Ballistic switching and rectification in single wall carbon nanotube Y junctions

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Transport properties of various semiconducting zig-zag carbon nanotube Y junctions are studied for the investigations of rectification and switching. Our results indicate that such junctions, when symmetric, can support both ballistic rectification and/or the ballistic switching operating modes. Although structural symmetry of the Y junction is found to be a necessary condition for rectification, it may not be sufficient in all cases.
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Multiterminal nanotube junctions are interesting for their potential use in nanoscale transistor or amplifier applications. In particular, in three-terminal T or Y junctions, a gate voltage supplied through the third terminal can be used to control current flow in the primary channel which is driven by a bias voltage applied across the first two terminals. Earlier experimental observations of carbon nanotube Y junctions[1,2] were followed by controlled production of these junctions using template[3] and pyrolysis[4] based methods. Theoretical calculations had previously predicted three-point single wall carbon nanotube (SWCN) to be stable.[5,6] The existence of branching in nanotubes resulting in potential electronic device applications is just one of many exciting useful features envisioned for this form of carbon. It is interesting to investigate if the SWCN Y junction can operate in the ballistic rectification (BR) and/or the ballistic switching (BS) mode(s) in a way analogous to that observed in Y-branch switches (YBS)[7] made from materials other than carbon nanotubes, as for example in YBSs based on the InP/InGaAs heterojunctions.[8]

The conductance measurements performed on the template and pyrolysis produced Y junctions have shown intrinsic nonlinear and asymmetric current–voltage ($I-V$) behavior at room temperature.[4,9] In particular, the rectification properties of Y junctions were demonstrated by Papadopoulos *et al.*,[3,9] in the experimentally measured $I-V_b$ characteristic of Y junctions biased in a configuration in which the bias-voltage V_b was set equal to

$$V_b = V_S - V_L = V_S - V_R ; \quad V_L = V_R = 0.00, \tag{1}$$

where V_j, $j=S,L,R$ denotes applied voltages in the stem (S), the left (L), and the right (R) branch of the Y junction, respectively. The labeling is illustrated in Fig. 1(a). Papadopoulos *et al.*,[4,9] attributed the observed rectification properties to doping effects in analogy to the operation of a field effect transistor. Subsequent computer simulations based on YBS and Y junctions satisfying a C_{2v} or D_{3h} symmetry and biased as in Ref. 3 have, however, shown that the observed

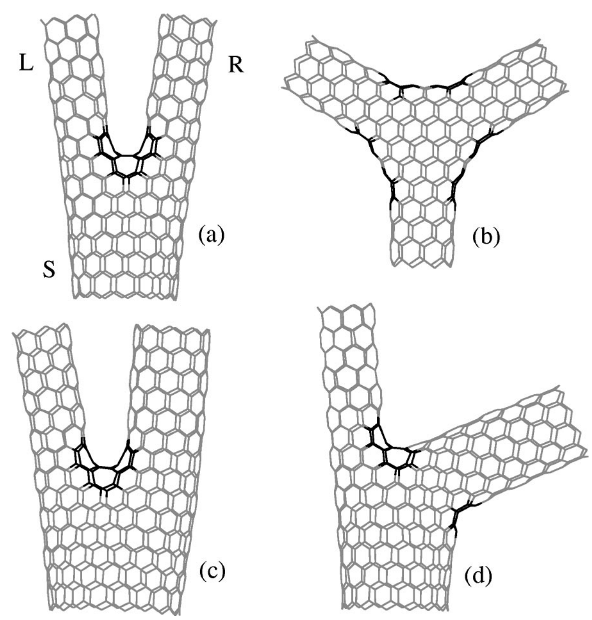

FIG. 1. The four different Y junctions studied in this work. They consist of: (a) a (14,0) stem branching into two (7,0) tubes symmetrically, (b) three (8,0) branches, (c) a (17,0) stem branching into (10,0) and (7,0) tubes with an acute angle between them, and (d) another (17,0) stem branching into (10,0) and (7,0) tubes, but with a different angle between the branches than in (c). In (a), S, L, and R denote stem, left and right branches, respectively of the Y junction. Defect rings are shown in dark.

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rectification can be assigned to features of the ballistic propagation.[8,10–12] The question still remains whether the BR mode is a result of symmetry or is it an intrinsic property of the Y junction.

Switching properties of Y junctions, analogous to those observed in YBS based on InP/InGaAs heterostructures,[8] have not been reported so far to the best of our knowledge. It is, therefore, very worthwhile to investigate if Y junctions can provide an additional support for a BS mode.

