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Effect of twisting and stretching on magneto resistance and spin filtration in CNTs

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***Abstract*—Spin dependent quantum transport properties in twisted carbon nanotube and stretched carbon nanotube are calculated using density functional theory (DFT) and non-equilibrium green's function (NEGF) formulation. Twisting and stretching have no effect on spin transport in CNTs at low bias voltages. However, at high bias voltages the effects are significant. Stretching restricts any spin-up current in antiparallel configuration (APC) which results in higher magneto resistance (MR). Twisting allows spin-up current almost equivalent to the pristine CNT case resulting in lower MR. High spin filtration is observed in PC and APC for pristine, stretched and twisted structures at all applied voltages. In APC, at low voltages spin filtration in stretched CNT is higher than in pristine and twisted ones with pristine giving higher spin filtration than twisted CNT.**

***Index Terms*—Twisted carbon nanotube (twisted CNT), stretched carbon nanotube (stretched CNT), magneto resistance (MR), spin efficiency.**

I. INTRODUCTION

Spintronics involves investigations associated with the electron's spin, magnetic moment, in addition to charge. Magnetic junction has usefulness in magnetic device applications, for example, magneto-resistive random access memory (MRAM), read head of hard disk drive, programmable logic and so on [1, 2]. Two Probe magnetic junction is a three-layer device in which nonmagnetic material is sandwiched between two electrodes. Electrodes are basically made up of ferromagnetic materials. The ferromagnetic material is chosen because of its unique electronic properties, that is the spin-up and spin-down electrons pass from one electrode to other electrode through magnetic junction with different Fermi energies. Carbon nanotube (CNT) was discovered in 1990s [3]. CNT has high electrical conductivity and thermal conductivity. It can be metallic or semiconductor [4 - 7], and it is one of the best nanomaterial that plays important role in electronics and spintronic based devices. The quantum transport properties of pristine CNT are reported in [8].

It is understood that during fabrication process some defects may occur in CNTs. Defects such as twisting of CNT, stretching of CNT, bending of CNT, can inevitably occur. CNTs can also get radially expanded and axially elongated during transfer to the substrate. Due to twisting and stretching defects CNTs can undergo change in the transmission spectrum and band structure. It is therefore of interest to understand how twisting and stretching in CNTs affect its spin transport properties.

In this paper, a comparative analysis of spin transport in twisted CNT, stretched CNT, and pristine CNT is done. Current-voltage characteristics, transmission spectrum, magneto résistance, and spin efficiency of twisted and stretched CNTs are calculated using DFT and NEGF. The results are compared with pristine CNT to understand the effect of twisting and stretching on magneto resistance and spin filtration in CNTs.

II. SIMULATION METHOD AND SETUP

Fig. 1 and 2 show the two-probe geometry of magnetic junction made up of twisted carbon nanotube and stretched carbon nanotube sandwiched between two CrO_2 HMF electrodes.

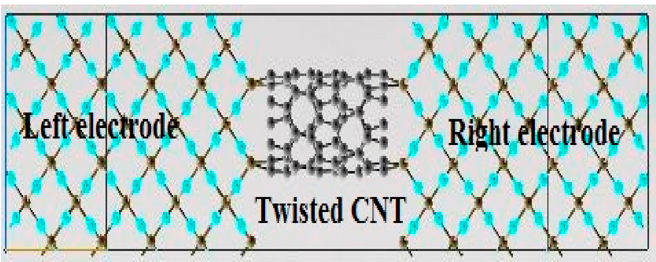

Fig. 1 Two-probe geometry in which twisted CNT is sandwiched between CrO_2 electrodes.

