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ORIGINAL ARTICLE

Design of nanoscale self switching diodes with high rectification ratio based on two-dimensional semiconductor hBCN

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Abstract

In this paper, we present a new self-switching diode (SSD) realized with a two-dimensional semiconductor hexagonal boron carbon-nitrogen (hBCN) monolayer. Channel length and width are 4.5 nm and 1.23 nm respectively. The device operation is simulated based on the Extended Huckel method and Nonequilibrium Green's Function (NEGF) Formalism. The simulation results indicate non-linear I-V characteristics of the nano-diode and a current rectification ratio near 11250 that is higher than previous SSD structures reported before. Also, the effects of channel width on the electrical characteristics of SSDs are investigated. It can be found that the bandgap value of hBCN plays an important role in the modulation of current in the channel. Transmission pathways are provided under reverse and forward biases to show channel opening and pinch-off conditions. The results indicate that hBCN is a promising material for the realization of self-switching diodes (SSDs).

Keywords: *Extended Huckel Method; Nanoscale Self Switching Diode; NEGF; Rectification Ratio; Transmission Pathways.*

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INTRODUCTION

Realization of a diode at the nano-scale for high-frequency application has been a challenge. Self-switching diode (SSD) which is a two-dimensional rectifier was introduced that can operate at nanoscale dimensions.

SSD performance is based on surface effects and was developed by song *et al.* [1]. The structure consists of a nanochannel between two L-shape insulating trenches. Surface states in the wall of trenches induce the depletion region along the nanochannel. Similar to a p-n junction diode, this depletion region is modulated by bias voltage. Fabrication of SSDs needs very minimal lithography steps. Also, neither doping junction, nor tunneling barrier is required for rectifying performance.

The SSDs are basically three-dimensions (3D) bulk materials such as silicon [2], ZnO [3], and ITO [4], in which the electrical conduction resulting from the self-induced field effect is carried out via two-dimensional electron gas.

To make the SSD channel smaller in size, two-dimensional materials such as graphene [5, 6], MoS_2 [7], and silicene [8] have been reported. Also, SSDs with V-shaped insulating trenches were simulated and compared with L-shaped insulating ones [9]. The simulation results indicate that SSDs based on two-dimensional graphene and silicone, do not show high rectification ratios [5-8]. Indeed, self-switching diodes rectify current based on a field-effect mechanism and hence require a bandgap for strong rectification. Graphene and silicene can only have a small bandgap lower than

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0.3 V [5, 8]. Indeed, the low rectification ratio is the main drawback of these devices due to low channel bandgap. In this paper, two-dimensional Hexagonal boron carbon-nitrogen (hBCN), is used as channel material to increase the current rectification ratio.

hBCN is a promising two-dimensional material for next-generation electronics [10-12]. Its electronic properties can be changed by tuning the relative fraction of the three elements [12]. Although its structure is similar to graphene, it exhibits a large bandgap around 1.9 eV [12], which is necessary for field-effect transistor (FET) operation [13]. Indeed, due to the larger bandgap, the hBCN nanoribbon is more suitable than graphene for SSD realization and a higher rectification ratio is expected.

In some research, the possibility of hBCN as a material channel in FET [13], and also as a tunneling barrier in tunneling transistors [14] has been investigated. In this paper, we implement SSDs using hBCN and study their transport properties and current value by using NEGF formalism that has not been investigated yet. Also, the rectification ratio of the device is calculated and compared with other reported devices.

To analyze the rectification behavior of the device, we use quantum simulation-based on extended Huckel (EH) tight-binding model with non-equilibrium Green's function (NEGF) formalism. In this method, the tight-binding model is based on the EH approach as implemented in ATK's semi-empirical (SE) package, in which the tight-binding Hamiltonian is parameterized using a two-center approximation, where the matrix elements are described in terms of overlaps between Slater orbitals at each site. The used weighting scheme of the orbital energies of the offsite Hamiltonian is according to Wolfsburg [15]. This semi-empirical approach is used instead of the computationally expensive Density Functional Theory (DFT) based approach for large device structures.