In this letter, we report results of our calculations of quantum conductivity of SWCN Y junctions which show ballistic switching in two different bias voltage configurations. All three arms of the Y junctions are taken to be in contact with the paramagnetic transition metal leads consisting of bulk Ni in the ⟨001⟩ orientation. Quantum conductivity calculations of SWCN Y junctions are carried out using the familiar Landauer expression.[13] The transmission function $T(E)$ is obtained using the Green's function formalism which incorporates the interaction of SWCN with metal leads.[14] We use the tight-binding (TB) formulation for both the Hamiltonian and the Green's function. The TB Hamiltonian consists of $N_{at}N_{\mathrm{orb}}\times N_{at}N_{\mathrm{orb}}$ matrices, where N_{at} is the number of atoms in the embedding subspace and N_{orb} is the number of orbitals on each atom. Contrary to previous works on quantum transport which use only one π-electron orbital per atom, we use $N_{\mathrm{orb}}=4$ for carbon that includes 1 s and 3 p orbitals. Additionally, we use $N_{\mathrm{orb}}=9$ for Ni that includes 1 s, 3 p, and 5 d orbitals. This Hamiltonian has been used with success in the treatment of transition metal systems as well as their interactions with graphite and nanotubes.[15,16]

The transmission function has the form $T(E)=T_{ij}(E)$ where the indices i,j indicate the three branches of the Y junction. Having obtained the functions $T_{ij}(E)$, we next use the formalism of Landauer and Buttiker[13,17,18] to calculate the current I_i passing through the branch i for $i=S,L,R$ in terms of the applied branch voltages V_i, $i=S,L,R$.

Following Hieke and Ulfward,[8] we examine the Y junctions by simulating their setup in the two measurement configurations described in Ref. 8. In the first configuration, we put

$$V_L=-V_R=V_b;\quad I_S=0.00 \tag{2}$$

and obtain the dependence $V_S=f(V_b)$ subject to the condition that the stem current I_S be zero. In the second configuration, we put

$$V_L=-V_R=V_b;\quad V_S=0.00 \tag{3}$$

and obtain the dependence $I_S=f(V_b)$ subject to the condition $V_S=0.00$. The results of our calculations are presented in Figs. 2 and 3.

The four different Y junctions studied in this work are shown in Fig. 1. They are all "zig-zag" nanotubes and include, (a) a (14,0) stem branching into two (7,0) tubes symmetrically, (b) three (8,0) branches, (c) a (17,0) stem branching into (10,0) and (7,0) tubes with an acute angle between them and, (d) another (17,0) stem branching into (10,0) and (7,0) tubes, but with a different angle between the branches than in (c). The defect rings are shown in dark. All these Y junctions are semiconducting. This allows us to make direct comparison with experiment since the chemical vapor deposition method used to produce the Y junction is known to result in semiconducting tubes.[3]

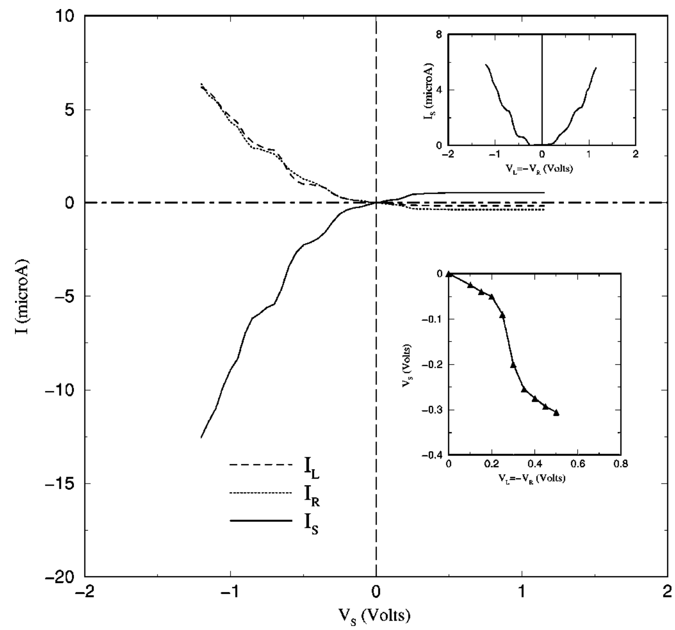

FIG. 2. Stem (I_S) and branch (I_L and I_R) currents vs bias voltage in the bias configuration described by Eq. (1) for the symmetric (14,0)–(7,0)–(7,0) Y junction. Top inset: Stem and branch currents vs bias voltage in the bias configuration described by Eq. (3). Bottom inset: The dependence $V_S=f(V_b)$ when the Y junction is biased according to Eq. (2). The current is taken to be positive when flowing towards the junction and negative otherwise.