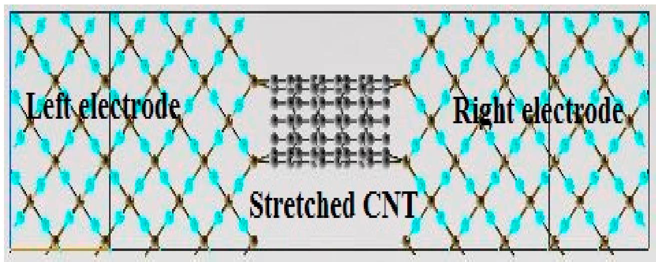

Fig. 2 Two-probe geometry in which stretched CNT is sandwiched between CrO_2 electrodes

The above two-probe geometry is simulated using Atomistix software [9-12] to obtain current-voltage characteristics (see Fig. 4 and 5) and transmission spectrum (Fig. 8 and 9) in both configurations (PC and APC). The electronic transport properties are calculated using self-consistent calculations. The self-consistent calculations are performed on the basis of DFT and NEGF formulation. The spin polarized generalized gradient approximation (SGGA) is set in the simulation because current is due to movement of spin polarized electrons. Pristine, twisted, and stretched CNTs are also shown in Fig. 3.

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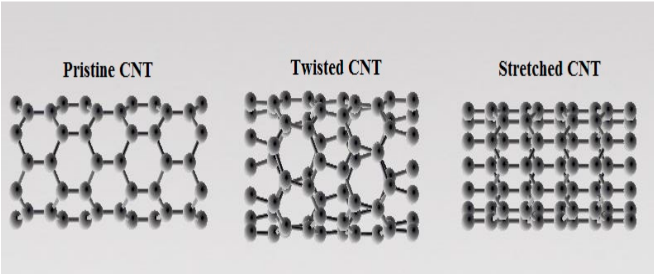

Fig. 3 Pristine, twisted, and stretched (in x-y) CNTs are shown.

A zigzag (6, 0) twisted CNT and zigzag (6, 0) stretched CNT with bond length 1.421 Å between carbon atoms and length 15.629 Å is considered in simulations, as in [8].The bond length between carbon and chromium is kept ~2.09 Å [8]. The I-V characteristics and transmission spectrums are acquired by simulating this geometry. The parameters used in the simulation are in accordance with [13-15]. The basis set used is double zeta polarized for carbon nanotube and single zeta polarized for both CrO_2 electrodes. The mesh cutoff and electrons temperature are considered as 150 Ry and 1800 K. The k point sampling in x, y, and z direction is considered as 3, 3, 100, as in [8]. The relative spin in parallel configuration for half metallic ferromagnetic atoms of both electrodes and carbon atoms of twisted or stretched CNT are considered as 1 and 0 respectively. Therefore, in PC spin sequence is 1, 0, 1. Whereas, in antiparallel configuration, the right electrode atoms spin is considered as -1, so spin sequence is 1, 0, -1.

The transmission spectrum indicates the probability of an electron moving from left electrode to right electrode under the influence of applied voltage. The current can be evaluated by using relation [1, 9-11]:

$$I\uparrow(\downarrow) = e/h \int_{-\infty}^{+\infty} T\uparrow(\downarrow)(E, V_B)\,[F(E-\mu_L)-F(E-\mu_R)]\,dE$$

Where $T\uparrow(\downarrow)(E, V_B)$ represents Transmission coefficient, E as Energy, F as Fermi-Dirac distribution function, μ_R and μ_L are the chemical potential for right and left electrodes.

III. Results And Discussion

For PC and APC configurations, the current-voltage characteristic is shown in figure 4 and 5. In Fig. 4, for PC, I↓ is always less than I↑ in all the three structures (pristine, twisted, and stretched). The spin-up current increases with increase in bias, with spin-down current being negligible in all the three structures as shown in Fig. 4. The total equilibrium conductance of pristine, twisted and stretched CNTs at zero bias are found as $0.48G_0$, $0.59G_0$ and $0.58G_0$, respectively, where G_0 represents conductance quanta, $G_0 = 2e^2/h$ [1].

In Fig 5, both I↑ and I↓ in APC are almost zero for applied voltage range of 0 to 0.8 V for all the three structures, but spin up current increases slowly above applied voltage of 0.8 V while spin down current stays around zero. The total equilibrium conductance of pristine, twisted and stretched CNTs is found as 2.18 G_0, $2.64G_0$ and $7.0G_0$, respectively.

