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Effect of carrier number in density of states and quantum capacitance of with and without disorder GNR-FET on drain current

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ABSTRACT

In this paper with and without disorder grapheme nanoribbon (GNR) channel is being considered for different electrical parameters (Current, Number of carriers at steady state, Density of states, Quantum Capacitance). Due to increase in drain potential from 0 V to 0.7 V, the carrier concentration changes in channel region. Because of the dependence of channel potential on carrier concentration, the constant value carrier concentration cannot be considered to calculate drain current. Self-consistent field (SCF) method is utilized to calculate channel potential for the proposed model. The change in carrier concentration of channel is related to quantum capacitance. Quantum capacitance has a significant effect when drain to source bias is low. Density of states (DOS), dependent current expression is derived for with and without disorder grapheme nanoribbon (GNR) channel based field effect transistor (FET). Energy broadening due to the contact between grapheme nanoribbon (GNR) and metal leads is also considered to show effective carrier collection. The model also presents the short channel effect of device. The simulation of current-voltage, Density of states (DOS) using MATlab 2014a software is carried out.

1. Introduction

Recently, graphene has become a highly studied electronic material with many potential uses in electronic devices, optics, and sensing applications [1–7]. Transport property of graphene is one of the brilliant concerns to give attention [8]. Metal induced DOS broadening inside the metal-graphene contact regions enhances the current transport. Efforts have been given for the transport property (such as the minimal conductivity, localization effects, and signatures of relativistic behaviour of the charge carriers). Different transport properties of grapheme allow deriving suitable current relation of GNR-FET. The quantum capacitance (QC) [9,10] is also another important parameter for graphene channel. For design and fundamental understanding of the graphene based electronics device QC plays important role. In fact Quantum capacitance also gets deflected because of disordered graphene channel. For Electronics applications semiconducting behaviour of graphene is needed. Graphene's properties are highly affected by its geometry (such as its width and length). Graphene is different from conventional semiconductors for different reasons. First of all graphene is 2D atomically thin layer of carbon atoms. Neutral graphene is a semi metal with zero density of states at the Fermi energy of zero gap. For ideal graphene it is true, but in real

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case density of states exists at Dirac point or at Fermi energy because of substrate and impurity in environment. The third point considered in this paper is the electronic band structure near the Fermi energy level of conically shaped. Perfect electron-hole and internal valley symmetry is required for isomorphic two dimensional mass less Dirac fermions [11]. For designing low dimension structures and achieving large on-off (resistant) ratio uniform band is required at very low temperature. Also, it shows very small resistance at Dirac point [12–15]. The GNR channel which is considered in this paper is monolayer (as the monolayer interlayer coupling doesn't exist) graphene strip of finite width W. On the basis of edge configuration graphene fall in two categories (zigzag and armchair). Recent transport experiments with graphene ribbons [16,17], confirm that ribbons with $W = 20$ nm present a thermally activated conductivity indicating the presence of a gap. Because of imperfect edge configuration it is hard to fabricate real ribbons which are metallic intrinsically.

In this paper SCF (self-consistent field) [18–21] method is used to calculate the channel potential. Because channel potential and number of carriers at steady state are interdependent. Direct calculation of channel potential may not be accurate. So a rigorous and effective method is required to calculate channel potential that is SCF. When we connect metal lead to graphene channel the channel effective density of states doesn't remain the same. It varies and takes a shape of parabola instead of sharp energy level that is because of energy broadening. So energy broadening is also important factor for the proposed model. Finally monolayer graphene is used as channel for the modelling of GNR FET, known as graphene Nanoribbon FET. Energy broadening of channel has been taken in to consideration to get current relation.

2. Proposed model

A single layer of graphene has been used in this paper and screening effect may be ignored. Graphene is one atom thick carbon allotrope in which carbon atom has sp^2 hybridization. It has honeycomb lattice. For every honeycomb one electron is free for transport charge from source to drain. The current voltage characteristics, Number of carriers at steady state, quantum capacitance for disordered graphene channel with variable energy has been modelled. Also in this paper all characteristic parameter of predestine graphene (i.e. without disordered) has been simulated. The comparisons of the different characteristic parameters are shown in observation section. Researchers have published different works to define current-voltage relation of GNR FET [18–20]. But still improved method is needed for modelling purpose. The optimized device characteristic parameters could be useful for practical applications. A device model 'A' has been proposed for optimum performance.

