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Usefulness of Spin Transport in BN Doped CrO_2-Graphene-CrO_2 Magnetic Tunnel Junction

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Abstract— We investigate the spin-dependent electronic transport properties of Magnetic tunnel junction (MTJ) consisting of Boron (B) and Nitrogen (N) doped graphene nanosheet sandwiched between two CrO_2 half-metallic-ferromagnet (HMF) electrodes. A large value of tunnel magnetoresistance (TMR) was obtained as compared to un-doped graphene MTJ structures reported in past. The use of HMF electrodes further raises the TMR comparison to MTJs with metallic and ferromagnetic (FM) electrodes, which suggest HMF electrodes as a suitable candidate over metallic and FM electrodes for implementing graphene sheet based MTJs. A high value of TMR ~100% is obtained at zero bias voltage, which remains constantly high at higher bias voltages in the range of 0 V to 1 V. The higher value of TMR abilities suggests its usefulness in spin-valves and other spintronics based applications.

Index Terms—Magnetic tunnel junction (MTJ), Graphene nanosheet, Boron-Nitrogen doping, Half-metallic-ferromagnetic (HMF) electrodes, Tunnel magnetoresistance (TMR)

I. INTRODUCTION

Spintronics or spin electronics refers to the utilization of electrons quantum property called spin in addition to charge and mass of an electron. The various applications of spintronic based devices in the fields like programmable logic elements, magneto-resistive random-access memory (MRAM), non-volatile information storage devices and other reconfigurable circuits make giant magneto-resistance (GMR) and tunnel magneto-resistance (TMR) effects in spintronics an attractive field to study [1] [2]. In a basic magnetic tunnel junction (MTJ) device, a thin tunnel barrier separates two ferromagnetic (FM) layers which act as source and drain electrodes. The magnetic configurations (parallel or antiparallel) of the two electrodes can be controlled by imposing an external magnetic field, thereby changing the electrical resistance of the MTJ [2] [3]. Therefore, the tunneling current for the two configurations is different which gives rise to TMR effect. Due to spin-dependent tunneling, a high conductance in case of parallel configuration (PC) and low conductance in antiparallel configuration (APC) of two electrodes is obtained [4].

The effectiveness of a spintronic device depends on the spin polarization of the tunneling current. To ensure highly spin-polarized current source, use of half-metallic-ferromagnetic (HMF) electrodes has been suggested in [5] [6] and in several other research works. By using HMF electrodes, a large value of magnetocurrent ratio, high TMR and efficient spin filtration were obtained in [5]. In [6], a

silicon (Si) channel based spin-MOSFET with HMF source and drain electrodes is demonstrated. The high value of TMR is necessary for using the structure in spin-valves and other spintronic based devices.

In MTJ, the tunnel barrier sandwiched between the ferromagnetic electrodes generally consists of metal oxides. Various theoretical and practical investigations have been conducted on MTJs using metal oxides like Al_2O_3, MgO, HfO_2 and Y_2O_3 [4], but the presence of material inter-diffusion and the defects in such oxides limit their performance [7] [8]. Recent studies have proposed to use graphene as a viable alternative to metal oxides as tunnel barriers. Graphene has gained noticeable attention due to its excellent in plane charge and spin transport properties [7]. The long electronic mean path, low spin orbit coupling, spin relaxation mechanism and extraordinary carrier mobility of graphene increases its utility in spintronics based applications [7-10]. Recent simulations of first graphene based MTJ [11] suggests that the use of graphene in spintronic devices can lead to large TMR. Graphene based MTJ demonstrated in [7] shows that improved spin-polarized current is obtained by using graphene as tunnel barrier in place of metal oxides.

The effect of Boron (B) and Nitrogen (N) co-doping in graphene sheets results in bandgap opening [12-14]. The bandgap opening is useful for implementing graphene based switches and other devices. Therefore, it is of interest to study the effects of BN co-doping on spin transport in graphene based MTJs with HMF electrodes. In this paper, we investigate the spin-transport properties of BN co-doped CrO_2-Graphene-CrO_2 MTJ and compare it with pristine graphene based MTJ.

