Simulation of Quantum Capacitance in Graphene Nanoribbons Considering Channel Width Variation

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***Abstract* - Graphene nanoribbon (GNR) relinquishes the zero band gap technology provides the promising candidates in electronic conduction. Lessening the width in nano scale as a ribbon creates considerable bandgap. The effect of changing the width of GNR, classical capacitance follows the linear curve need higher analysis of quantum capacitance in different regime using variation of width method. Persistence of quantum phenomena is observed through comparison of quantum capacitance and classical capacitance in nano scale device. In this paper at first we will observe the band gap energy for varying GNR's width.We will also calculate classical capacitance by varying again GNR's width.But classical capacitance does not give full information when electron goes through GNR channel.For this we will calculate a capacitance formed in GNR by varying GNR's width called quantum capacitance considering two regime named as degenerate and nondegenerate regime.From this we will get information that among classical capacitance, quantum capacitance in degenerate and nondegenerate regime which one dominates or is dominated over another. Upon this a compromise of between width of GNR and capacitance is the better designing of GNR based device in nanotechnology.**

***Keywords - graphene nanoribbon, bandgap, classical capacitance, quantum capacitance* degenerate and nondegenerate regime.**

I. INTRODUCTION

A new class of materials in the carbon family which also recognized as promising building blocks for nano-electronic devices is the utilization of the patterned graphene which constitutes an array of sufficiently narrow graphene nanoribbons [1, 2]. GNRs are one dimensional (1D) structures with confinement of carriers in two directions. According to the edges GNRs are classified as zigzag and armchair [3].

Having two open edges at both sides GNRs are different from Carbon Nanotubes (CNTs). The edges of GNRs are most of the time hydrogen terminated and have no major impact on the bandstructure of GNRs as the edges not only remove the periodic boundary condition along the circumference of CNTs, but also make GNRs more vulnerable to defects than CNTs [4, 5]. Along with CNTs offers better electrical properties such as higher carrier mobility compared to GNRs, we chose to use GNRs instead of CNTs due to the reason that the chirality of CNTs is very difficult to control during the fabrication. On the other hand the chirality of GNRs is easier to manage during the fabrication [6, 7]. Through the geometrical nature, the semiconducting properties of GNRs can be predicted which is the width dependent on its number of dimmer lines (N) in which the semiconducting property in GNRs occur when N = 3p or N = 3p+1, where p is an integer [8, 9, 10, 11]. For future digital electronic application GNR is very suitable due to not only its small size but also its overall potential characteristics, especially the electronic properties [12]. Armchair GNRs show semiconducting behaviors with a direct energy gap. The quantum confinement effect (QCE) which can be characterized by [energy gaps] versus [width]. Besides the QCE, the edge effects play an important role to force the armchair GNRs to be semiconductors [13]. The capacitance formed between the channel and gate is one of the most important characteristics of FET device in which the knowledge and well understanding of the capacitance will in turn greatly help to understand fundamental electronic properties [14]. By the device geometry and a dielectric constant of the medium the capacitance in classical approach is completely determined but quantum effects will give prominent impact to the device performance once the transistor approaches the size of nanoscale device and hence the quantum capacitance must be taken into consideration [15, 16, 17, 18]. Although graphenes first isolation as a single-layered sheet of graphite, it has attracted enormous interest due to its extraordinary electronic properties [19, 20]. Especially the extremely high mobility in graphene has made it as a promising candidate for transistors [21, 22].

Our analysis is based on variation of width method in GNR when decreases it opens the bandgap giving the transistor cut into conduction. We will investigate importance of GNR's width on classical capacitance but for clear understanding we will go through the quantum capacitance in various regime.At later we will compare the quantum and classical capacitance of GNR based device.

II. PROPOSED METHOD

The names ―"armchair" and ―"zigzag" refer to the shape of the edge in the transport direction of the GNR and follow the standard GNR literature convention, which is opposite to the CNT convention [23]. Recent studies have shown that GNRs can be either metallic (N=3p-1) or semiconducting (N=3p or 3p+1), depending on the atomic structure of their edges. An armchair ribbon(A-GNR) is cut so that the edge looks as if it consists of repeated armchairs. The width of an armchair ribbon can be defined in terms of the number of dimer lines (N): [24]

$$W_{ac} = (N-1)\frac{\sqrt{3}}{2}a \quad (1)$$

Where a=1.42A° the nearest neighbor distance.

