ORIGINAL ARTICLE

SAMRIDDHI Volume 14, Issue 3, 2022 Print ISSN: 2229-7111 Online ISSN: 2454-5767

Study and Modeling of Graphene-Boron Nitride Heterostructures

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Abstract

When we talk about nano devices, the molecule and its interface with electrodes play a key role. So, one of the major objectives is to select an organic nanomaterial with extensive applications, which requires smart synthesis of appropriate materials and an understanding of their properties. Here we modeled a device, which not only adds another "protuberance" to learn about the transport properties of the molecule but also helps in grasping its use as a considerable material for future flexible electronics. Modeling of materials at the nano-level not only provides fundamental insight into the properties of crystalline defects but also gives a reasonable understanding of phase stability and learning of processes like atomic diffusion interface migration. For the development of devices at a mesoscopic and macroscopic level and with atomistic input parameters, this recognition serves as a guide. We tried to model how the layers of one type of molecule and the interaction of two different types of molecular layers control the junction charge transport characteristics.

Keywords: Band gap, Boron-Nitride, Graphene, Interface, Molecular Junction, NEGF, Two probe system.

SAMRIDDHI : A Journal of Physical Sciences, Engineering and Technology (2022); DOI: 10.18090/samriddhi.v14i03.14

Introduction

Here we present theoretical as well as experimental studies about the electronic and electric transport properties in graphene-based systems. Our work/results presented give better insight into the design or rationalization of molecular electronic devices and the dreams of Flextronics/Molecular Electronics.[1-4] The subject of this work is the modeling and analysis of electrical properties in graphene and its interaction with boron-nitride. When it comes to the advantages of using this model, it allows comparison in experiments with fixed parameters.[5-8] By using these experiments we can find many molecules with similar properties. One must consider how intra and inter molecules interaction affects the geometry of the system, the distribution of the electronic charge, and the broadening of the electronic levels. The method we used to study carrier transport in the nano-scale region uses NEGF formalism.[9-12] The model we used consists of a junction of two different types of molecules layer i.e., graphene and boron-nitride. Further variation in band gap for different inter-layer distances and electric field orientation is studied.

Graphene-Boron Nitride Heterostructures

Due to progress in the development of devices[13-15] at the molecular level, periodic systems, especially thin films with their distinguished electrical and mechanical properties, have gained wide attention. For example, graphenes band structure shows zero gaps at the Dirac point and band gaps of more than one layer configuration are tunable for the applied electric fields but depend upon the symmetry of layers.[16, 17] Graphene due to its planer structure with carbon rings, demonstrates suitable electrical properties for its application in switchable devices. We already know that BN has a sizeable band gap and it is quite stable at the chemical level, so it will be very interesting to study the graphene/BN layer for their electronic structures under the effect of the applied electric field. It is interesting to study these materials for their application in switchable devices.[18-22]

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How to cite this article: Amardeep, Lamba, V.K. (2022). Study and Modeling of Graphene-Boron Nitride Heterostructures. *SAMRIDDHI : A Journal of Physical Sciences, Engineering and Technology,* 14(3), 337-340.

Source of support: Nil

Conflict of interest: None

Computational Models and Simulations

The models we used for calculations are in Figure 1. We have investigated the response of the molecular system using two probe systems. We have taken two probe models with nanostructure and electrodes and optimized it for input. We used NEGF and DFT, i.e., a combination of both methods, along with ATOMISTIX TOOLKIT, i.e., ATK package, to gain knowledge about the electronic properties of our model.

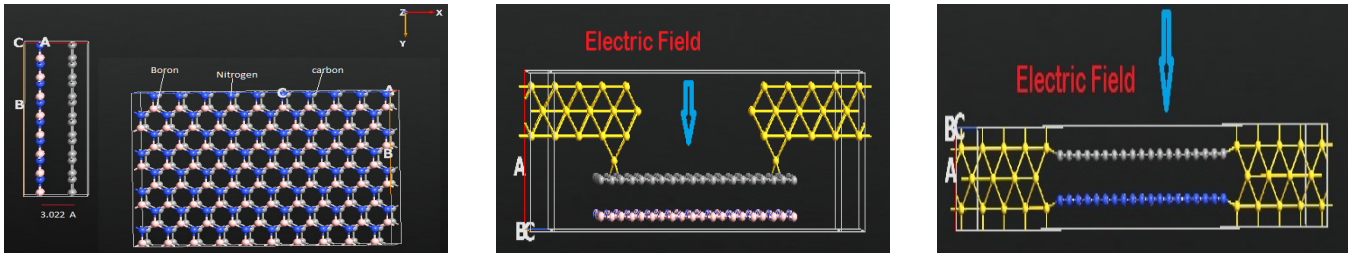

Figure 1: Graphene-Boron-Nitride Model.