II. SIMULATION METHOD AND SETUP

A two-probe geometry of MTJ using BN co-doped graphene nanosheet as tunnel barrier and CrO_2 as left and right HMF electrodes is built [see Fig. 1] and is simulated to obtain I-V characteristics and transmission spectra for parallel (PC) as well as antiparallel configuration (APC).

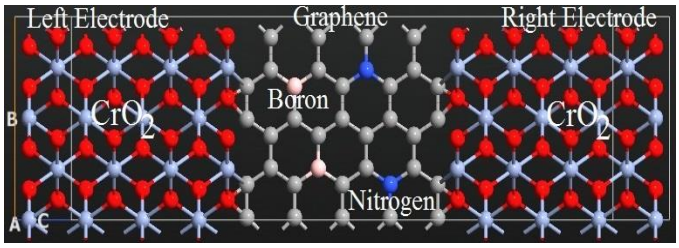

Fig. 1. MTJ consisting of BN co-doped graphene nanosheet sandwiched between CrO_2 (Left-Right) HMF electrodes.

The software package used for the simulation is Atomistix toolkit [15] which utilizes self-consistent calculations based on the combination of non-equilibrium Green's functions (NEFG) and density-functional theory (DFT) to realize the quantum transport properties of materials and devices. Since the I-V characteristics are a consequence of spin-polarized electron transport, therefore the exchange correlation considered in the simulations is spin-polarized generalized-gradient-approximation (SGGA).

In the simulations, graphene nanosheet with C-C bond length of 1.39 Å [16] and width (along the central region) 9.654 Å is used [see Fig. 1]. Left and right HMF electrodes are assumed to be perpendicular to graphene nanosheet and are made up of $5 \times 5 \times 5$ CrO_2 layers. The spacing between graphene nanosheet and CrO_2 HMF electrodes is found by setting the designed structure to relaxation. In order to minimize the total energy of the system, Quasi-Newton geometry optimization technique is used for relaxing the system with force tolerance set to 0.05 eV/Å [2] [17] [18]. As a result of relaxation, the carbon atoms (C) of graphene nanosheet forms bond with chromium (Cr) and oxygen (O_2) atoms of HMF electrodes. C-Cr and C-O bonds with bond lengths of ~2.201 Å and ~1.28 Å are formed as a result of this relaxation.

In order to obtain the I-V characteristics and transmission spectrum, the relaxed geometry is simulated using self-consistent calculations. The simulation parameters considered in the simulation are in accordance with the parameters used in [4] [17-20] and other research works. The parameters considered are as follows: The basis set used is double zeta polarized for central region as well as left and right electrodes. The k-point sampling of 3, 3 and 100 is selected in x, y and z directions. Mesh cut-off is 150 Ry and an electron temperature of 1200 K is chosen for faster self-consistent convergence. The spin of the left electrode is fixed to spin-up, while for the right electrode it is fixed to spin-up for PC and spin-down for APC.

The transmission coefficient T (E, V) indicates the probability of an electron having certain energy E to travel from one electrode to another under the influence of external bias voltage V and can be calculated by using the mathematical equation [19]:

$$T(E,V) = Tr[\ \Gamma_L(E,V)\ G^{\dagger}(E,V)\ \Gamma_R(E,V)\ G(E,V)\ ]$$

where $\Gamma_{L/R}$ is the electrode coupling matrix. The spin-polarized current through the device can be calculated using transmission coefficients by the relation [2] [19] [21]:

$$I\uparrow(\downarrow) = e/h \int T\uparrow(\downarrow)(E, V)\ [F(E - \mu_L) - F(E - \mu_R)]\ dE$$

where $T\uparrow(\downarrow)(E, V)$ defines transmission coefficient for up (↑) and down (↓) spin channel, F defines Fermi–Dirac distribution and $\mu_L(\mu_R)$ defines chemical potential of left (right) electrodes.