Fig. 1 is the schematic representation of the proposed device model. Where Fig. 1(A) shows cross sectional view of the device, Fig. 1(B) top view of channel with different parameters, and Fig. 1(C) broadening of graphene channel. The device has length $l = 1$ nm, variable width W = 1–4 nm, and thickness of oxide/Graphene layer is 1.5 nm (refer to Fig. 1)(B). Insulating layer material 'Graphane' is obtained by complete hydrogenation of graphene. It is dielectric in nature with band gap of 3.5 eV for armchair and 3.7 eV for zigzag. For better lattice matching with graphene nano ribbon graphene dielectric is considered. So, the leakage current will decrease significantly. Silicon is used as substrate for modelling. Energy broadening is undertaken to derive the I-V relation. Coupling between Metal-Graphene can broaden the zero DOS near the contact Dirac point but if the intrinsic graphene DOS is large, the effect of broadening is weakened. Current transport enhances as drain Dirac point's

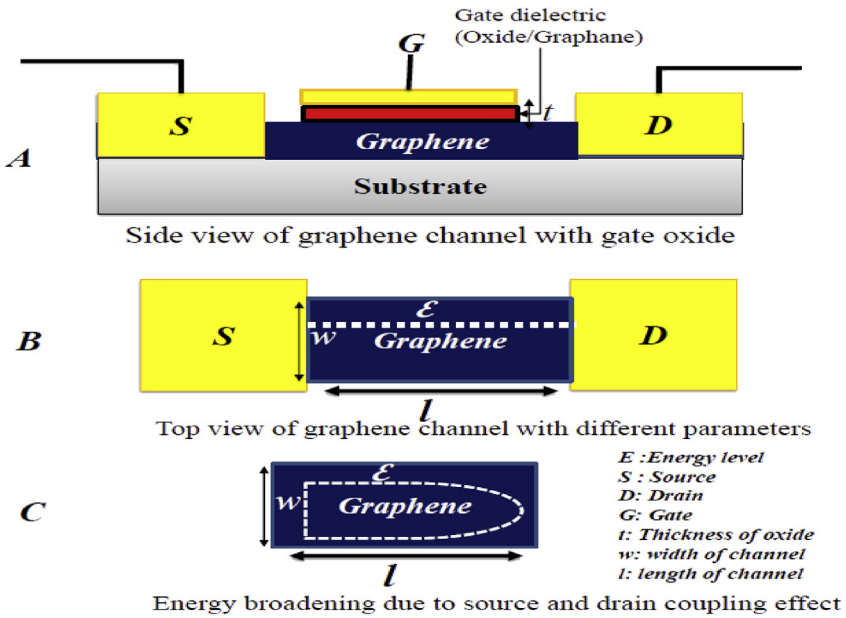

Fig. 1. (A) Cross sectional view of Device, (B) Top view of channel with different parameters, (C) broadening of graphene channel.

increases due to metal induced DOS broadening inside the Metal-Graphene contact regions. When metal lead coupled with GNR at the drain or source region, then the spilling of density of states occur, and that is why the sharp energy level gets broadened. This will add uncertainty in transport phenomena, and contribute to Quantum capacitance also.

3. Mathematical modelling and simulation

The Dispersion relation for Single layer graphene $E_k = \hbar k v_F$[24] here$v_F \approx 10^8$ m/s is Fermi velocity, $\hbar$ is reduced plank's constant, k is Boltzmann constant. This dispersion relation is defined for linear region. Since it is known that graphene is not disorder free material it has different edge disorder as well as defects in bulk. The Density of states for disorder at Dirac point is because of electrons and holes puddles arises due to impurity in environment; substrate impurity has been derived in this paper.

It is assumed that charged impurities creates a local electrostatic potential. That fluctuates randomly through the surface of graphene channel. It is also assumed that disorder potential introduces variation in Density of states of channel. The potential because of these charged impurities assumed to follow Gaussian distribution$P(S)$ parameterized by parameter σ (standard Deviation of distribution). DOS for disordered graphene is calculated by convolution for $\boldsymbol{E} > \boldsymbol{0}$ as follows [22,23].

$$D(E) = \int_{-\infty}^{\infty} D_0(E-S)*P(S)dS \tag{1}$$

$P(S)$ is Gaussian distribution function it shows potential due to electrons and holes puddles at Dirac point with parameter $\boldsymbol{S}$. Where, S is Average Value of the distribution. When drain potential is applied, electron availability can be defined using S.

