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Simulation of Voltage Applied Effect on Carbon-Doped Boron Nitride Nanoribbon Hydrogen Gas Sensing Performance

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Abstract: Advanced materials have been widely investigated for numbers of electronics application. The aim is to provide higher device performance and mitigating the short channel effect. In this work, the performance of hydrogen sensing on carbon-doped boron nitride nanoribbon (BC_2NNR) is investigated in response to different gate voltage applied, V_{gs}. The simulation is done to see the variation in the density of state (DOS) and the variation in the I – V characteristic. From the simulation, a significant effect is found when the Hydrogen gas was attached to different atom positions within the BC_2NNR surface. A notable difference in sensitivity was achieved when V_{gs} is varied from 0 V to 2 V. In fact, a sensitivity of 85.07 % was achieved when the hydrogen molecule was attached to carbon atom. The result presented here may become guideline for experimentalists fabricating BC_2NNR for gas sensing application.

Keywords: DOS, FET, I-V characteristic, pristine BC_2NNR

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1. INTRODUCTION

Recent advancement in electronics industry have led to a widespread study reported on the use of advance nanomaterial and non – planar devices architecture. Number of efforts have been done particularly on investigating the potential use of nanomaterial such as graphene, carbon nanotube, phosphorene, and boron nitrite (BN) in switching and sensing application. Boron nitrite on one of the materials often studied for various gas sensing application [1]–[3]. A nature of wide band gap in BN has limited use in sensing [4]. However, substitutional and adsorption doping technique has made it possible to engineer BN bandgap allowing possible use in electronics application like gas sensing [5]. A modified version of BN namely hexagonal boron carbon nitride can be formed through alloying process have expand its physical and electrical properties for many devices application.

There is an increased number of studies pertaining to carbon doped boron nitrite (BC_2N) physical and electrical properties [6], [7]. One of the applications using BC_2N is gas sensing particularly on hazardous gas [8] which requires a material with high sensitivity, high selectivity, fast response, and rapid recovery time [9], [10]. In a study by Nematollahi et al. [11], they simulated using density functional theory (DFT) to investigate the effect of CO oxidation on Si-doped carbon-doped boron nitride nanosheet (BC_2NNS) and Si-doped carbon-doped boron nitride nanotube (BC_2NNT). Their results shows that Si-doped BC_2NNS offers highly activated substrate to CO oxidation compared to Si-doped BC_2NNT. In another study, Esrafili et al. [12] performed a simulation study related to the effect of CO and SO_2 molecule on BC_2N for N_2O reduction. The edge of BC_2N is also found to have considerable effect on the electronic properties of the devices [13], [14]. For example, Lu et al. [14] found that H-passivated armchair BC_2NNR reveal to have remarkable electronic and magnetic properties. In fact, modification of the material properties by introducing dopant or defect may directly affect these properties. For example, when dopant is introduced on BC_2N, the charge transfer and binding energy exhibit significant changes [15]. This is supported by a study by Mishra et al. [15] demonstrated that CO_2 binds strongly with an optimal storage of 44 wt % (weight percent) for a monolayer of BCN compared to CH_4, N_2, and H_2 adsorption. It is found that when BC_2N sheets are doped with boron, the adsorption energies for CO_2 and CH_4 considerably increase [15].

Previous works on boron nitrite-based sensing devices result in promising outcome and should be further investigate. This study focusing on evaluating Hydrogen based gas sensor using carbon-doped boron nitride nanoribbon (BC_2NNR). Number of works has been done related to hydrogen gas sensor [16], [17] where they noted binding energy relation with the presence of electric field. In this work, the hydrogen sensing sensitivity is evaluated by applying different values of back gate voltage. This is to see how the gas molecules reacted upon different gate biased. This is studied through computational simulation and the details of this is presented in the next section.