III. RESULTS AND DISCUSSION

In Fig. 2 and Fig. 3, we compare I-V curves for pristine and BN co-doped graphene based MTJ for PC and APC. It can be seen that for PC the spin-up current (I↑) in BN co-doped structure is more as compared to pristine structure in the bias voltage range of 0 V to 0.8 V, however, I↑ is much less in case of APC for all the bias voltages in the range 0 V to 1 V. The spin-down current (I↓) in the un-doped (pristine) structure is of the order of ~0.4 microamperes. When BN doping is introduced, I↓ decreases by ~4 orders in PC, and in case of APC I↓ decreases by ~2 orders. The total current (I↑ + I↓) in PC is much larger than the total current obtained in APC [see Fig. 2(c) and Fig. 3(c)]. The total equilibrium conductance of $0.195G_0$ is obtained in BN doped structure and $0.32G_0$ in pristine structure for PC, however, for APC these values are $0.000044G_0$ and 0.032G0, where conductance quantum $G_0 = 2e^2/h$ [2].

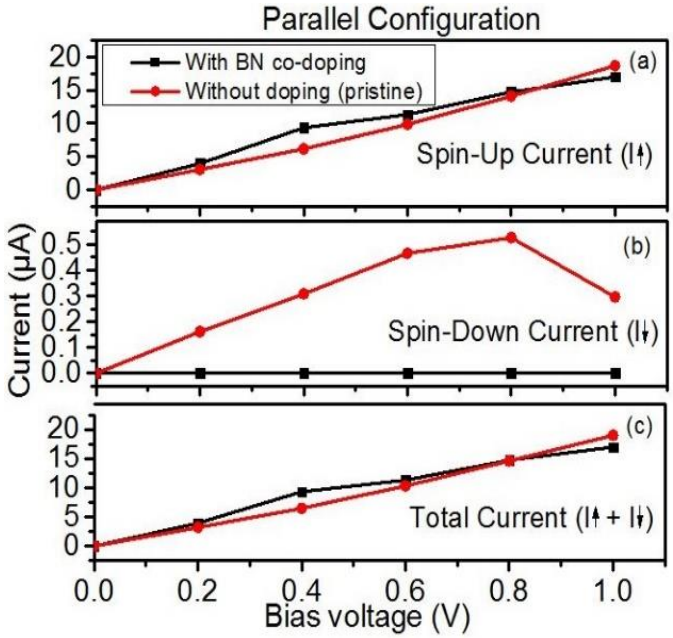

Fig. 2. I-V curves showing comparison of tunneling current between pristine and BN co-doped graphene based MTJ for parallel configuration (PC). (a) I↑ in doped structure is slightly more than I↑ in pristine (un-doped) structure in the bias range of 0 V to 0.8 V. (b) I↓ is much larger in un-doped structure. (c) Total current (sum) in doped structure is slightly less than the current in un-doped structure at higher bias voltages (after 0.8 V).

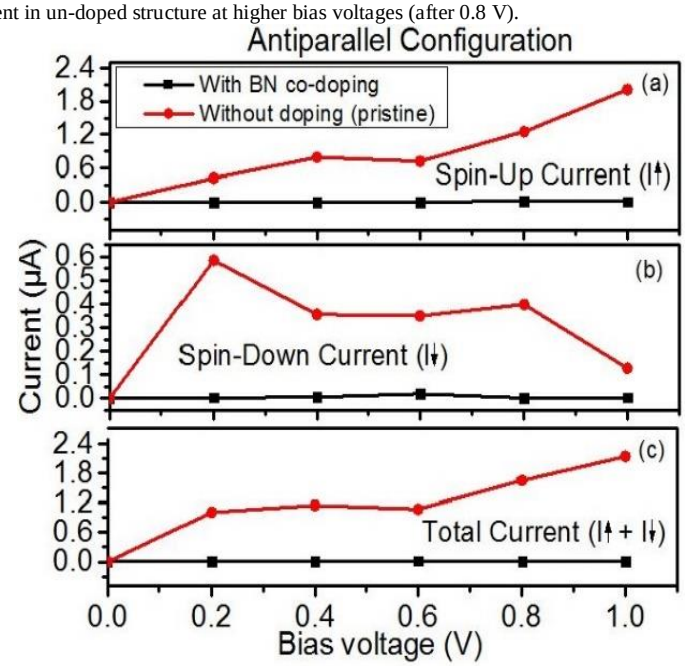

Fig. 3. I-V curves showing comparison of tunneling current between pristine and BN co-doped graphene based MTJ for antiparallel configuration (APC). (a) I↑ is larger in un-doped structure. (b) I↓ is larger in un-doped structure. (c) Total current (sum) is larger in un-doped structure.