By using this method, turn-on voltage, and rectification ratio are investigated. We show that the presented device achieves a rectification ratio of 11250 which is higher than previously proposed SSD devices.

MATERIALS AND METHODS

The schematic top view of hBCN SSD is shown in Fig. 1. In this structure, there are two L-shaped trenches defining the nanochannel between them. Two side gates in this structure induce an electric field into the channel and are used to control the conductance of nano-channel using the self-induced electric field. The purpose of hBCN as a channel material is expected to enhance field effect control because of its large bandgap in comparison with previous 2D structures. The proposed device is a nanoscale device with sub-10nm dimensions, incorporating a channel with 4.5 nm length and 11 atoms wide (1.23 nm), and two atom side gates that are 4 atoms wide each (0.37 nm).

We note that the hBCN nanoribbon channel can have either armchair or zigzag edges, and in this study, we consider armchair one. This depends on L-shaped trenches orientation.

In order to get an insight into device operation, Fig. 2 explains the principle operation of the device. The majority carriers in this device are electrons. Without bias voltage, depletion regions

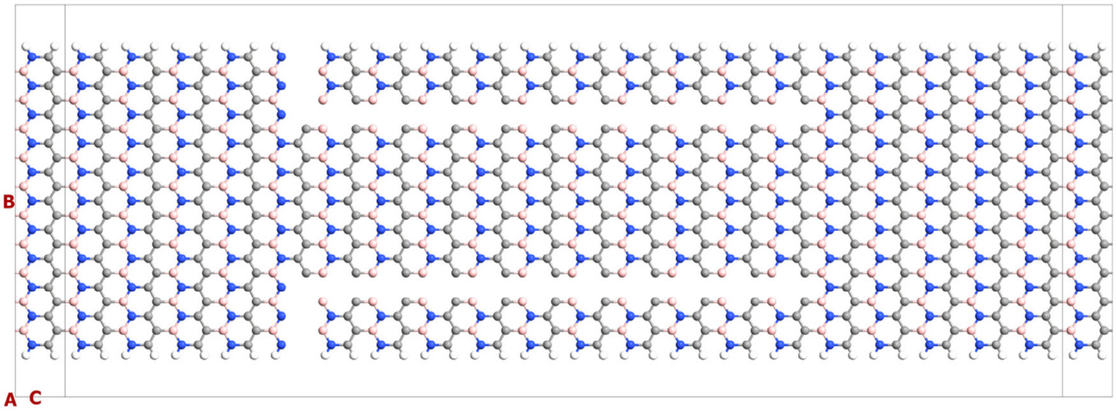

Fig. 1. Top view of the hBCN self-switching diode. Showing the L-shaped insulating trenches and nano-channel.

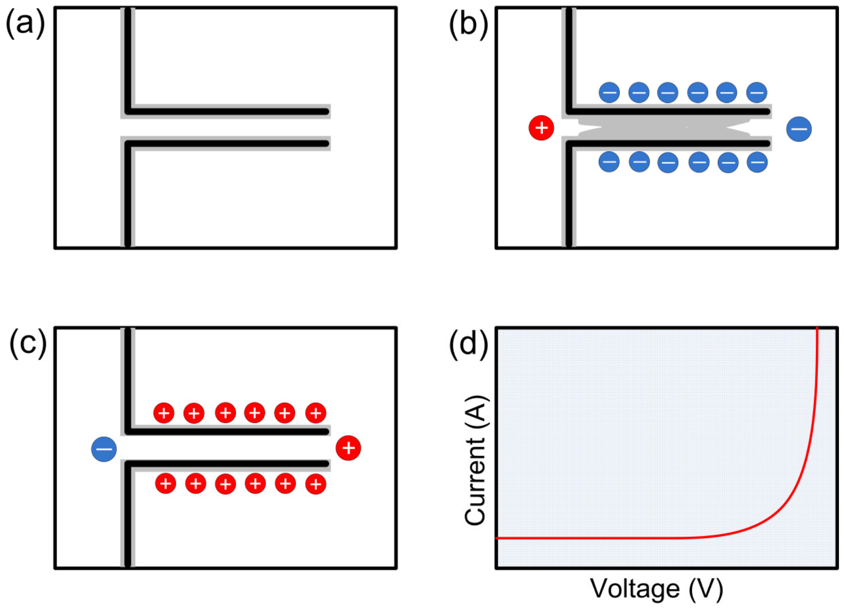

Fig. 2. Schematic diagram showing the principle operation of hBCN SSD (a) under zero bias voltage, (b) reverse bias voltage and (c) and forward bias voltage. (d) The expected I-V characteristics of a SSD.