$$P(S) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left(\frac{-S^2}{2\sigma^2}\right) \tag{2}$$

Here $D_0(E)$ is homogeneous density of states [15]. It is defined below-for $\mathbf{E} > \mathbf{0}$

$$D_0(E) = \frac{2E}{\pi\hbar^2 v_F^2} \tag{3}$$

$$D(E) = \frac{1}{\sigma\sqrt{2\pi}}\int_0^{\infty}\frac{2(E-S)}{\pi\hbar^2 v_F^2}\exp\left(\frac{-S^2}{2\sigma^2}\right)dS \tag{4}$$

$$D(E) = \sqrt{\frac{2}{\pi}}\times\frac{1}{\pi\hbar^2 v_F^2}\left[\int_0^{\infty} E\exp\left(\frac{-S^2}{2\sigma^2}\right)dS - \int_0^{\infty} S\exp\left(\frac{-S^2}{2\sigma^2}\right)dS\right] \tag{5}$$

$$\text{Put } z = \frac{S^2}{2\sigma^2} \text{ we get } D(E) = \sqrt{\frac{2}{\pi}}\times\frac{1}{\pi\hbar^2 v_F^2}\left[\frac{E\sigma\sqrt{\pi}}{\sqrt{2}} - \sigma\right] \tag{6}$$

After calculation, the density of states with disorder is

$$D(E) = \sqrt{\frac{2}{\pi}}\times\frac{1}{\pi\hbar^2 v_F^2}\left[\frac{E\sigma\sqrt{\pi}}{\sqrt{2}} - \sigma\right] \tag{7}$$

From capacitive model given above C_G, C_D may be calculated. Schematic representation of capacitance model for GNR-FET is shown in Fig. 2.

$$C_G = \frac{\varepsilon_0\varepsilon_r}{t}W*l \tag{8}$$

C_D is calculated using C_G, as $C_D = 0.05C_G$ which is one of the models Parameter.

Here $\varepsilon_r\varepsilon_0 = \varepsilon$ called permittivity of oxide/Graphane used between Gate electrode and channel, 'W' and 'l' is width, length of graphene flake. Thickness of oxide/Graphane layer is 't' which is grown just above the Graphene Flake.

Electrostatic potential for insulate channel (U_L) is obtained by Laplace equation. It is only justified if there is a few number of energy states between electrochemical potentials of source and drain of device. Since graphene is not an insulator so there will be change in charge density in channel and Poisson's equation is used to solve. Let's assume $\Delta\rho$ be the change in electrons density in the channel because of biasing of electrodes, then the form of Poisson's equation would be-

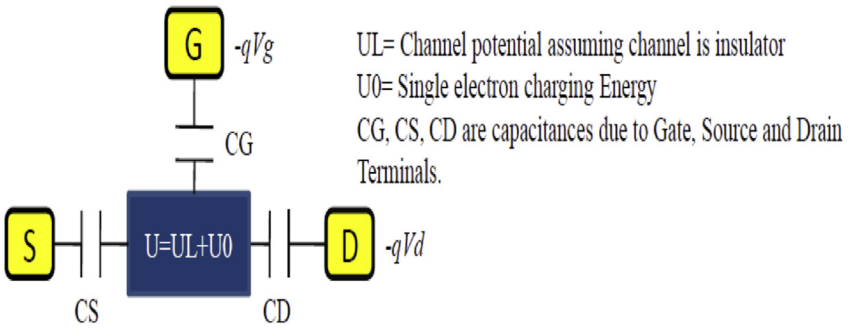

Fig. 2. Equivalent Capacitance Model of GNR FET with total energy 'U' of the channel.

$$\vec{\nabla}\cdot(\varepsilon_r\vec{\nabla}\varphi) = \frac{-\Delta\rho}{\varepsilon_0} \tag{9}$$

Here ε_r and ε_0 are relative permittivity of oxide and permittivity of vacuum respectively. U_0 is single electron charging energy defined as change in potential energy, By adding a single electron to the channel.

The channel is connected to the two gate electrodes by the familiar parallel plate capacitors. The capacitance (per unit area) is proportional to the effective dielectric constant ε and inversely proportional to the distance t between the centres of the channel. Gate capacitance for the input potential is

$$C_{in} = \frac{\varepsilon}{t} \tag{10}$$

Due to increased drain bias carrier concentration at channel start to boost. Because of this significant change in carrier concentration from equilibrium concentration quantum capacitance is appeared.

