Study of Electronic Properties of Single and Bilayer Graphene gr/hBNHeterostructure

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Abstract: As very high mobility of graphene on conventional silicon oxide is being deteriorated, sorequiresanother 2D oxide to maintain the mobility and quality of the pristine graphene layer. Research and survey proves Hexagonal boron nitride (hBN) as one of the suitable 2D atomically flat layered substrate which allow graphene device fabrication without any degradation in graphene ballistic transport.This paper presents electronic properties of single and bilayergraphene, gr/hBN(hexagonal Boron Nitride) heterostructure. The electronic band diagram, current density and charge carrier density with respect to the thickness of graphene layer over gr/hBNheterostructure is being presented.

Keywords: *band diagram, bilayer graphene, electronic properties, graphene, gr/hBN heterostructure, hexagonal Boron Nitride.*

I. Introduction

Graphene is of high interest 2D material for electronics application [1-2], because of its very high electron mobility [3-5] of 200000cm^{2}V^{-1}S^{-1} in its pure suspended state. It is just out of imagination thoughts that an atomically thick/thin material could be thermally stable. Although graphene shows marvellous electronics qualities in its pristine thin film form but these properties is being deteriorated by the supporting semiconductor material and oxides [6-7]. The mean free path greater than 2 microns at high carrier density 10^{12} cm^{-2}with big low down in intrinsic mobility to extrinsic mobility from 2 x 10^5 to 4 x 10^4 cm^2/Vsec for graphene at room temperature seeks to find a new substrate choice for graphene based electronics[6]. Graphene electronic devices exhibits much inferior characteristic on SiO_2 as expected of intrinsic graphene properties [7].Thus the Research advancements come in terms of various 2D Dielectric materials like BN, BCN, etc.Specially hBN(hexagonal Boron Nitride) is found best suitable 2D material supports graphene flack and provide wonderful Gr/hBN interface along with keeping graphene's superb electronic qualities[8-10]. A dangling bond free smooth surface and atomically match structure of hBN is an appealing substrate for graphene electronic applications [8]. Even after solving substrate issue graphene based field effect device lagging regularly for bandgap,which is very useful to graphene device logicapplications. Bilayer graphenegr/hBNheterostructurei.e. graphene layers stacked with hBN layer as insulating isomorph of graphite produce a bandgap along with a good current ON/OFF ratio[11-15]. Gr/hBN heterostructure in its lateral tunnelling structure is compared with gr/MoS_2heterostructure and shows approximate current ON/OFF ratio 50 [11]. Another different structure named as encapsulated means a graphene layer capture by a hBN oxide at both top and bottom end also explore the scope and possibility of gr/hBN heterostructure and provide great results towards the graphene electronics [12-13]. Another work [14] compare gr/hBN heterostructures with (graphene nanoribbon) GNR/hBN heterostructure suggests that gr/hBN heterostructures are better graphene structure option for graphene based electronics devices.

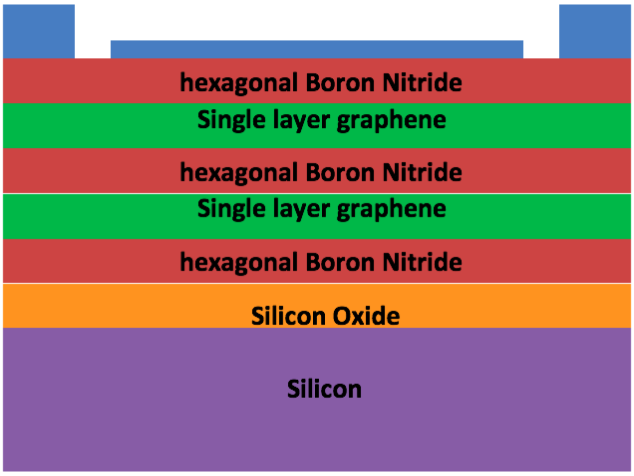

Figure 1 (colour online)Single layer Gr/hBN Heterostructure Fits for GFETs, with soucre, drain at top ends and gate in top middle with Ag/Cu metal.

Literature[16-21] has been explored gr/hBN heterostructure elecrtonically such as electronic highways(tranaports)in bilayer graphene[16], study of gr/hBN Van der Walls heterostructures[17-18] lineter layer or layer by layer dirac fermions fromation, crossectional images and buried interface properties [19], STM-Scanning Tunneling Microscopy based locale electronic properties [20] and inter layer tunneling insight [21] of gr/hBN heterostructures.