are created around these insulating trenches, as a result of the majority carrier repulsion due to surface states of L-shaped trenches as shown in Fig. 2(a). By applying a negative voltage, negative charges besides the gate, repulse electrons from the channel and widen the depletion region as shown in Fig. 2(b). On the other hand, by applying a forward bias, the depletion region narrows down is due to positive charge accumulation within the side gates as shown in Fig. 2(c). This carrier accumulation in the channel leads to an increase in the current. The current-voltage curve indicates the rectification as a diode as shown in Fig. 2(d).

RESULTS AND DISCUSSIONS

The atomic structure was optimized using the Density Functional Theory (DFT) as implemented in the ATK package. The Generalized Gradient Approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional was adopted to describe the exchange-correlation interaction [15]. The Atomic positions and lattice constant were relaxed until all atomic forces were less than, 0.01 eV/Å.

The current between contacts is calculated as [16-17]:

$$I=\frac{2e}{q}\int_{-\infty}^{+\infty}T(E,V)\left[f_0\left(E-E_{FC}\right)-f_0\left(E-E_{FA}\right)\right] \qquad (1)$$

Where $T(E,V)$ is the transmission probability of incident electrons with energy E from cathode to anode [18-19]. $f_0\left(E-E_{FC/FA}\right)$ is the Fermi-Dirac distribution function of electrons in cathode and anode regions, respectively[16].

The mesh points in real space calculation are defined as1×10×50 with 50 sample points along the length(transport direction) and 10 points along the width(induced electric field direction). I-V curve of SSD is shown in Fig.3. The asymmetrical shape of the curve clearly shows the diode behavior of the device and hence achieves rectification. It can be found that positive bias enhances the current while negative bias suppresses.

One of the important parameters of a diode is turn-on voltage. At turn-on voltage, conductance rises abruptly. According to Fig.3, the turn-on voltage is near zero that is similar to an ideal diode. The calculated maximum forward to reverse current rectification ratio is calculated according to the following equation:

$$Rectification\,ratio_{max}=max\left[\frac{I(+V)}{I(-V)}\right] \qquad (2)$$

Where V is the bias voltage, and I(V) is the current corresponding to that bias voltage. The rectification ratio of the device is reported in Table I and is compared with the previous 2D SSD. From

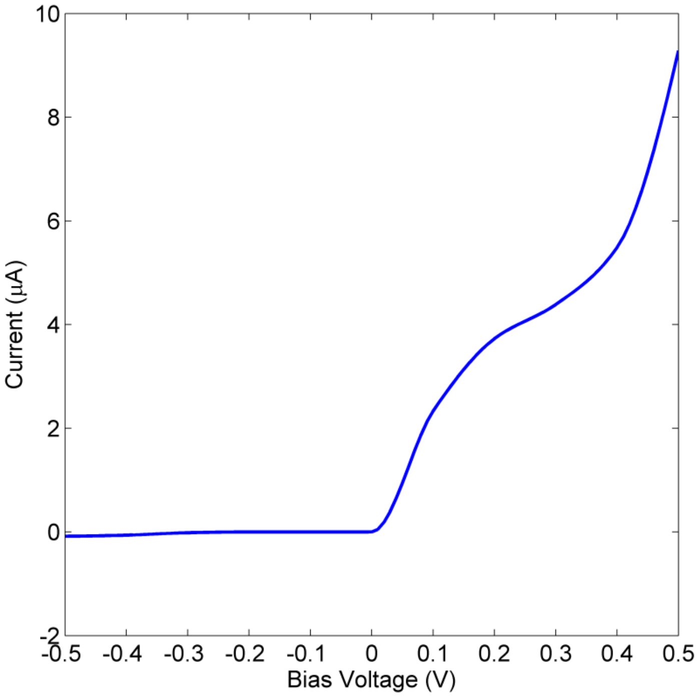

Fig. 3. I-V characteristics of the hBCN self-switching diode.