The width of a zigzag ribbon is demonstrated as

$$W_{zz} = (N-1)\frac{3}{2}a \quad (2)$$

Where a=1.42A° the nearest neighbor distance

As we have seen in [27] that quantum capacitance can be calculated varying energy constant including conduction energy along with Fermi energy. Assuming that Fermi level lies in middle between conduction and valence band we will analyze in depth of device structure mainly width from which quantum capacitance is calculated. For this at first we have to look upon some influencing parameter. Although armchair GNRs have three typical families (corresponding to N = 3p, 3p+1, 3p+2, respectively. where p is any integer) with distinguished energy gaps, they have similar band shapes .The relations between E_G (band gap) and width of GNRs can be derived as following [25]

$$E_G = 2\pi t\sqrt{3}\left(\frac{p}{N+1} - \frac{2}{3}\right) \quad (3)$$

Here we have considered only two structure like $N=3p$ or $N=3p+1$ for observing only semiconducting properties. And $t = -0.2\,eV$ hopping parameter.

Now the classical capacitance, $C_c$given by the expression of gate insulator capacitance, C_{ins}[26]

$$C_{ins} = N_G \varepsilon_o k\left(\frac{W_{ac}}{t_{ox}} + \alpha\right) \quad (4)$$

Where N_G is the number of gates, k is the relative dielectric constant of the gate insulator here 3.9 for SiO_2, ε_0 is the permittivity of vacuum, t_{ox} represents the gate insulator (oxide) thickness here 4nm and $\alpha = 1$ is a dimensionless fitting parameter.

An important quantity in the design of nanoscale devices is the quantum capacitance begins with fermi probability function is given by

$$f(E) = \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1} \quad (5)$$

In the nondegenerate condition, 1 from the denominator of the fermi probability function is neglected and thus the quantum capacitance in nondegenerate regime $C_{QND}(non\deg)$ at room temperature as a function of Fermi energy model is [27]:

$$C_{QND}(non\deg) = \frac{e^2}{3ta\pi}\left(\frac{x + \frac{E_G}{2k_B T}}{\sqrt{x + x\frac{E_G}{k_B T}}}\right)\exp(\eta) \quad (6)$$

Also by neglecting exponential term in degenerate regime of quantum capacitance appears as

$$C_{QND}(\deg) = \frac{e^2}{3ta\pi}\left(\frac{x + \frac{E_G}{2k_B T}}{\sqrt{x + x\frac{E_G}{k_B T}}}\right) \quad (7)$$

Where $k_B = 8.6 \times 10^{-5}\, eV/K$ (Boltzmann constant),T = Room temperature in *K*.

$$x = E - \frac{E_G}{2} \quad (8)$$

And

$$\eta = \frac{E_C - E_F}{k_B T} \quad (9)$$

Where E_C is the conduction band energy and E_F Fermi level energy .Here we have assumed these two energy is very close to each other.

III. Simulated Studies

A. Width of GNR

Width of the edge of GNRs is derived by their no. of dimer line which is obtained from equation (1).

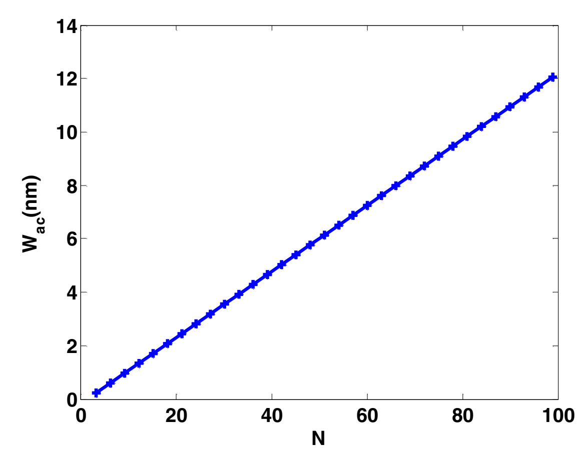

Fig.1. Width of Armchair nanoribbon in (nm) vs. Number of dimer line.

We have seen that as equation (1) denotes straight line for increasing number of dimer line in the armchair structure it increases the width of GNR.