Figure 1 shows a gr/hBNi. e. graphene layer of atomic thickness is encapsulated by the hexagonal Boron Nitride layer of almost same thickness, and so provide a stable structure with appropriate band gap and much needed and improved current on-off ratio.

This paper is organsized in four sections, section-I introducesgraphene (2D material) properties and its pros and cons of substrate for graphene like hBN. section-IIdiscuss and explains the band diagram electronically band, current density and charge carrier density with respect to the thickness of graphene layer stacked overhBN, gr/hBNheterostructure followed by simulation results. Section-III concludes the paper that gr/hBN heterostructure is the appealing graphene electronic device structure. Final section IV cover references.

II. Results and Discussion

This section discusses and demonstrate single layer graphene, bilayer and graphene heterostructure (encapsulatedby top and bottom of hBN layers) electronic properties developed by AFORS-HET CAD tool. Electronic properties of single layer of thickness (.342nm) [2] and bilayer graphene of thickness (.684nm), with band gap of approx. 0.24 eV and encapsulation of them with the single layer hBN layer at the top and bottom end (gr/hBN) heterostructure is being explain graphically. Bandgap and other basic properties such as N_v, N_c, electron affinity and permittivity of the single layer and bilayer graphene is given in [1]. Bandgap, thickness and other basic properties of hBN layer is accounted on behalf of[7]where thickness almost same as (0.334nm)as of graphene layer,but with the band gap of 5.97 eV[9].

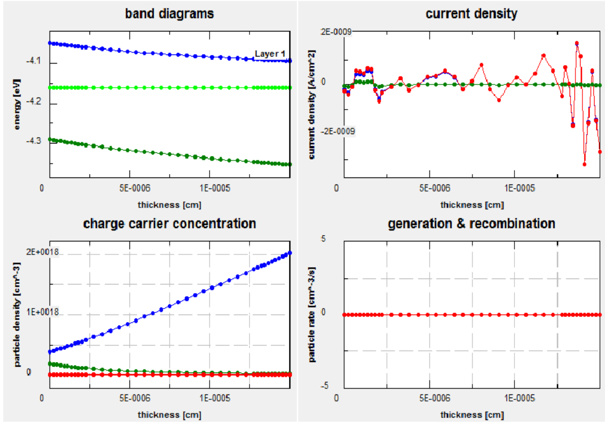

Figure 2.aSingle layer graphene electronic properties with band diagram, current density and charge carrier concentration along with zero rate of generation and recombination of charge carriers versus thickness of the particular layer.

Figure 2.a and 2.c graphically explore the bandgap, current density of am-bipolar nature graphene and the change in concentration of the graphene single layer and encapsulated graphene layer by the hBN layer top and down respectively, over the thickness of material layers.

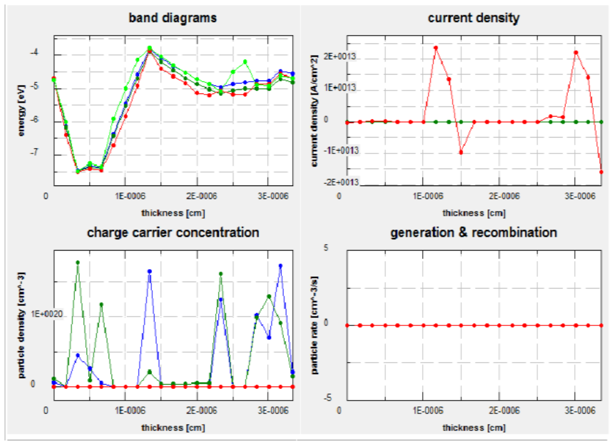

Figure 2.bBilayer graphene electronic properties with band diagram, current density and charge carrier concentration along with zero rate of generation and recombination of charge carriers versus thickness of the particular layer.