Table 1. Comparison between rectification ratios of various 2D SSDs.

Device	Rectification Ratio
Undoped MoS_2 SSD [12]	6
Doped MoS_2 SSD [12]	70
Silicene SSD [13]	200
Optimized graphene nanoribbon SSD [10]	5000
This Work	11250

the results, we find that forward bias current is 11250 times greater than reverse bias current presenting a strong rectification ratio. To analyze the transport mechanism through the device, we calculate the transmission pathways in the device. These pathways indicate the transmission of charge between individual atoms locally and are represented by lines along the bond lengths. The transmission pathway is calculated in cases, i.e, forward bias and reverse bias.

Fig.4 shows the transmission pathway under forward bias while Fig.5 shows it under reverse bias. The figure shows that under a reverse bias, the continuous transmission pathway through channel does not exist. This situation is named channel pinch off. From the figure, we can find that even under pinch-off situation small current can flow because of tunneling from the side gates through the insulating trenches.

On the other hand, by applying forward bias, the strong continuous pathway of transmission can be observed that confirms channel opening. Besides the main current, the unwanted tunneling current also exists in this case.

But conduction through channel dominates. Thus the simulation results indicate that the highly enough bandgap value of hBCN enables complete channel pinch off in forward bias and strong channel opening in reverse bias. Our results suggest that hBCN is a promising material for the realization of monolayer self-switching devices.

From Fig. 5, the tunneling transmission pathway from the side gates to the channel can be observed. A study about SSD has shown that hydrogen passivation of the edges, leads to a decrease in the undesirable tunneling current

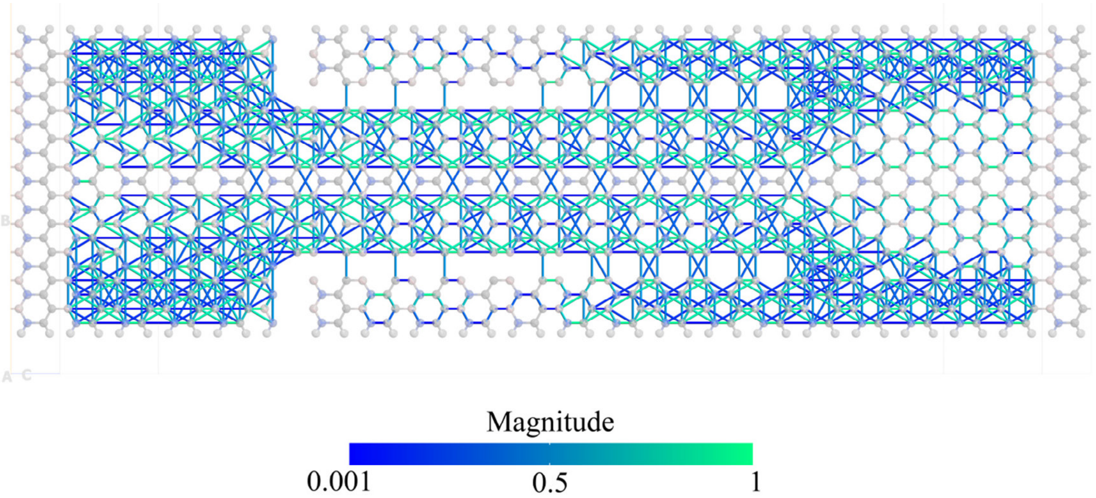

Fig. 4. Transmission pathways plot for the hBCN SSD under forward bias voltage of +0.5V.