B.Bandgap Energy

GNR has finite electronic properties which depend on their channel width .In order to go to the conduction band from valence band the electron must have to achieve an amount of energy which is equal to the bandgap energy. This bandgap energy is inversely proportional to the channel width which obtained from equation (3) by putting the value of N+1 and is seen in the curve given below.

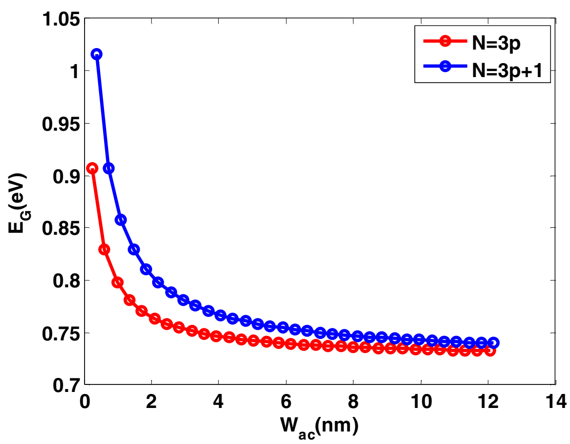

Fig. 2.Bandgap Energy in (eV) vs. Width of GNR in (nm) for N = 3p, 3p+1.

From the above Fig.2 it is seen that as the width of GNR is increasing the band gap is decreased. This behavior shows inverse relation between bandgap and width of GNR as the equation (3) indicates. But it is realistic for choosing 4-8 nm GNR where the band gap in between 0.74-0.76 eV

C.Classical capacitance

The effects of classical capacitance give insignificant impact on the device performance once the transistor approaches the size of nanoscale device. It is proportional to device dimension (width) hence the quantum capacitance must be taken into consideration. The classical capacitance is achieved by the equation (5).

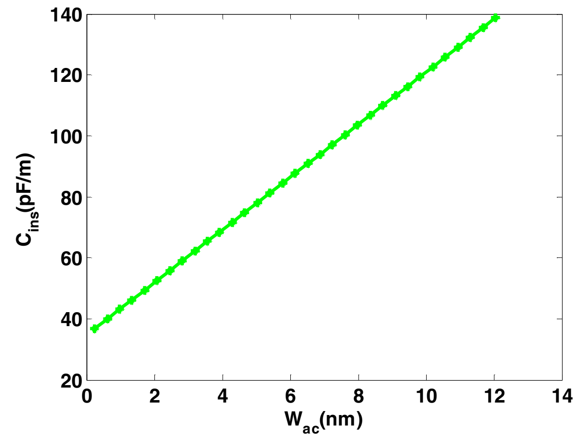

Fig. 3.Classical capacitance (pF/m) vs. Width of GNR in (nm).

We have seen that classical capacitance increases for the corresponding increase in width of GNR.

D.Quantum capacitance

Nondegenerate regime:

In non-degenerate regime at room temperature when the width of A-GNR increases the quantum capacitance of the channel linearly decreases for N=3p and N=3p+1.The quantum capacitance is obtained from the equation (7).

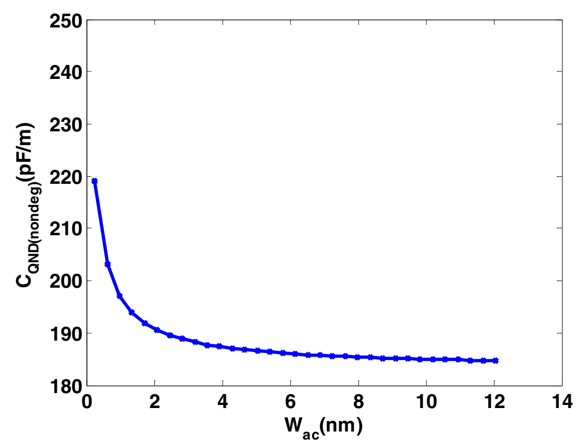

Fig. 4.Quantum capacitance (pF/m) vs. Width of GNR in (nm) when N=3p.