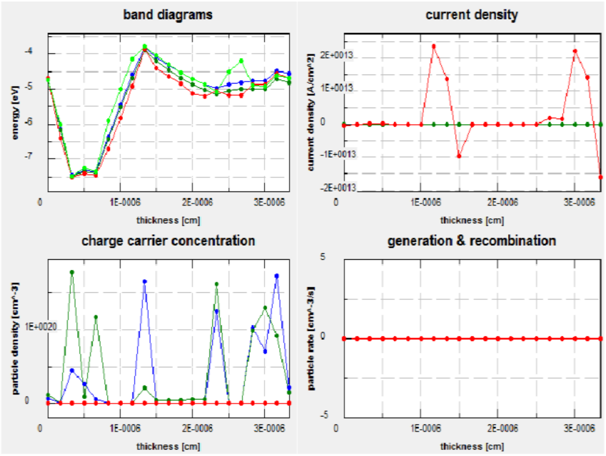

Figure 2.c Single layer graphene encapsulated by single hBN layers on top and bottom, electronic properties with band diagram, current density and charge carrier concentration along with zero rate of generation and recombination of charge carriers versus thickness of the particular layer.

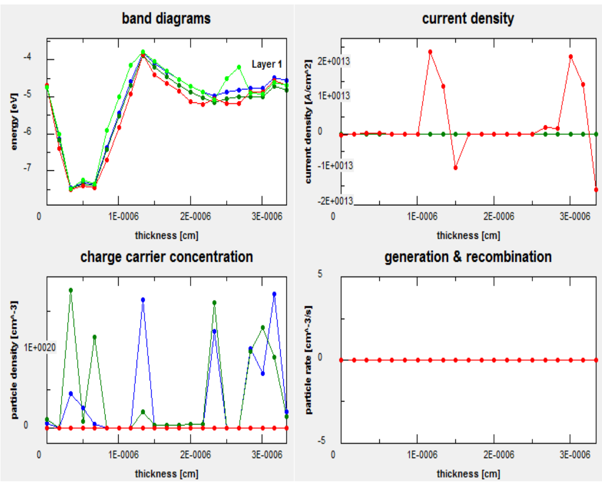

Figure 2.d bilayer graphene encapsulated by single hBN layers on top and bottom graphene, electronic properties with band diagram, current density and charge carrier concentration along with zero rate of generation and recombination of charge carriers.

Similarly, 2.b and 2.d explain results, like bandgap, current density carrier concentration and recombination and generation during the transport with the layer for bilayer graphene and encapsulated bilayer graphene by the hBN layer top and down respectively, over the variation of thickness of material layer.

III. Conclusions

The electronic properties of single layer and bilayer graphene, along with graphene over hBN layer (gr/hBNheterostructure) are studied and well demonstrated. The electronic band diagram, current density and charge carrier density with respect to the thickness of graphene layer over gr/hBNheterostructure have been presented.

IV. References

[1] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, and S. V. Dubones, I. V. Grigorieva and A.A. Firsov "ElectricFieldEffectinAtomically Thin Carbon Films,"*Sci. Report*, vol. 6, no. 3, pp. 183–191,2004.

[2] K. S. Novoselov and A. K. Geim, "The rise of graphene,"*Nat. Material*, vol. 6, no. 3, pp. 183–191, 2007.

[3] F. Schwierz, "Graphenetransistors,"*Nat. Nanotechnology*, vol. 5, no. 7, pp. 487–496,2010.

[4] A. K. Geim, "Graphene: status and prospects"*Science*, vol. 3, no. 734, pp. 1530-1534,2009.

[5] K. S. Novoselov, V. I. Falko, L. Colombo, P. R. Gellert, M. G. Schwab and K. kim "A roadmap for graphene,"*Nature*, vol. 490, no. 11, pp. 192–200,2012.

[6] J. H. Chen, C. Jang, S. Xiao, M. Ishigami, and M. S. Fuhrer, "IntrinsicandextrinsicperformancelimitsofgraphenedevicesonSiO2,"*Nat. Nanotechnologoy*., vol. 3, no. 4, pp. 206–209,2008.

[7] C. R. Dean, A. F. Young, I. Meric, C. Lee, L. Wang, S. Sorgenfrei, K. Watannabe, T. taniguchi, P. Kim, K. L. Shepard and J. Hone, "Boron nitride substrate for high-quality graphene electronics,"*Nat. Nanotechnologoy*, vol. 5, no. 10, pp. 722–726,2010.

[8] C. R. Dean, A. F. Young, I. Meric, C. Lee, L. Wang, G. H. Lee, K. Watannabe, T. taniguchi, P. Kim, K. Shepard and J. Hone, "Graphene based heterostructures",*Solid State Communication*, vol. 152, no. 5, pp. 1275–1282,2012.