Further, we computed change in conductance using two probe systems and studied the effect on charge transport using the NEGF approach.

Results And Discussion

Figure 1 shows the band structures of graphene/BN and BN/BN bi-layer. We found that their band structures demonstrate large dissimilarity from each other. The band structure for the graphene/BN bi-layer depends upon the carbon atoms near the Fermi level. Further increasing randomly the number of boron atoms the band gap decreases. The change in band gap in the Graphene-boron-nitride layer is dominated by the morphology of carbon atoms and significantly influences the change in the HOMO-LUMO band gap and molecular orbital levels. From the figures, we can say that both systems exhibit modulation of their band gaps, when an external field is applied. Also, the band structure gives an idea that the conduction bands are affected more strongly than valence bands.

We have studied the change in band gap with the applied electric field. The band gap of graphene/BN and BN/BN also varies with the distance between the layers as shown in Figures 2 to 5 and Table 1. It is clear from the figures that bi-layer systems exhibit modulation of their band gaps by the external field orientation and distance between the layers of the system.

Due to the applied electric field band gap in the graphene layer ranges from 0 to 205 meV. In the graphene-boron-nitride hybrid system, when the electric field was applied initially, the band gap increased linearly with the electric field. Later, it increased exponentially as shown in Figure 3. But when we talk about BN/BN bi-layer systems the case is just the opposite. This band gap shows a decrease with an increase in the applied electric field as in Figure 4. Also when we talk about relative change in band gap it is higher for graphene/BN bi-layer system as compared to BN/BN bi-layer system as per Figure 5.

From the above figures, we can state that the band gap of Graphene/BN is dominated by the graphene layer.

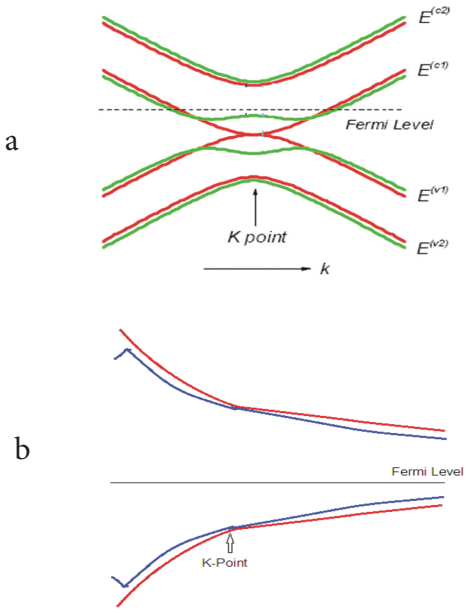

Figure 2: Band structures of (a) Graphene/BN and (b) BN/BN layers.

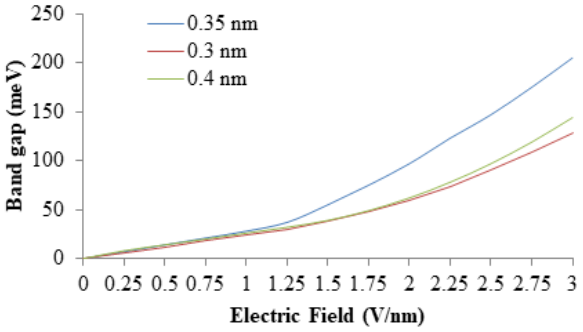

Figure 3: Band gap variation of Bi-layer Graphene at a different inter-layer distance with the applied electric field.