The electrostatic relation is given as:

$$U = U_L + \frac{q^2}{C_E}(N - N_0) \tag{11}$$

where, N_0 is carrier concentration at steady state, N is instantaneous carrier concentration, U_L is the channel potential is obtained by the Laplace equation assuming zero charge. While $(N - N_0)$, the extra electron density relative to the number N_0 required to keep it neutral. The quantum relation can be expressed as [16].

$$N = \int_{-\infty}^{\infty} D(E-U)f_0(E-F)dE \tag{12}$$

where $D(E-U)$ is the density of states (per unit area) shifted by the potential$U$. This is a non-linear relation and around certain point nearby linearism is achieved. For example, a "neutral potential" $U = U_N$ can be defined for $N = N_0$ and keeps the channel neutral [16].

$$N_0 = \int_{-\infty}^{\infty} D(E-U_N)f_0(E-F)dE \tag{13}$$

Any increase in potential (U) will raise the energy levels and reduce carrier concentration *(N)*. While a decrease in potential (U) *will* lower the energy levels and increase carrier concentration *(N)*. For small deviations from the neutral condition can be expressed as [2].

$$(N - N_0) = \frac{C_Q[U_N - U]}{q^2} \tag{14}$$

$$C_Q = -q^2\left[\frac{dN}{dU}\right]_{U=U_N} \tag{15}$$

where C_Q is called the quantum capacitance and it depends on the density of states. Channel potential is constant throughout the operation. Because it is depends on change of carrier from steady state value. Carrier concentration (N) is also dependent on potential of channel. So, these both quantities are interdependent. A rigorous method is needed to calculate channel potential energy. This method is SCF (Self consistent field calculation).

To start with some potential (U) is assumed, the value of carrier concentration (N) using equation (16) is calculated. It is shifted version of density of states. Now putting the value of carrier concentration (N) in equation (11) potential (U) is found. Final potential value was compared with initial potential. If new potential (U) is not close to initial potential is done using a suitable algorithm. Like equation (18), the value of U will be in fraction of K_BT. When the value of potential energy reaches to K_BT the iteration is stops.

Using equations (16) and (17) current-voltage (I-V_{ds}) characteristics of GNR FET is done.

$$N = \int_{-\infty}^{\infty} D(E-U)\frac{\gamma_1 f_1(E) + \gamma_2 f_2(E)}{\gamma_1 + \gamma_2} dE \tag{16}$$

$$I = \frac{q}{\hbar}\int_{-\infty}^{\infty} D(E-U)\frac{\gamma_1\gamma_2}{\gamma_1 + \gamma_2}[f_1(E) - f_2(E)]dE \tag{17}$$

Here $\gamma = \gamma_1 + \gamma_2$ is total channel broadening, $U = U_L + U_0$ total potential energy of channel. $U_L = C_G/C_E(-qV_G) + C_D/C_E(-qV_D)$ is Laplace potential obtained by solving Laplace equation by assuming channel as insulator (please refer Fig. 2). $U_0 = q^2/C_E$ is single electron charging energy. $f_1(E)$ and $f_2(E)$ are Fermi Dirac distribution of Source and Drain. F_S and F_D are electrochemical potential for source and Drain respectively. C_G, C_D and C_E are gate, drain and total capacitance respectively.

$$f_1(E) = \frac{1}{1+\exp\left(\frac{E-F_S}{K_BT}\right)}, f_2(E) = \frac{1}{1+\exp\left(\frac{E-F_D}{K_BT}\right)}$$

$$U_{new} = U_{old} + \alpha(U_{calc} - U_{old}) \tag{18}$$

4. Observation

The performance of GNR FET has been studied. An analytical method is introduced to achieve a better understanding of the Graphene nanoribbon FET. The results will be applied to identify how GNR FET parameters vary with drain to source voltage as well as effects of Disorder on conduction properties of GNR FET.

By increasing the value of disorder it has been observed that DOS is decreasing since disorder increase impurity level of grapheme channel. It is seen in Fig. 3 that at 0.4 value of disorder DOS parameter is same that of without disorder DOS. For higher disorder value density of states (DOS) are reduces. This is due to the reduction of effective density of states (EDOS).