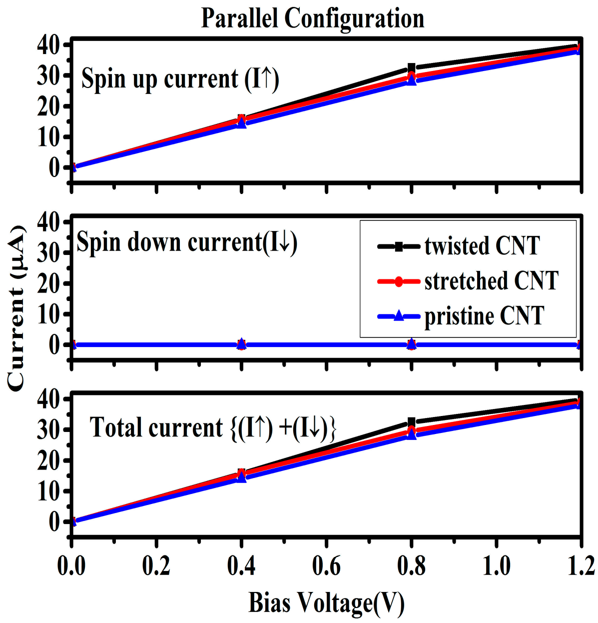

Fig. 4 Comparison of current-voltage curves in PC for all the three structures. The total spin current of twisted CNT is greater than that of stretched CNT and total spin current of stretched CNT is greater than that of pristine CNT.

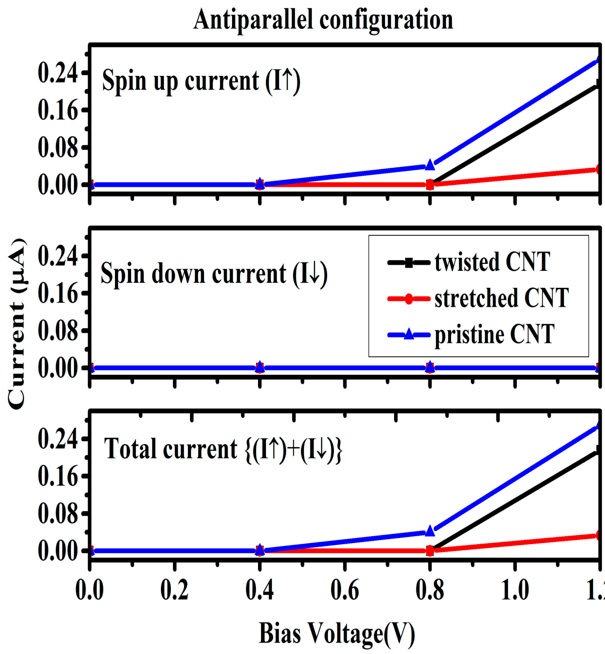

Fig. 5 Comparison of I-V curves in APC for all the three structures. Total spin current for all the three structures are zero for low biases but for higher biases spin down current remains zero and spin-up current of pristine CNT is greater than that of twisted CNT and spin-up current of stretched CNT is greater than that of pristine CNT.

The MR is calculated by utilizing the usual definition, MR = $(I_{PC}-I_{APC})/I_{PC}$ [16], where I_{PC} and I_{APC} are the total currents in parallel configuration and antiparallel configuration. From the current-voltage curve it can be seen that at zero volts, total current in all the three structures is zero and MR is calculated

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by utilizing equilibrium conductance. The MR obtained at zero bias is ~100%. At low bias I_{APC} is negligible for all three structures, however, at high bias voltages I_{APC} marginally increases in case of pristine and twisted CNTs and is greater in pristine CNT (see Fig. 5). For stretched CNT, I_{APC} remains negligible even at high bias voltages. This results in higher MR in stretched CNT than in twisted and pristine CNTs (see Fig. 6). Physical phenomenon behind higher MR in stretched and twisted CNTs can be directly associated to the number of electronic states available near Fermi level. There are almost negligible states in all the three structures, due to which current is very small in them. However, least number of states in twisted structure (see Fig. 9(a)) results in high resistance (see Fig. 6) and low I_{APC} (see Fig. 5).

