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# Simulation of Energy band gap opening of Graphene Nano Ribbons

Anas M M[1], Roy Paily[2]
[1](ECE Dept., MITS/ MG University, India)
[2](ECE Dept., IIT Guwahati/ IIT Guwahati, India)

***Abstract:*** *Graphene nanoribbons are among the recently discovered carbon nanostructures, with unique characteristics for novel applications. One of the most important features of graphene nanoribbons, from both basic science and application points of view, is their electrical band gap [1]. In this research, we study the tunability of band gap in single and double layer Graphene nano ribbons (GNRs) of specified widths and edge geometries. The calculations are carried out using Tight Binding quantum mechanical simulations for obtaining the optimized atomic configurations of the nanoribbons and their electronic structures. Our calculations show that for single-layer graphene nanoribbon with a width of 12A$^0$, the one with armchair edge is semiconducting with a band gap of 0.25 eV whereas the one with zigzag edge is metallic. For bilayer nanoribbons, two different stacking configurations (AA and AB) are considered.*

***Keywords:*** *AA, AB, BLG, Eg, GNR, STM.*

## I. Introduction

The fact that carbon forms many allotropes, compounds, and intricate net-works, is essential to the existence of life on earth. There is no surprise, therefore, that carbon compounds and allotropes are the most studied and researched materials in the world. The capability of carbon atoms to from complicated networks is fundamental to organic chemistry. Even elemental carbon shows complicated bonding, forming a number of allotropic structures. Diamond and graphite are the two most ancient and well understood materials. It is due to the unusual bonding of carbon that diamond is considered to be one of the hardest naturally occurring materials known to humans. Recently discovered allotropes like fullerenes and nanotubes are the center of focus for many scientists researching in the fields of chemistry, physics, biology, and material science [2]. Thus far, I mentioned three dimensional (diamond, graphite), one dimensional (nanotubes) and zero-dimensional (fullerenes) symmetric allotropic structures of carbon. Until recently the two dimensional from was missing, resisting any attempt of experimental observation.


Fig. 1 allotropes of carbon

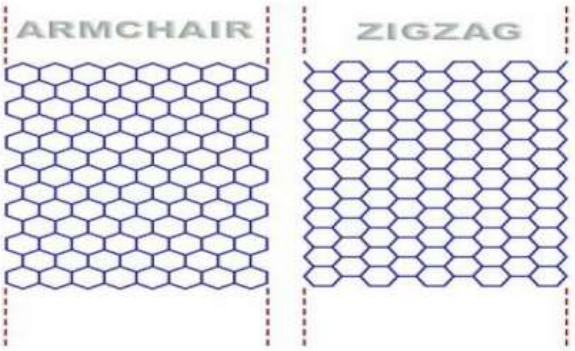


Fig. 2 two different variation of graphene nano ribbon according to edge geometry

The missing two dimensional structures is now called graphene. Graphene is planar hexagonal arrangement of carbon atoms (fig:2). It is the name given to a flat mono-layer of carbon atoms arranged tightly in honeycomb lattice, which is the building block of graphitic materials (nanotubes and fullerenes contain pentagons). Graphene is the starting point of all calculations and structural studies on graphite, carbon nano-tubes and fullerene. Importantly, in the mid-1930s two scientists Landau and Peierls proposed that 2D crystals of carbon (graphene) could not exist and were thermodynamically unstable [3].

## II. Width and band-gap opening of single layer GNR

The origin of energy gaps for armchair is ascribed to both quantum confinement and the crucial effects of edges. The electronic states of GNRs largely depend on the edge structures (armchair or zigzag, with armchair being the picture on bottom). Zigzag edges provide the edge localized state with non-bonding molecular orbitals near the Fermi energy. They are expected to have large changes in optical and electronic properties from quantization. Calculations based on tight binding predict that zigzag GNRs are always metallic while armchairs can be either metallic or semiconducting, depending on their width. However, Extended Huckel calculations show that armchair nanoribbons are semiconducting with an energy gap scaling with the inverse of the GNR width [4]. Indeed, experimental results show that the energy gaps do increase with decreasing GNR width. Graphene nanoribbons with controlled edge orientation have been fabricated by scanning tunnelling microscope (STM) lithography [5].