Fig. 4 shows change of density of states versus Energy for different value of width with constant disorder value of 0.4. Density of states (DOS) is proportional to the width of graphene nano ribbon. The effective densities of states (EDOS) also increase in the energy band. For increasing the width of the GNR channel from 1 m to 4 nm DOS is increasing accordingly.

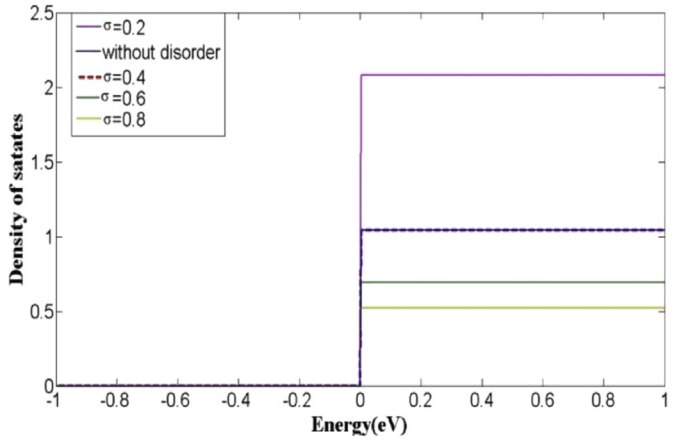

Fig. 3. Change of density of states as a function of Energy for different value of disorder.

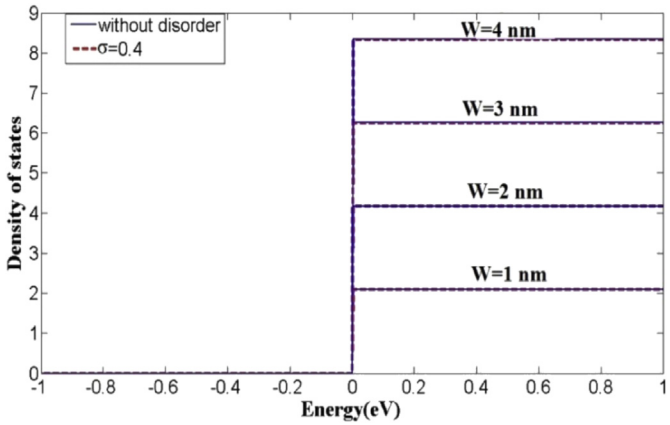

Fig. 4. Change of density of states versus Energy for different value of width with constant disorder value of 0.4.

Disorder value has been considered 0.4 at this particular disorder value the disordered graphene plot is assembling the non-disordered GNR FET plot. So, by increasing width of the channel we can increase the DOS of channel.

In order to obtain an analytical relation for the contact current, an explicit analytical equation for the electric potential distribution along the GNR channel is presented. The channel current is being simulated as a function of various physical and electrical parameters of the device including effective mass, length, temperature, and applied bias voltage. Research papers are published for steady state characteristics of GNR FET [25,26], in this paper Disordered graphene is chosen to model steady state carrier concentration. In addition comparison of Steady state carrier concentration for disorder and without disorder graphene channel is shown in Fig. 4 which makes this model more practical. Here in Fig. 5 it is observed that for $V_{gs} = 0.5\ V$ the current is starting increasing with positive slope. It is not saturating by increasing the drain Voltage. It shows the sub-threshold effect. The fact behind it is that the device size is small the effective field along the channel will be greater so the velocity overshoot occurs and the device current is not saturating. This performance is known as ballistic (for short channel) performance.

Considering the relation between current and density of states (DOS) of channel, the main current-voltage characteristics are modelled. A numerical solution of the presented analytical model in the preceding section is employed. Rectified current–voltage characteristic of GNR FET is plotted as shown in Fig. 6 ((a), (b), (c)) for different values of gate to source voltage with disorder value of 0.4.

In Fig. 6(a), it is observed that for $V_{gs} = 0.5\ V$, the current starts to increase with positive slope. But as the value of V_{gs} increases more than 0.5 V, drain current saturated after certain drain potential. The saturation is seen in Fig. 6 (b) & (c). It is due to the increase of effective channel area.