2. METHODOLOGY

The simulation is performed using Quantum Atomistix Toolkit (ATK) from Synopsys (version T-2022.03-SP1). Armchair BC_2NNR layer was constructed by using Nanoribbon Plugin Tool in QuantumATK. The number of atoms determining the width of the BC_2NNR layer is fixed to 12 – dimer line while four unit – cells representing the length, L is obtained by repeating atoms along the C – axis. The hydrogen gas molecules were introduced within the surface by attaching to three different positions namely carbon atom, boron atom and both boron and nitrogen atoms. The temperature was kept constant at 298 K. Figure 1(a - c) presented the structure 12-BC_2NNR with the presence of H_2 located at carbon, boron, and nitrogen atom respectively. To set – up the device configuration, left and right electrodes were connected at both end of the layers representing the source and the drain region. This is showed in Figure 2. In this study, silicon dioxide, SiO_2 is chosen as gate dielectric, with permittivity of 3.9 εo, a thin metallic layer represent as gate potential was set to 0 V and work function of 5.1 ε.

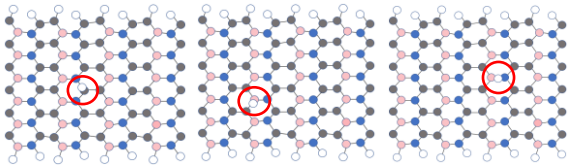

Figure 1. Illustration of 12-BC_2NNR with the presence of H_2 gas in red circle located at (a) carbon atom, (b) boron atom, and (c) both boron and nitrogen atom. White ball, grey ball, pink ball, and blue ball represent hydrogen atom, carbon atom, boron atom, and nitrogen atom, respectively.

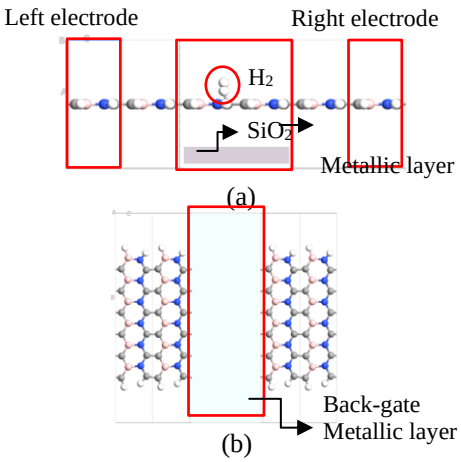

Figure 2. Two probes of BC_2NNR based FET with H_2 gas (a) side view and (b) back view.

In all calculation, the linear combination of atomic orbitals-based density functional theory was used. The Perdew-Zunger formalism of local density approximation was used to compute the exchange-correlation electron. All calculations were performed using the double-zeta polarized basis set. The density mesh cut-off energy was set to 75 Hartree to ensure numerical accuracy. For the electronic structure calculation, the Brillouin zone (BZ) was sampled with a k-point sampling of 1 × 1 × 100. The geometries of all atomic structures in the unit cells were initially optimized using the limited-memory Broyden-Fletcher-Goldfarb-Shanno algorithm. geometry optimization is performed using LBFGS to relaxes the structure and finds the minimum energy structure in the modelled layer. To prevent artificial inter-ribbon interactions, a vacuum region of 10 Å was added along the non-periodic boundary.

3. RESULT AND DISCUSSION

Figure 3 compare the evolution of the projected density of states (DOS) between bare BC_2NNR and with the presence of hydrogen molecules at three different positions simulated from energy of -2 eV to 2 eV. It can be observed from Figure 3 (a) that bare BC_2NNR behave typically like one dimensional material where there is a staircase characteristic as the energy increase. This trend can hardly be seen when the hydrogen molecules was attached to BC_2NNR layers. For example, there is a spike when hydrogen molecules were attached at carbon around energy level of 1.4 eV and 58 eV^{-1}. The DOS on the positive side of the energy level for hydrogen attached to boron and both boron and nitrogen atom have very minimum changes. This can be seen in Figure 3 (c – d) where energy state is found around 2 eV, 1.4 eV, -0.6 eV, -1.5 eV and -1.9 eV.