[9] K. Watannabe, T. Taniguchi, H. Kanda, "Direct-bandgap properties and evidance for ultraviolet lasing of Graphene on hexagonal boron nitride single crystal", *Nature Material*, Vol. 3, no. 5, pp. 404-409, 2004.

[10] Pedro C. Feijoo, Francisco Pasadas, José M. Iglesias, El Mokhtar Hamham, Raúl Rengel, and DavidJiménez,"Radio Frequency Performance Projection and Stability Tradeoff of h-BN Encapsulated Graphene Field-Effect Transistors,". *IEEE Trans. Electron Device*,vol. 66, no. 3, pp. 1567–1573,2019.

[11] J. S. Moon, H. C. Seo, F. Stratan, M. Antcliffe, A. Schmitz, R. S. Ross,

A. A. Kiselev, V. D. Wheeler, L. O. Nyakiti, D. K. Gaskill, Kang-Mu Lee, and P. M. Asbeck, “Lateral Graphene Heterostructure Field-Effect Transistor,” *IEEE Trans. Electron Device*, vol. 34, no. 9, pp. 1190–1192,2013.

[12] Tarun Chari, Inanc Meric, Cory Dean, and Kenneth Shepard, “Properties of Self-Aligned Short-Channel Graphene Field-Effect Transistors Based on Boron-Nitride-Dielectric Encapsulation and Edge Contacts,” *IEEE Trans. Electron Device*, vol. 62, no. 12, pp. 4322–4326,2015.

[13] H. Pandey, M. Shaygan , S. Sawallich, S. Kataria, Z. Wang, A. Noculak, M. Otto, M. Nagel, R. Negra, D. Neumaier, and Max C. Lemme, “All CVD Boron Nitride Encapsulated Graphene FETs With CMOS Compatible Metal Edge Contacts,” *IEEE Trans. Electron Device*, vol. 65, no. 10, pp. 4129–4134,2018.

[14] N. Ghobadi and M. Pourfath, “A Comparative Study of Tunneling FETs Based on Graphene and GNR Heterostructures,” *IEEE Trans. Electron Device*, vol. 61, no. 1, pp. 186–192,2014.

[15] I. Meric, C. R. Dean, N. Petrone, Lei Wang, J. Hone, P. Kim, and K. L. Shepard, “Graphene Field Effect Transistor Based on Boron-Nitride Dielectric,*Procc. of the IEEE* Vol. 101, No. 7, July 2013.

[16] Z. Qiao,J. Jung,Q. Niu, and A. H. MacDonald “Electronic Highways in Bilayer Graphene,” *ACS nano Lett.*, vol. 28, no. 4, pp. 282–284, 2007.

[17] B. Hunt, J. D. Sanchez-Yamagishi, A. F. Young, M. Yankowitz, B. J. LeRoy, K. Watanabe, T. Taniguchi, P. Moon, M. Koshino, P. Jarillo-Herrero, R. C. Ashoori , “Massive Dirac Fermions and Hofstadter Butterfly in a van der Waals Heterostructure ,” *Sci. Report*, vol. 140, no. 6, pp. 1427–1430,2013.

[18] K. S. Novoselov, A. Mishchenko, A. Carvalho, A. H. Castro Neto, “2D materials and van der Waals heterostructures” *Science*, vol. 353, no. 7, pp. 461-473,2013.

[19] S. J. Haigh1, A. Gholinia1, R. Jalil2, S. Romani, L. Britnell, D. C. Elias, K. S. Novoselov, L. A. Ponomarenko, A. K. Geim and R. Gorbachev“Cross-sectional imaging of individual layers and buried interfaces of graphene-based heterostructures and superlattices,”*Nature Material*, Vol. 11, no. 7, pp. 764-767.

[20] Regis Decker, Yang Wang, Victor W. Brar, William Regan, Hsin-Zon Tsai, Qiong Wu, William Gannett, Alex Zettl, and Michael F. Crommie, “Local Electronic Properties of Graphene on a BN Substrate via Scanning Tunneling Microscopy,” *ACS nano Lett.*, vol. 11, no. 5, pp. 2291–2295, 2011.

[21] S. Kang*et al.*, "Insights into interlayer tunnel FET performance improvement: Lessons learned from graphene hexagonal boron nitride heterostructures," *2016 74th Annual Device Research Conference (DRC)*, Newark, DE, 2016, pp. 1-2.