But if the gate potential is more then, channel area reduces substantially. So, it is seen in Fig. 7 (a) when $V_g = 1.2$ V, the Drain current starts after a certain Drain voltage because of the fact that below $V_g = 1.2$ V, the device channel is treated as narrow ohmic channel. But increase in Gate voltage is broadening the channel states. Increased drain voltage is needed to start (on) the device. This phenomenon is known as enhancement type of FET. When gate voltage is increases from 1.2 V to

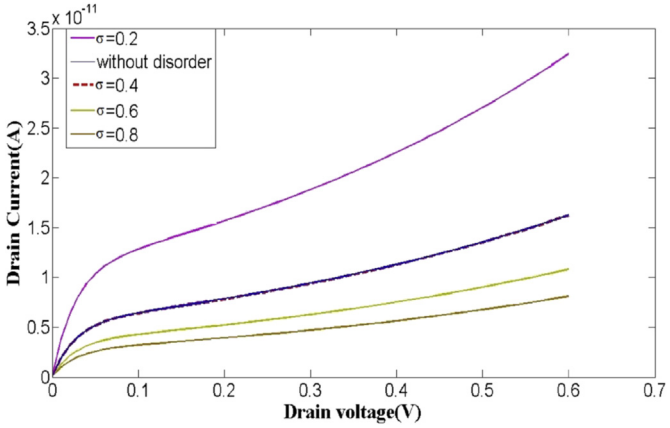

Fig. 5. Drain Current (A) Vs Drain Voltage (V) for Different value of Disorder parameter σ.

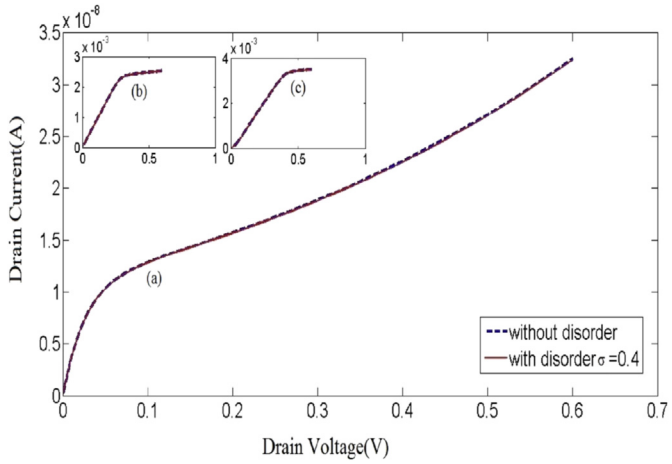

Fig. 6. Change of drain current with drain voltage for different gate voltage (Vg), (a) Gate voltage. Vg = 0.5 V for, (b) Gate voltage. Vg = 1 V, (c) Gate voltage. Vg = 1.1 V.

1.5 V, then it needs more drain voltage than previous one. From Fig. 7 (b) and (c) it is observed that the current is decreasing in very large amount, leads to abruptly change in differential trans-conductance because of very less carrier concentration at the channel.

From Fig. 8, it is observed that by increasing width of channel, the current increases effectively due to by increased width 'W' of the channel causing reduced channel resistance. Also density of states (DOS) is directly proportional width 'W' and, Drain current is directly proportional to density of states (DOS). So increase of drain current with the increase of channel width is relevant and justified.

From Fig. 9, it is observed that Number of carrier at steady state decreases significantly when there is increase in disorder. At $\sigma = 0.4$ the disordered Graphene channel plot is following the plot of Graphene channel without disorder. So, it is desired that to fabricate the device having environment impurity as less as possible.

It is seen in Fig. 10, that when value of width (W) increases the number of carriers (N) at steady state increases proportionally. Because, DOS is directly proportional to Width of channel and Number of carriers at steady state is directly proportional to DOS of channel.

From Fig. 11 (a), (b) & (c) it is observed that for increased gate voltage the carriers increases after certain drain voltage. The carriers at 0 drain voltage increases because of induced carrier for gate potential. When drain potential starts to increase the carriers start to decrease. This is because of drain voltage, recombination starts in channel after a certain drain voltage. The number of carriers again starts increasing because of extra carrier induced by Drain bias.