From the I-V plots shown in Fig. 2 and Fig. 3 , TMR vs. bias voltage plot is obtained [see Fig. 4] as per the common definition [2]: TMR = $(I_{PC} - I_{APC})/I_{APC.}$ Here, I_{PC} and I_{APC} represents total currents in PC and APC, respectively. Since the current is zero at zero bias voltage (Vb = 0), therefore, TMR at zero bias is calculated using equilibrium conductance. Fig. 4 compares the TMR values for pristine and BN co-doped graphene based MTJ, which shows that TMR of ~100% can be obtained for BN co-doped structure at all bias voltages. High TMR indicates perfect tunneling magneto resistance effect is possible with this structure. On the other hand, a maximum possible TMR of ~90% was obtained at a bias voltage of 0.6 V for un-doped structure. The physical reason for higher value of TMR in doped structure is the bandgap opening in BN doped graphene [12-14]. Large bandgap results in high TMR, which has also been suggested in [2] for V-doped BNNTS. High TMR in case of BN co-doped structure indicates its usefulness in spin-valves and in other spintronics based devices. Furthermore, TMR for BN co-doped structure remains constantly high (100%) at higher bias voltages. However, in [7] [8] [11], a reduction in TMR (reduced to zero) with increase in bias voltage was reported for graphene based MTJ.

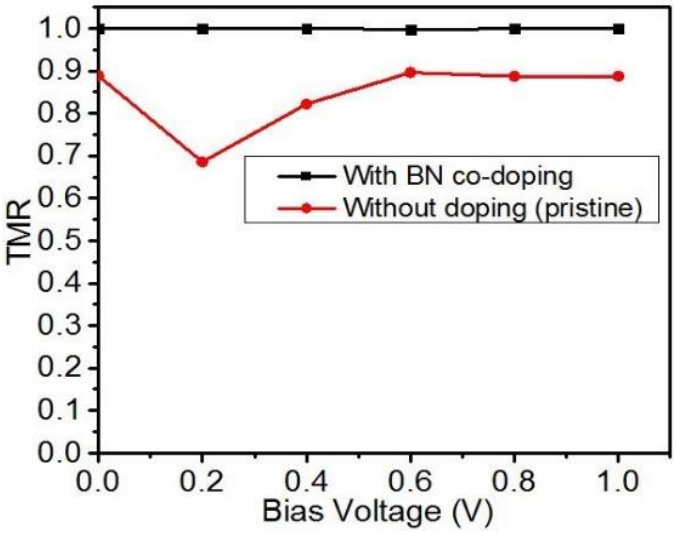

Fig. 4. TMR curves showing comparison between pristine and BN co-doped graphene based MTJ. High values of TMR ~100% at all bias voltages in BN co-doped structure indicates perfect tunneling magnetoresistance effect.

To further investigate the I-V characteristics of Fig 2 and Fig. 3, we study the bias dependent transmission probability curve in Fig. 6 and Fig. 7. In the case of PC with spin-up channel, there is finite transmission probability at all bias voltages [see Fig. 6 (a)]. These transmission probabilities do not change much with applied bias. In the case of PC with spin-down channel, there is a large transmission gap around Fermi level [see Fig. 6 (b)]. Therefore, the current is expected to be larger in spin-up than in spin-down channel, which is also justified by I-V characteristics of Fig. 2. In the case of APC, there is no transmission at all for spin-up and spin-down channel [see Fig 7 (a) and (b)]. Hence negligible current is expected for APC structure, which is also justified by I-V curves of Fig. 3. The spin-up and spin-down current values are important in determining the TMR.

IV. CONCLUSION

In conclusion, the spin-dependent electronic transport properties of BN co-doped graphene based MTJ are investigated and are compared with pristine graphene based MTJ. High TMR (~100%) is obtained with BN co-doped structure in comparison to the un-doped structure. High TMR in doped structure is attributed to an increase in bandgap with doping. Furthermore, high TMR achieved in BN co-doped graphene based MTJ suggest its importance over un-doped structure in spin-valves and other spin based applications.

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