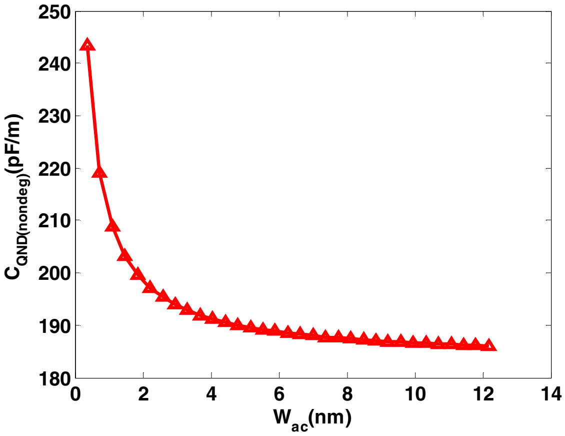

Fig. 5.Quantum capacitance (pF/m) vs. Width of GNR in (nm) when N=3p+1.

Now if we integrate quantum capacitance in non-degenerate regime for N=3p and N=3p+1 the Fig.6 will be

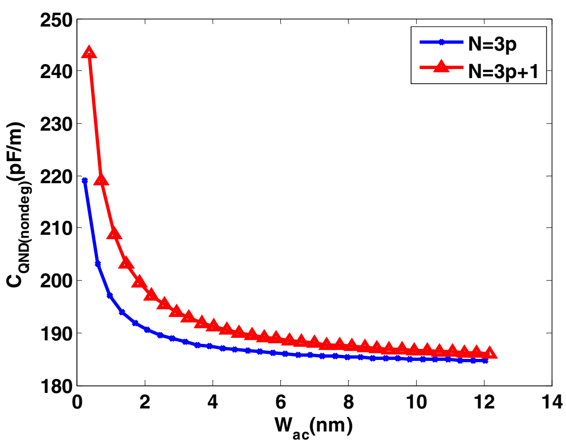

Fig. 6.Quantum capacitance (pF/m) vs. Width of GNR in (nm) when N=3p and 3p+1

We have seen that for N=3p the quantum capacitance in non-degenerate regime is 219.12 pF/m to 184.73 pF/m. And for N=3p +1the quantum capacitance in non-degenerate regime is 243.30 pF/m to 186.05 pF/m. So it can be said that large structure (N=3p+1) capacitance will be more than the small (N=3p) structure.

Degenerate Regime:

In degenerate regime capacitance values also decreases as the width of A-GNR increases .It is drawn from equation (8).

Here individual response curve is shown in Fig.7, first quantum capacitance in degenerate regime for N=3p .

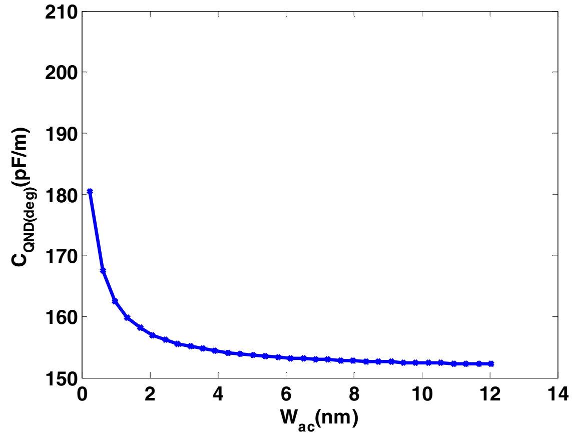

Fig. 7.Quantum capacitance (pF/m) vs. Width of GNR in (nm) when N=3p.

Again for N=3p+1 the quantum capacitance in degenerate regime is shown in Fig.8.

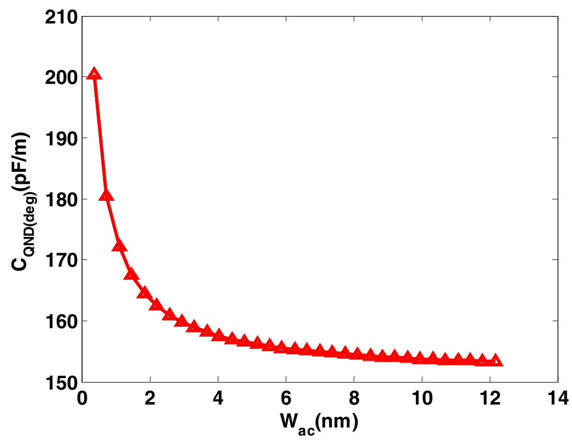

Fig. 8.Quantum capacitance (pF/m) vs. Width of GNR in (nm) when N=3p+1.