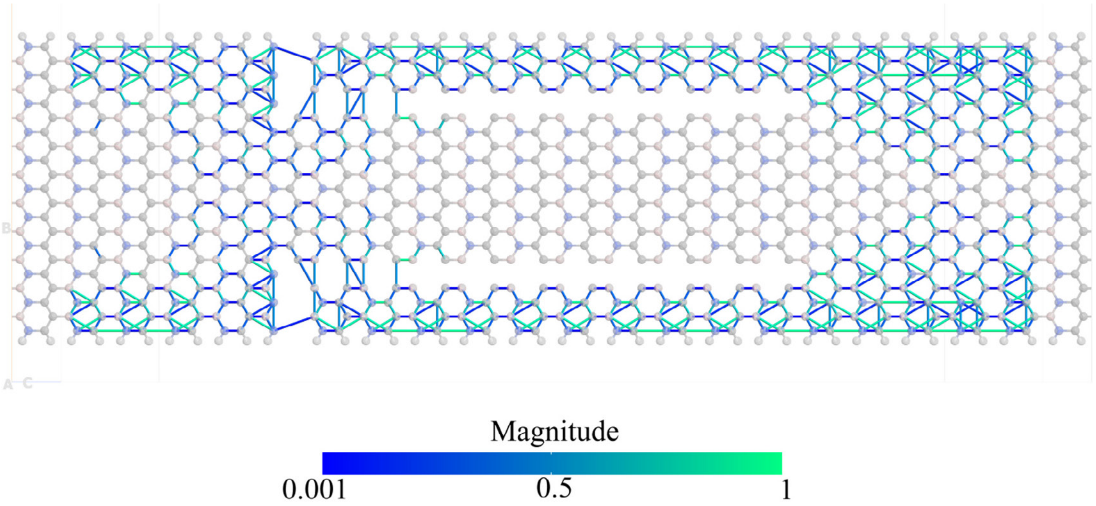

Fig. 5. Transmission pathways plot for the hBCN SSD under reverse bias voltage of -0.5V.

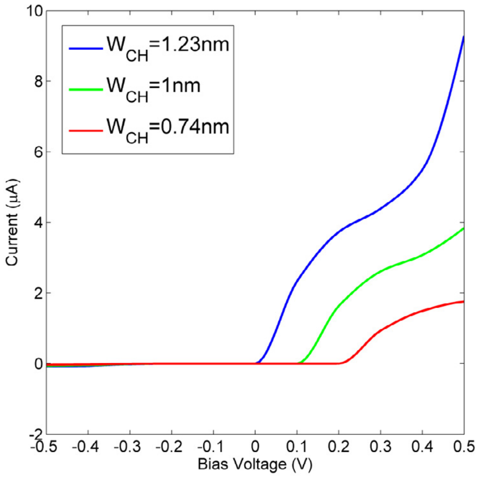

Fig. 6. Current-voltage characteristics of the hBCN self switching diode with different channel widths.

through the insulating region [16]. Thus hydrogen passivation can increase the overall rectification ratio.

Fig. 6 shows the I-V characteristics of three SSDs with the same channel length (L=4.5 nm), but different channel widths. From the figure, it can be found by increasing channel width, the turn on voltage increases, and the rectification ratio decreases. Indeed, for narrower widths, the channel is fully pinched off under equilibrium conditions because of surface charges in the wall of trenches. Therefore, a higher positive voltage is needed to drive a current through the channel. Although wider channels increase the forward current and reduce the SSD turn-on voltage, the reverse current increases. As mentioned before, in this paper only hBCN nanoribbons with armchair edges are considered. Thus analysis of hBCN SSDs with zigzag edges is suggested for future works.

CONCLUSION

By using quantum mechanical simulation hBCN SSDs were proposed and analyzed. It can be found that complete pinch off channel in reverse bias and strong channel opening in forward bias is achievable due to highly enough hBCN bandgap. Thus high rectification ratio was obtained. It was found that the hBCN SSD suffers from an unwanted tunneling current that limits the rectification ratio. The results confirm that SSD turn-on voltage can be tuned by changing channel width. These results show that hBCN SSD can be used in next generation terahertz detectors and various diode applications.

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CONFLICTS OF INTEREST

The authors do not have any conflicts of interest.

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