\left(\frac{R k_B T_L}{\hbar v_s}\right) \quad (12)$$

where, R is characteristic length of electron in magnetic field which is expressed as $R = \sqrt{\frac{\hbar}{eB}}$ is constant which is independent of properties of material. Hence, the electron mobility under the impact of magnetic field is calculated by

$$\mu_{mag} = \frac{1}{ne\rho_{mag}} \quad (13)$$

3. Results and Discussion

The Present work explores the impact of magnetic field on electronic transport behavior through transition metal (Zn) doped graphene nanoribbon wherein the effect of magnetic field under constant applied electric field (0.1 mv/nm) is considered with minor doping concentration of zinc in aGNR. We have investigate the electron mobility and scattering rate under the impact of various intensities of magnetic field and constant applied electric field with the help of equations (11) and (13). In our previous work [24], the electron mobility for manganese doped graphene was calculated using Eq. (9) without considering magnetic field. The reference values of the parameters for pristine armchair graphene nanoribbon utilized for these calculations are: $\rho = 7.6 \times 10^{-4}$ gm/cm^2, $v_s = 2 \times 10^4$ m s^{-1}, $e = 1.6 \times 10^{-28} gm$ and w= 20 nm. We have performed the calculations of electron transport parameters for 1% of zinc doping because armchair graphene nanoribbon with the doping concentration of above 1% of transition metal possesses charge transfer semiconductor behavior and also possesses a finite minute energy band gap whereas the higher

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concentration leads macroscopic antiferromagnetism. The electron mobility variation with temperature as

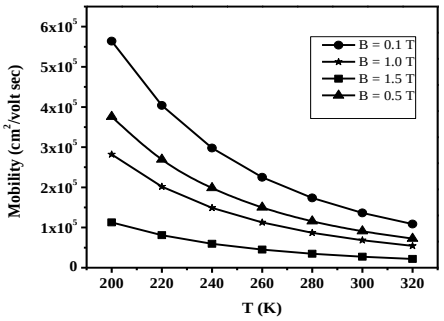

Figure 1 Variation of electron mobility with temperature under various intensities of magnetic field for Zn doped aGNR with electric field of 0.1 mV/nm

well as strength of magnetic field is shown in Fig. 1 wherein it has been shown that the electron mobility while traversing through the nanoribbon diminishes with the rise in magnetic field intensity. Moreover, It seems from Fig.1 that the electron mobility decreases with increase in lattice temperature. The responsible parameter for this is the electronic effective mass. In fact, the effective mass of electron significantly increases under the effect of zinc doping concentration with respect to pristine armchair nanoribbon under the effect of both electric and magnetic fields. The main reason behind the rise of

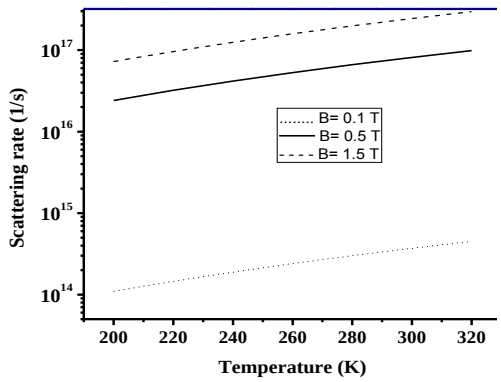

Figure 2 The variation of electron scattering rate with temperature under various magnetic field intensities for Zn doped armchair graphene nanoribbon.

effective mass of electron is that as the electron effective mass increases the corresponding Fermi velocity of electron also increase because effective mass is of electron directly reduces the Fermi velocity under the impact of doping concentration. Moreover, we have observed that the Fermi velocity of electron and electron scattering rate via acoustical deformation potential (ADP) scattering mechanism are also impacted by electron effective mass which reveals in Fig. 2. From Fig. 2, it is observed that the increasing magnitude of applied magnetic field rises electron scattering rate. The rise in magnetic field strength, increases the electron effective mass which in turn increases the electron scattering rate.

4. Conclusion

In summary, in the present work, we have calculate the electron mobility and scattering rate under the effect of magnetic and electric fields. This study helps to understand magnetic field effect on electron transport in better manner for transition metal (Zn) doped armchair GNR. We observe that the higher magnitude of magnetic field reduces electron mobility down to considerable amount. In addition to this we also observed that the energy scattering rate of electrons traversing through zinc doped nanoribbon rises with increasing strength of magnetic field intensity. This is due to the fact that as the magnetic field strength increases, it leads to further increase the electron effective mass. Thus, the rise of electron effective mass in turn increases the energy scattering rate of electrons. The results of the present work are important for future implementation of graphene based nanoribbon in space applications where temperature have its large variation scale. Hence, the optimum magnitude of magnetic field intensity is desirable for the electron transport study through transition metals doped armchair GNR.

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