If we integrate quantum capacitance in nondegenerate regime for N=3p and N=3p+1 the Fig.9 will be

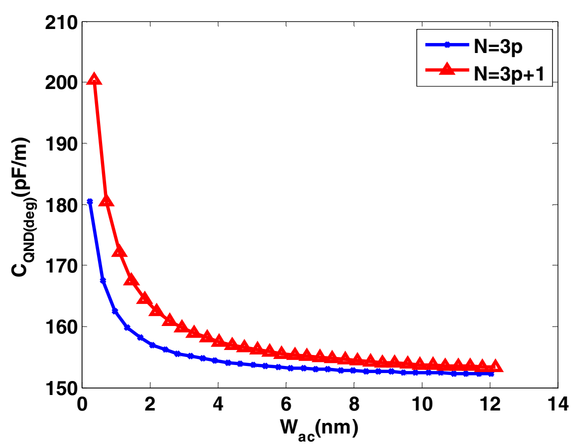

Fig. 9.Quantum capacitance (pF/m) vs. Width of GNR in (nm) when N=3p+1.

Here we have seen that for N=3p the quantum capacitance in degenerate regime is 180.52 pF/m to 152.18 pF/m .And for N=3p +1the quantum capacitance in non-degenerate regime will be 200.43 pF/m to 153.27 pF/m. Again it can be said that large structure (N=3p+1)capacitance will be more than the small (N=3p) structure.

IV. CONCLUSION

In this paper "quantum capacitance" is discussed in both nondegenerate and degenerate regime which may be useful in modeling electronic devices. In nanoscale, models must include quantum capacitance (non-degenerate regime, degenerate regime) in order to properly capture the device behavior in case of fully turned-on devices which dominates over the classical capacitance. In fully turned on transistor which indicates bandgap opening in GNR depends on width of GNR where quantum capacitance in non-degenerate regime dominates the classical capacitance and quantum capacitance in degenerate regime. But in fabrication it is necessary how width of GNR can be design for a required quantum capacitance. From the above Fig.6 and 9 we see that if the GNRs width is between 4-8nm then it will satisfy all types of classical capacitance, quantum capacitance in degenerate and nondegenerate regime with a minimum amount of quantum capacitance. In future from current, voltage through the device can be calculated for N=3p+1 and N=3p considering channel width .

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REFERENCES

[1] G. Liang, N. Neophytou, D. E. Nikonov, and M. S. Lundstrom, "Theoretical study of Graphene Nanoribbon Field-Effect Transistors," Technical Proceedings of NSTI Nanotechnology Conference and Trade Show, vol.1, 2007.

[2] G. chiau, N. Neophytou, D. E. Nikonov, and M. S. Lundstrom, "Performance Projections for Ballistic Graphene Nanoribbon Field-Effect Transistors," IEEE Transaction Electron Device, vol. 54, pp. 677-682, 2007.

[3] Nakada K., Fujita M., Dresselhaus G., and Dresselhaus M.S., "Edge state in graphene ribbons: Nanometer size effect and edge shape dependence," Physical Review B, vol. 54, pp. 17954–17961, 1996.

[4] M. Fujita, K. Wakabayashi, K. Nakada and K. Kusakabe, "Peculiar Localized State at Zigzag Graphite Edge," Journal of Physical Society ,vol.65, pp. 1920-1923 ,1996.

[5] A. Naeemi and J. D. Meindl, "Conductance Modeling for Graphene Nanoribbon (GNR) Interconnects", IEEE Electron Device Letters, vol. 28,pp. 428-431, 2007.

[6] G. L. Harris, P. Zhou,M. He and J.B. Halpren, "Semicondutor and Photoconductive GaN Nanowires and Nanotubes," Lasers and Electro-Optics Conference , vol. 239, pp.6-11 ,2001.

[7] G. Liang, "Widths Effects in Ballistics Graphene Nanoribbon FETs," IEEE International Nanoelectronics Conference, pp. 1187-1188, 2008.