Quantum capacitance is not significant at higher Drain bias. But at lower value of Drain voltage it plays a significant role in overall capacitance of device as well as in delay calculation. From Fig. 12 it has been observe that as drain to source voltage is

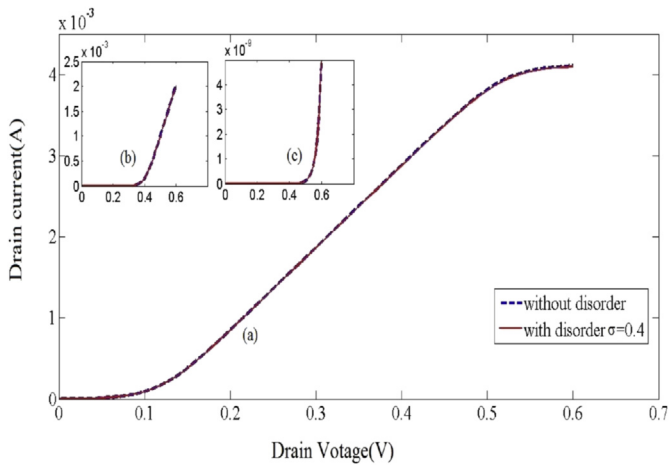

Fig. 7. Change of drain current with drain voltage for constant gate voltage (Vg). (a) Gate voltage. Vg = 1.2 V, (b) Gate voltage. Vg = 1.5 V, (c) Gate voltage. Vg = 2.0 V.

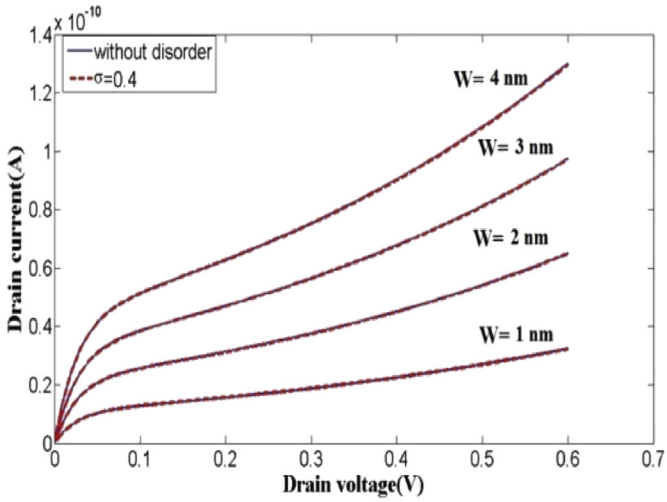

Fig. 8. Drain Current vs. Drain Voltage for different value of width W with constant value of disorder σ = 0.4 and without disorder Graphene channel.

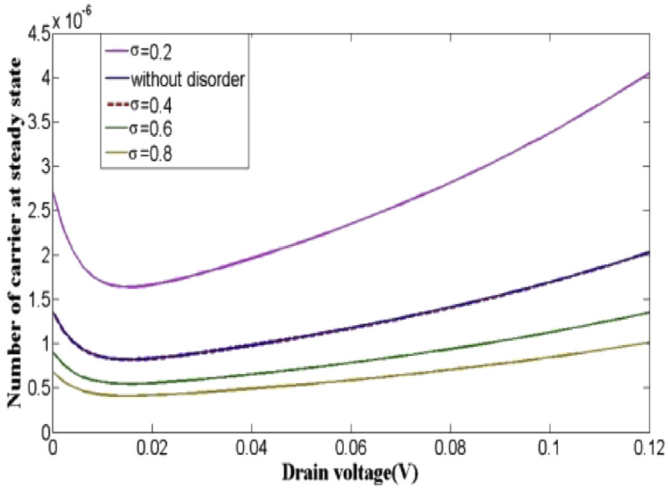

Fig. 9. Number of carriers at steady state vs. Drain Voltage for Different value of disorder with constant Gate voltage = 0.5 V.

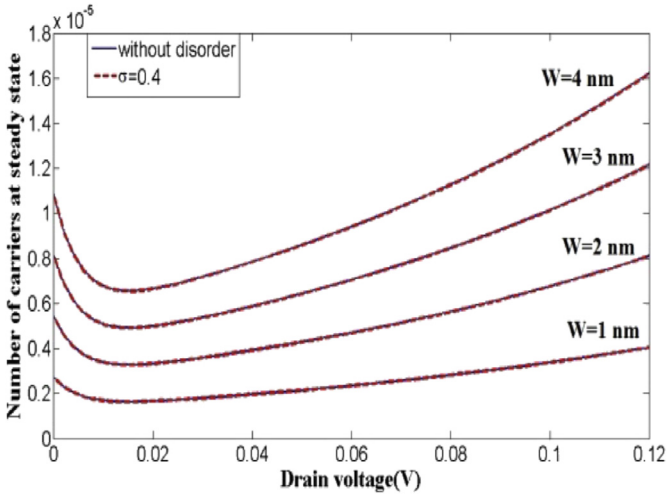

Fig. 10. Number of carriers at steady state vs. Drain voltage for different value of width 'W' with constant Disorder value of 0.4.