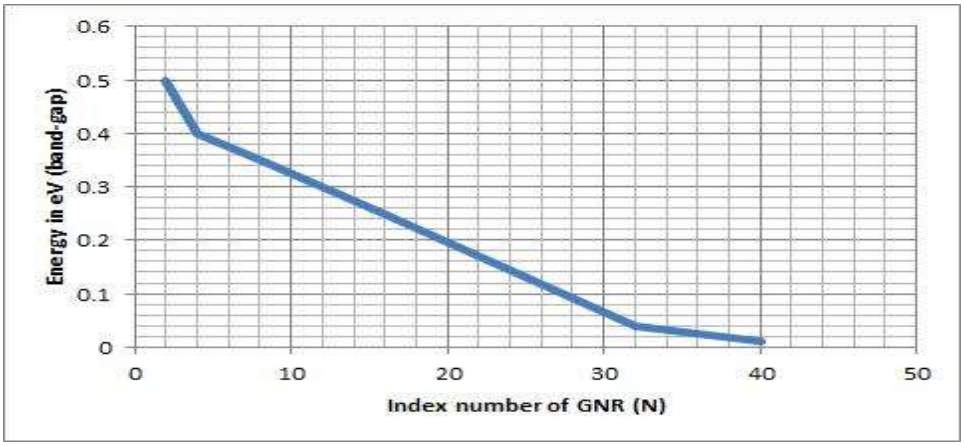


Fig. 3 Eg vs. N Curve

TABLE I Comparison of Index number (N) and band gap

| Index number(N) | Band gap(Eg) |
|---|---|
| N=2 | Eg=0.5eV |
| N=4 | Eg=.4eV |
| N=8 | Eg=.35eV |
| N=16 | Eg=.25eV |
| N=32 | Eg=.04eV |
| N=40 | Eg=.01eV |

From the table I and fig. 3 it is clear that bang gap GNR can be changed or tuned according the width of GNR.

## III. Bandgap Tunability due to stacking, interlayer spacing and perpendicular voltage

The topology of the AA stacked bilayer GNR appears to be the dominant factor in predicting its zero gap. Note that the existence of the energy gap in single layer zGNR is associated with the (unsaturated) dangling bonds associated with edge atoms. On the other hand, the interaction between edge atoms is facilitated by the topology of the AA stacked bilayer leading to crossing of the bands at Fermi level. For a large inter layer spacing of 10 $A^0$, each band is twofold degenerate due to negligible interaction between the two passivated single-layer GNRs.

The calculated band gap is the same as that of the single-layer GNR.Recent theoretical studies have predicted that a significant band gap could be induced by lowering the symmetry of the system through the application of a perpendicular electric field [6] [7]. One of the most remarkable properties of BLG is the ability to open a gap in the spectrum by electric field effect biased BLG.In the absence of an external perpendicular electric field unbiased BLG the system is characterized by four bands, two of them touching each other parabolically at zero energy, and giving rise to the massive Dirac fermions mentioned above, and the other two separated by an energy.

Based on the Bernal stacking model atom positions A1 and B1 for layer 1, and A2 and B2 for layer 2, are shown in Figure 3;each layer is a hexagonal carbon lattice and the inter plane distance is about 0.594 nm. The size of the band gap Eg can be controlled by adjusting carrier concentration and by applying an external electric field allow-ing the band gap spectrum to be controlled [8].The electronic structure of bi-layer graphene change significantly when a strong electric field is applied, particularly in the region around the K point.

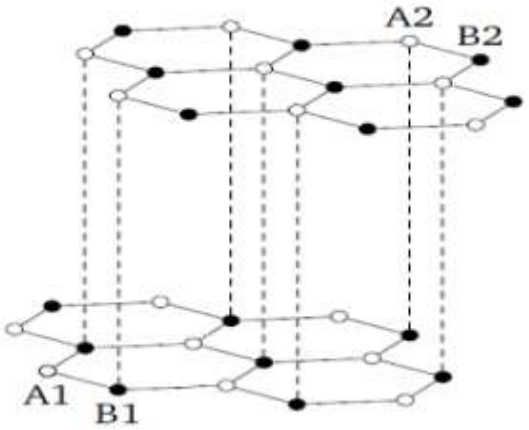


Fig 3. AB (bernal) Stacking

TABLE II Comparison of Index number (N) and band gap

| ELECTRIC FIELD(V/A) | Band gap(Eg) |
|---|---|
| V=0.3 | Eg=.12eV(more overlap) |
| V=0.5 | Eg=.15eV(more overlap) |
| V=1.0 | Eg=0.0eV(no overlap) |

## IV. Conclusion

Despite smaller energy gaps in bilayer GNRs (BLGNRs) in comparison with their single layer counterparts (SLGNRs) the fact that BLGNR systems have lower sensi-tivity to low frequency noise, accompanied by a unique property of tunable bandgap with perpendicularly applied electric field render them as more desirable candidates for nanoelectronic applications.It is observed that double layer graphene transistors have better gate voltage control over single layer graphene transistors. Better satura-tion region is obtained by using bilayer graphene channel for a channel length of 5nm and 8nm.Bilayer GNR system in the AA stacking configuration exhibits substantially enhanced electron transmission as well as tunneling current compared to single-layer GNRs.

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