[8] M. Choudhury, Y. Yoon, J. Guo and K. Mohanram, "Technology Exploration for Graphene Nanoribbon FETs," Design Automation Conference,2008.

[9] Z. F. Wang, Q, Li, Q.W. Shi, X.Wang, J. Yang, J.G. Hao and J. Chen, "Chiral Selective Tunneling Induced Negative Differential Resistance in Zigzag Graphene Nanoribbon: A theoretical study,"Applied Physics Letters ,vol.92,pp.133114, 2008.

[10] D. Unluer, F. Tseng, W. Ghosh and M.R.Stan, "Atomistic Deconstruction of Clear Performance Advantages of a Monolithically Patterned Wide-Narrow-Wide All-Graphene FET," Device Research Conference, pp. 75-76, 2009.

[11] P. Dietl, "Numerical Studies of Electronic Transport Through Graphene Nanoribbons with Disorder," Diploma Thesis, 2009.

[12] Z.Guo, D. Zhang, and X. Gong, "Thermal conductivity of graphene nanoribbons," Applied physics letters, vol.95, pp. 163103-163106, 2009.

[13] Y Son, M. Cohen and S. Louie "Energy gaps in graphene nanoribbons," Physical Review Letters, vol. 97, pp. 216803- 216806, 2006.

[14] A.A. Shylau, J.W. Klos and I.V. Zozoulenko, "Capacitance of Graphene Nanoribbons", Physical Review B,vol.80, pp.205402, 2009.

[15] P. Zhao, M. Choudhury, K. Mohanram, J. Guo, "Computational Model of Edge Effects in Graphene Nanoribbon Transistors", Nano Research,vol.1, pp. 395-402, 2008.

[16] Z. Chen and J. Appenzeller, "Mobility Extraction and Quantum Capacitance Impact in High Performance Graphene Field-effect Transistor Devices," IEEE International Electron Devices Meeting, pp. 1-4, 2008.

[17] Serge Luryi, "Quantum Capacitance Devices,"Applied Physics Letters, vol. 52, No. 6, 1988.

[18] D.L. John, L.C. Castro and D.L. Pulfrey, "Quantum Capacitance in Nanoscale Device Modeling," Journal of Applied Physics, vol. 96, 2004.

[19] A. K. Geim and K. S. Novoselov "The rise of graphene," *Nature Materials*, vol. 6, pp. 183–191, 2007.

[20] R. Ruoff "Calling all chemists," Nature Nanotechnology, vol.31, pp.10-11,2008.

[21]Y.-M. Lin, C. Dimitrakopoulos, K. A. Jenkins, D. B. Farmer, H.-Y. Chiu, A. Grill and Ph. Avouris- "100-GHz Transistors from Wafer-Scale Epitaxial Graphene,"Science, vol.327, pp.662,2010.

[22]X. Liang, Y. Jung, S. Wu, A. Ismach, D. Olynick, S. Cabrini and J. Bokor "Formation of Bandgap and Subbands in Graphene Nanomeshes with Sub-10 nm Ribbon Width Fabricated via Nanoimprint Lithography,"Nano Letters, vol.10, pp.2454–2460,2010

[23] M. R. Stan, D. Unluer, A.Ghosh, and F. Tseng, "Graphene Devices, Interconnect and Circuits –Challenges and Opportunities," IEEE Electron Device Letters, vol. 978, pp. 69-72, 2009.

[24] L. Feng Mao "Quantum capacitance of the armchair-edge graphene nanoribbon," Pramana journal of physics, vol. xx, no. x,pp.1-9,2013.

[25] H. Zheng, Z. Wang, T. Luo, Q.Shi, and J. Chen, "Analytical Study of Electronic Structure in Armchair Graphene Nanoribbons," Physical Review B,vol.75,pp.16, 2007.

[26] J. Guo, Y. Yoon and Y. Ouyang, "Gate Electrostatics and Quantum Capacitance of Graphene Nanoribbons," Nano Letters, vol.7,pp 1935-1940, 2007.

[27] Z. Johari, N.A. Amin, M. Taghi Ahmadi, D. C.Y. Chek, S.Mahdi Mousavi and R. Ismail "Modeling of Quantum Capacitance in Graphene Nanoribbon", Conference Proceeding in American Institute of Physics,vol.1341,pp.384-387,2011.