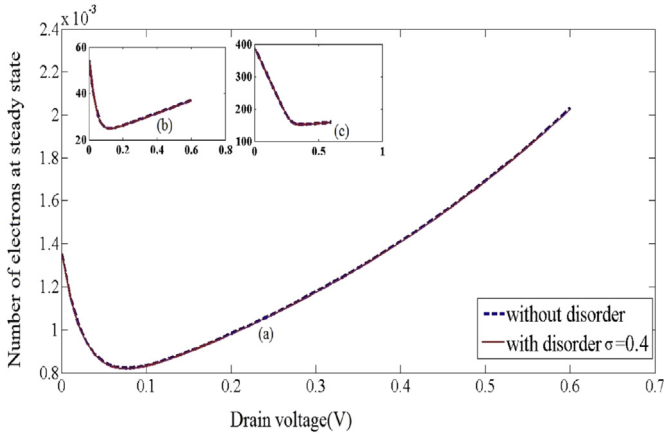

Fig. 11. Change of number of electrons at steady state with drain voltage (V) at different gate voltage (Vg). (a) Vg = 0.5 V, (b) Vg = 0.8 V, (c) Vg = 1 V.

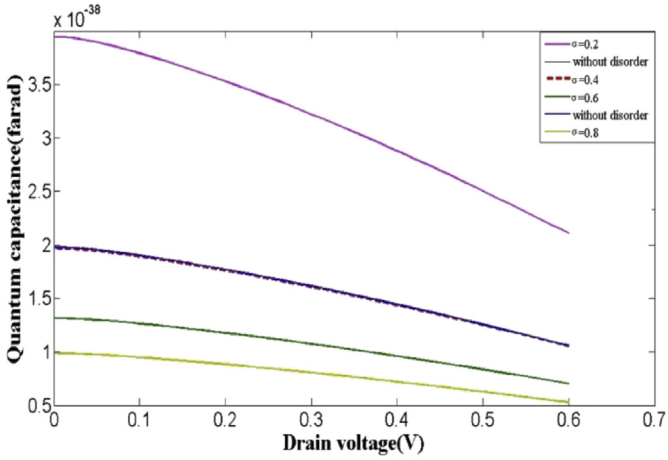

Fig. 12. Change of quantum capacitance with drain voltage for different value of disorder.

increasing Quantum capacitance is decreasing accordingly. As disorder has been considered for this Figure it can be observed that the quantum capacitance reduces. For disorder value of 0.4 the disorder plot of quantum capacitance is following the without disorder quantum capacitance. There would be a significant change in carrier concentration of channel which leads to a meaningful quantum capacitance value. After a certain Drain to source Bias the carrier change of the channel starts decreasing and leads to decrease in Quantum capacitance value.

5. Conclusion

Graphene has a number of desirable properties that can be utilized for electronic transport in different electronic devices. Single layer GNR is considered for the channel of FET. Since for miniaturization we cannot scale down a MOSFET after a certain limit because this will introduce lots of uncertainty in Device characteristics. So for small and tiny devices grapheme is a good approach. A device model is proposed for optimum performance. GNR FET in presence of electric field is considered. SiO_2 is advisable gate dielectric material is proposed for model. But for imperfect lattice match between GNR and SiO_2 leakage current would be a big issue. An alternate insulating material Graphene which is also an allotrope of carbon could replace SiO_2. Density of states for disordered graphene is analytically modelled for single layer of graphene with linear dispersion relation. Based on this structure simulation of junction current voltage characteristics of GNR FET is presented. The dependence of drain current on Drain to source voltage for different gate voltages are shown. Disorder and geometrical parameters such as width has been discussed. Dependence of other electrical parameters such as number of carriers at steady state, quantum capacitance has also been plotted in Figures for different value of V_g as well as for disorder. Comparison between Ideal and Disordered graphene has been shown. It is clear that Drain current, Number of carriers at steady state and Quantum capacitance are strong function of Disorder potential which fluctuate because of impurity in Environment and substrate impurity. In comparison it is seen that for Disorder parameter value of 0.4 the Disordered GNR FET has similar electrical

behaviour as Non Disordered GNR FET. So, it is concluded to keep the environmental impurity as low as possible or near about of 0.4.

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