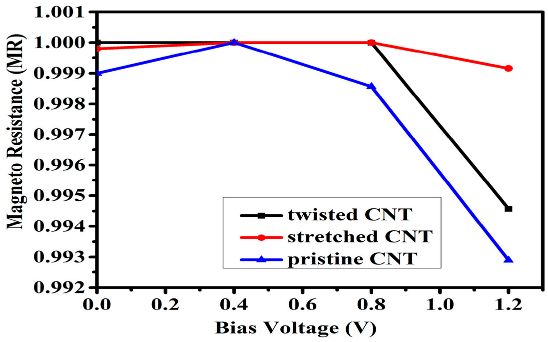

Fig.6 Comparative plots for magneto resistance with respect to applied voltages. For high bias voltage, MR for stretched CNT is higher than that of twisted CNT and MR for twisted CNT is higher than that of pristine CNT.

Spin injection factor (η) is calculated by utilizing following definition: $\eta = (I\uparrow - I\downarrow)/ (I\uparrow + I\downarrow)$ [2] and is plotted in Fig. 7.

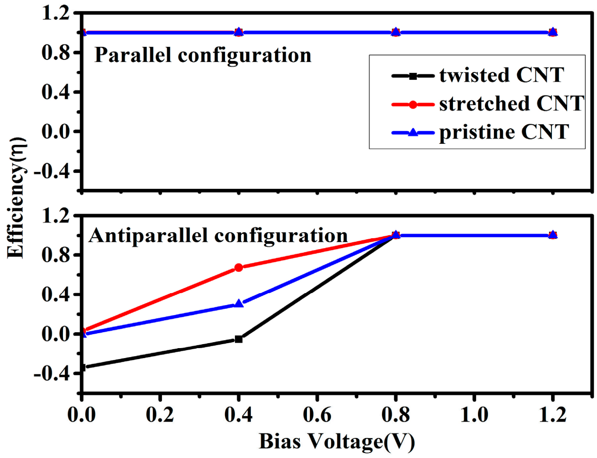

Fig. 7 Spin injection factor with respect to applied voltages for all the three structures in parallel configuration and antiparallel configuration.

At zero volts, total current in all the three structures is zero and spin injection factor is calculated by utilizing equilibrium conductance. Parallel configuration I↑ is nearly equal and I↓ is negligible in all the three cases (see Fig. 4) resulting in allowing only carriers with up-spin to propagate through the CNT and blocking the down-spin carriers, resulting in high spin filtration (η) in case of PC at all bias points. In APC, stretching increases the spin filtration at all bias points in comparison to pristine and twisted structures and is ~100 % at high bias voltages. However, twisting results in lower spin filtration than in pristine and stretched CNTs at low bias voltages and also negative due to I↓ being greater than I↑.

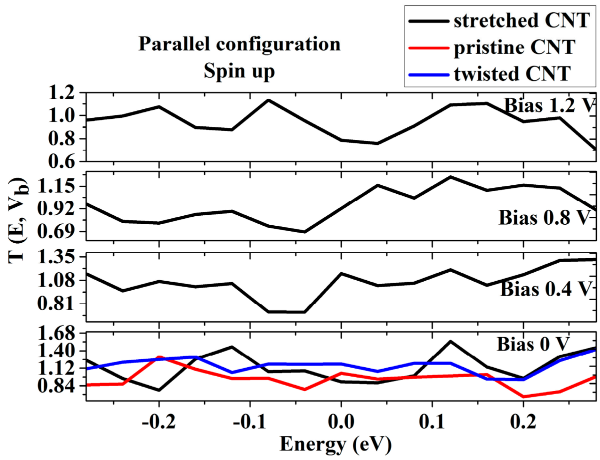

Fig. 8 (a)