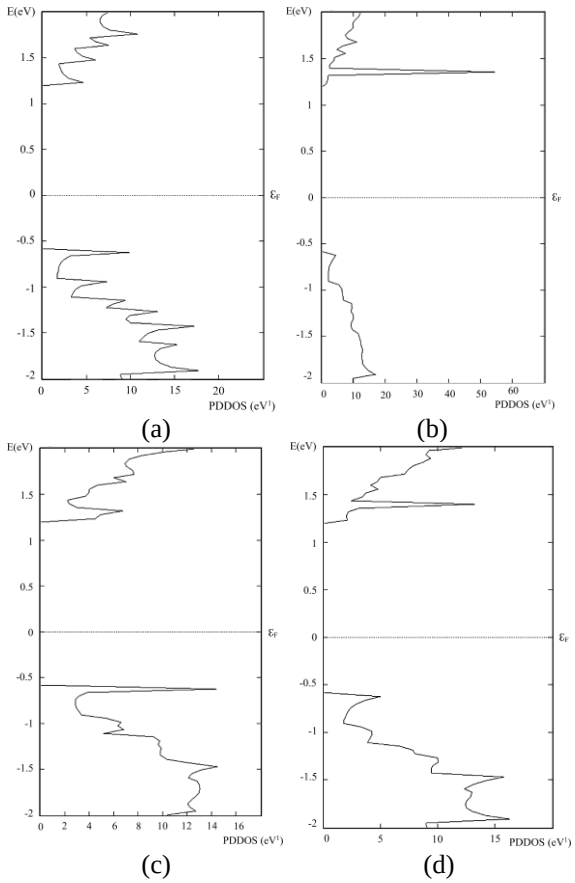

Figure 3. Device projected density of states (DOS) with (a) bare and presence of H_2 gas (b) carbon atom (c)

boron atom and (d) both boron and nitrogen atoms.

The presence of spike and new energy states upon introduction of gas achieve here has also been showed in other study when they studied propane and butane gas on GNR based FET [18]. This signifies the simulated FET devices demonstrated a considerable change in projected DOS towards the presence of these gas. The focus of this paper is to evaluate the effect of the applied gate biased on the device sensitivity. This is calculated from the changes in the current from the current-voltage (I-V) when hydrogen molecules were presence. The sensitivity is calculated using equation (1) [19].

$$\text{Sensitivity (\%)} = \left|\frac{I - I_O}{I_O}\right| \times 100 \qquad (1)$$

where I is the current with H_2 gas and Io is the current without H_2 gas molecules. The drain to source voltage, V_{ds} was swept biased, from 0 to 2 V. The sensitivity was calculated and listed in Table 1 below for V_{ds} = 2 V.

Table 1. Comparison of sensitivity for 12-BC_2NNR based FET at three positions for different V_{gs} applied taken at V_{ds} = 2 V.

V_{gs} (V)	Sensitivity (%)		
	Carbon	Boron	Boron and nitrogen
0	39.76	| -80.50 |	0.07
0.5	85.07	| -80.71 |	26.45
1	40.46	| -90.47 |	4.30
2	| -4.69 |	| -89.74 |	3.70

For clarity, the $I_{ds} - V_{ds}$ characteristic was shown from 1.7 V to 2 V as the data below 1.7 is very small. For the three different positions, the characteristic was displayed in Figure 4, Figure 5 and Figure 6 to observe the effect on different gate biased. For all cases, generally there is a nonlinear behavior on the current conduction with the presence of hydrogen molecules as the applied V_{gs} increase. The average threshold voltage in the presence of H_2 gas showed in back-gate controlled BC_2NNR are approximately 1.75 V. Appreciable variation in current can be seen particularly at highest V_{ds}.

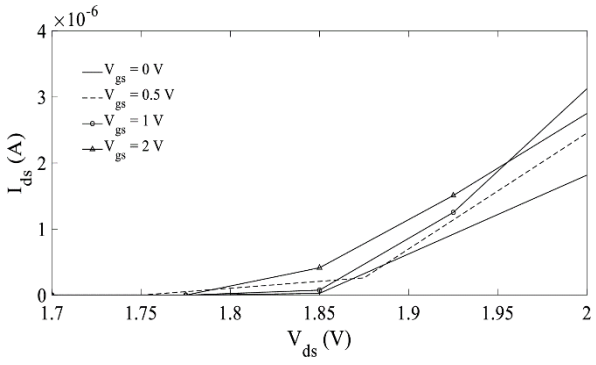

Figure 4. 12-BC_2NNR based FET in presence of H_2 gas on carbon atom.