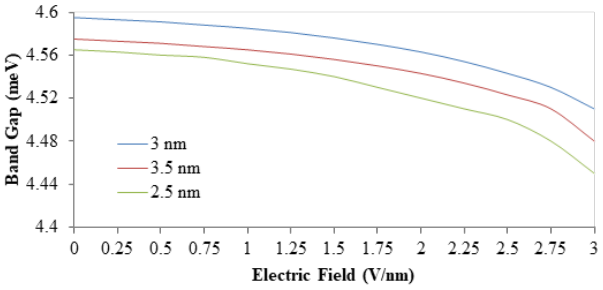

Figure 4: Band gap variation of Bi-layer Boron Nitride at a different inter-layer distance with the applied electric field.

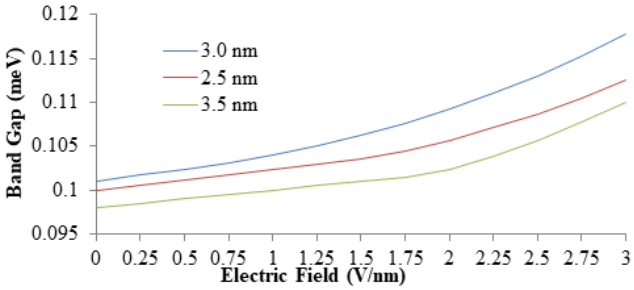

Figure 5: Band gap variation of Graphene/BN at a different inter-layer distance with the applied electric field.

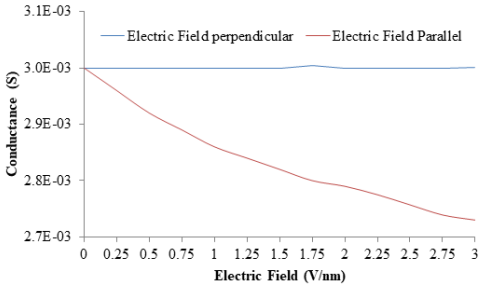

Figure 6: Conductance versus field orientation in Graphene/BN Bi-layer

Table 1: Inter length-dependent energy bands

System	*E(V/nm)*	*The band gap (eV) Interlayer distance (2.5nm)*	*The band gap (eV) Interlayer distance (3.0nm)*	*The band gap (eV) Interlayer distance (3.5nm)*
Graphene/BN	0	0.0970	0.1	0.101
Graphene/BN	0.5	0.0976	0.101	0.1025
Graphene/BN	1	0.0982	0.12	0.104
Graphene/BN	1.5	0.0987	0.104	0.106
Graphene/BN	2	0.0993	0.106	0.109
Graphene/BN	2.5	0.106	0.109	0.113
Graphene/BN	3	0.11	0.113	0.118
BN/BN	0	4.57	4.585	4.59
BN/BN	0.5	4.56	4.58	4.582
BN/BN	1	4.55	4.565	4.579
BN/BN	1.5	4.535	4.557	4.572
BN/BN	2	4.52	4.54	4.562
BN/BN	2.5	4.5	4.525	4.54
BN/BN	3	4.46	4.482	4.51

Figure 6 demonstrates that the field applied perpendicularly to the plane has no effect on conductance while conductance shows a decrease in it for the field applied parallel to the plane. Also, how the morphology of electrodes changes the charge transform should be considered carefully.

Conclusion

Charge transport through the junction is controlled by both the molecule and its interaction with electrodes. We have also studied the Effect on electric properties of Graphene-boron-nitride using a combined approach of density functional theory with NEGF. When we applied the electric field, the band gap initially increases linearly with the electric field and later increases exponentially. Further increasing randomly the number of boron atoms the band gap decreases. The distance between two layers also causes changes in the band gap and there is a direct relation between the two. Increase the distance between the layers higher will be the value of the band gap. The change in band gap in the Graphene-boron-nitride layer is dominated by the morphology of carbon atoms and significantly influences the change in the HOMO-LUMO band gap and molecular orbital levels. Further, we computed change in band gap for parallel and perpendicular orientation of the electric field and we found that band gap is independent of the perpendicular orientation of the electric field. When it comes to different application requirements for a specific purpose, this electric field orientation aspect can be quite useful.

Acknowledgment

Thanks for the support and encouragement from the RIC Department of I K Gujral Punjab Technical University, Jalandhar, Punjab, India.

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