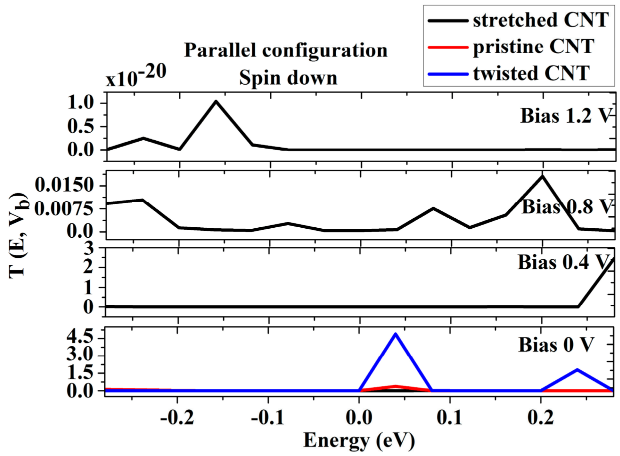

Fig. 8 (b)

Fig. 8 Transmission spectrum T (E, V_b) with respect to energy ranging from -0.3 eV to +0.3 eV for different applied voltages for PC. At zero volts, the comparative transmission probability for all the three structures shown separately for spin-up (see Fig. 8 (a)) and spin-down (see Fig. 8 (b)).

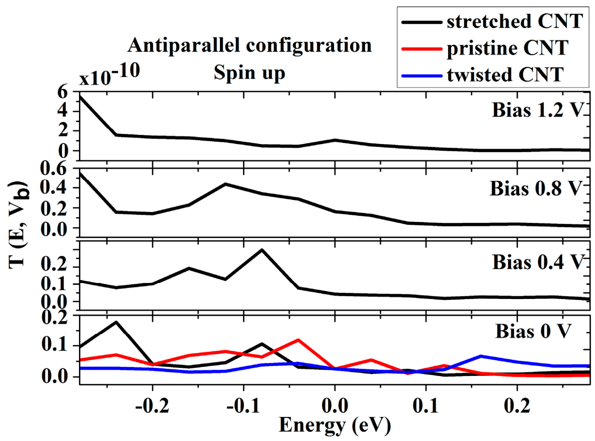

Fig. 9 (a)

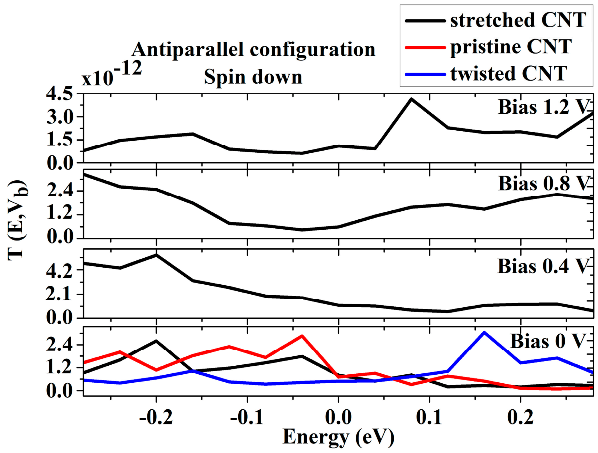

Fig. 9 (b)

Fig. 9 Transmission spectrum T (E, V_b) with respect to energy ranging from -0.3 eV to +0.3 eV for different applied voltages for APC. At zero volts, the comparative transmission probability for all the three structures shown separately for spin-up (see Fig. 9 (a)) and spin-down (see Fig. 9 (b)).

IV. Conclusion

The spin dependent quantum transport properties in twisted CNT and stretched CNT are investigated and it is found that magneto resistance (MR) of stretched CNT is higher than twisted CNT and MR of twisted CNT is higher than pristine CNT and high spin filtration is obtained in stretched CNT in comparison to pristine CNT. High MR and high spin filtration show the importance of twisted and stretched carbon nanotube for use in spin valves and other applications.

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