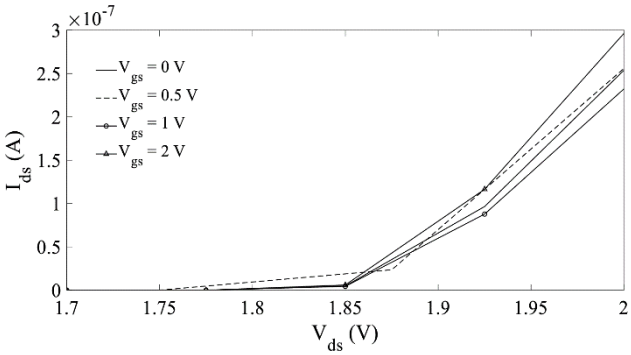

Figure 5. 12-BC_2NNR based FET in presence of H_2 gas on boron atom.

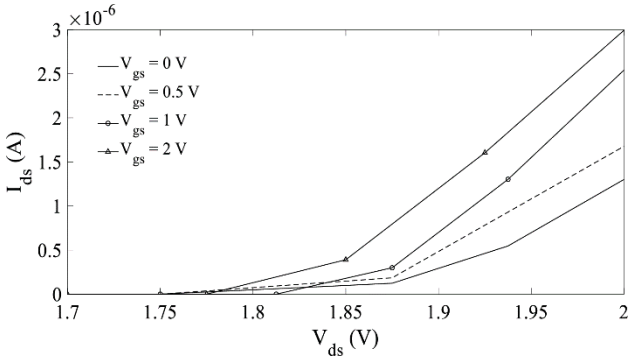

Figure 6. 12-BC_2NNR based FET in presence of H_2 gas on both boron and nitrogen atoms.

Graphene and BN has shared similar properties and has almost the same with some common characteristic due to the hexagonal structure. Rashid et al. [18] reported, the absorbed target gas molecules behave as charge carrier donors and acceptors for graphene. Hence, the increasing and decreasing of the charge carrier in the current through acted as donors and acceptors [20]. From Figure 4, back-gate controlled 12-BC_2NNR sensor appears to have better sensitivity. H_2 gas exposed at carbon atom may have acted like donors of charge carriers for BC_2NNR. Current conductivity shows about third quarter increment at V_{gs} = 0.5 V from 1.33 µA to 2.75 µA with (85.07 %). It then followed by V_{gs} = 1 V and 0 V with 3.42 µA (40.46 %) and 1.82 µA (39.76 %), respectively. Whilst a decrease in current conductivity at V_{gs} = 2 V with 4.69 %, showing H_2 gas exposed at carbon atom have acted like acceptors charge carriers for BC_2NNR.

On the other hand, H_2 gas exposed at boron atom shown in Figure 5 exhibit a huge drop of current conductivity for all V_{gs} with the highest drop of 90.47 % at V_{gs} = 1 V, 89.74 % at V_{gs} = 2 V, 80.71 % at V_{gs} = 0.5 V, and 80.50 % at V_{gs} = 0 V. It showed H_2 gas exposed at boron atom may have acted like acceptors and reduced the charge carrier concentration in BC_2NNR based FET. The most striking different is observed when hydrogen was attached to both boron and nitrogen as shown in Figure 6. For example, at V_{ds} = 2 V and V_{gs} = 0.5 V, the changes in current are 99.74 %, 83.74 % and 86.01 % compared to V_{gs} = 0 V, 1 V and

2 V, respectively. Hydrogen molecules attach to carbon (Figure 4) and both boron and nitrogen (Figure 6) serves better sensing performance compared to boron (Figure 5). Herein, H_2 gas may have acted as donors and increased the charge carrier concentration in BC_2NNR based FET. This indicates increases with 26.45 % in current conductivity with I_{ds} = 1.68 μA at V_{gs} = 0.5 V.

4. CONCLUSION

This paper studied the effect of the applied gate biased on back-gated BC_2NNR devices. Result indicates significant changes in the projected DOS upon introducing Hydrogen molecules for three different positions namely on carbon, boron, both boron and nitrogen. Generally, there is a current variation achieved when different gate biasing was applied. The device sensitivity calculated showed an upward increase of sensitivity when the hydrogen molecules attached to carbon atom on 12-BC_2NNR. Significant effect was observed at V_{ds} = 2 V where 85.07 % sensitivity is achieve compared to another position. The results presented can further be expanded to evaluate the gate biasing effect for multiple layers of BC_2NNR.

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