In the top inset in Fig. 2 we present the calculated $I_S=f(V_b)$ dependence obtained for the symmetric (14,0)–(7,0)–(7,0) Y junction biased according to Eq. (3) and shown in Fig. 1(a). This structure contains six heptagons clustered in the middle (shown in dark) in an otherwise hexagonal arrangement of carbon atoms. The symmetry in the currents

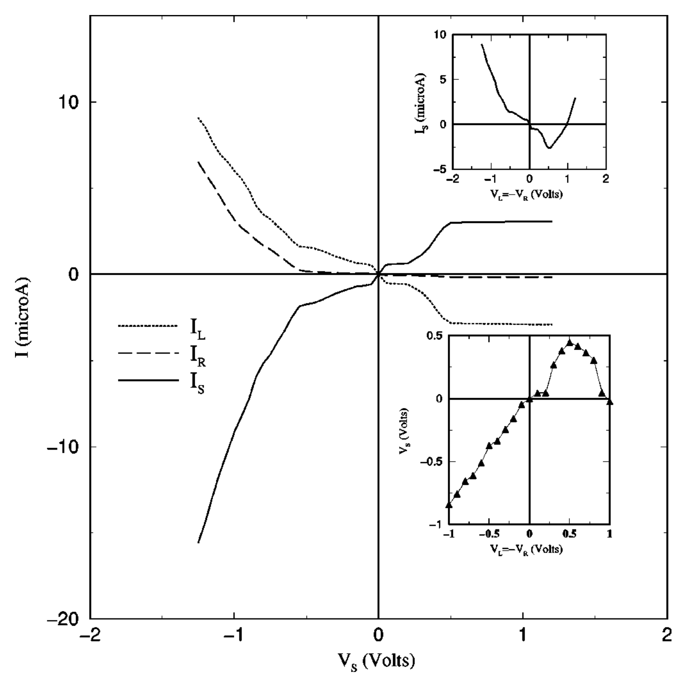

FIG. 3. The same quantities as in Fig. 2 but for the asymmetric (17,0)–(10,0)–(7,0) Y junction.

is evident in the figure indicating perfect switching. As can be seen in the figure, I_S is always positive regardless of whether the biasing is from the left or right branches. The structure in Fig. 1(b) is also symmetric, but the six heptagons are so distributed that there are two each on the outer side (shown in dark). When biased according to Eq. (3), the same perfect switching features are also present for this Y junction.

The calculated $I_S = f(V_b)$ dependence obtained for the asymmetric (17,0)–(7,0)–(10,0) Y junction [Fig. 1(c)] is shown in the top inset in Fig. 3. Although the arrangement of defects is identical to that in Fig. 1(a), there is asymmetry in the currents and the loss of the perfect switching feature.

The effect of the symmetry of the tube is also evident in the rectification efficiency of the Y junctions considered. Figure 2 shows the $I-V$ characteristics of the (14,0)–(7,0)–(7,0) Y junction [Fig. 1(a)] biased according to Eq. (1). As seen in the figure, there is perfect rectification. The $I-V$ characteristics of the asymmetric (17,0)–(7,0)–(10,0) Y junction [Fig. 1(c)], also biased according to Eq. (1), is shown in Fig. 3. The lack of rectification seen here lends strong support to the argument favoring structural symmetry of the Y junction for rectification in three-point junctions. We have also calculated the $I-V$ characteristics of the asymmetric Y junction shown in Fig. 1(d). This structure contains four heptagonal defects in the joint between the (7,0) and (10,0) branches and one octagonal defect in the joint between the (17,0) stem and the (10,0) branch. The defect regions are shown in dark. As expected, no rectification is obtained for this Y junction.

Further insights into the switching properties of carbon nanotube Y junctions can be gained by studying the $V_S = f(V_b)$ dependence of the Y junctions biased according to Eq. (2). The results are shown in the bottom insets of Figs. 2 and 3 for the symmetric (14,0)–(7,0)–(7,0) and the asymmetric (17,0)–(10,0)–(7,0) Y tubes, respectively. For the symmetric Y junction we find $V_S(-V_b) = V_S(V_b)$ and an approximate parabolic dependence of V_S on V_b as found in YBSs made from InP/InGaAs.[8] In the asymmetric Y junction we observe that $V_S(-V_b) \neq V_S(V_b)$ and no overall parabolic dependence. Results for the symmetric (8,0)–(8,0)–(8,0) nanotube [Fig. 1(b)] were similar to the (14,0)–(7,0)–(7,0) Y junction results. It is worth noting that in the (8,0)–(8,0)–(8,0) tube we find that the parabolic dependence, $V_S = f(V_b)$, is interrupted by a shallow dip for $|V_b| \in [0.1–0.3]$ V. This dip suggests the appearance of a negative differential resistance in the same range of V_b. However, the nature of the observed dip is not clear.

Our results, thus, clearly point to the important role played by the structural symmetry on the transport properties of the carbon nanotube Y junctions. Recently, Song *et al.*,[11] have observed rectification in a symmetric four terminal device made from InP/InGaAs heterojunctions when an asymmetric scatterer is introduced into it. They attributed the rectification effects to the artificial scatterer which breaks the device symmetry. We note, however, that the antidot in their work still retains the mirror symmetry. The Y junction with its heptagonal defects in our case may play a role similar to that of the antidot in their case. Furthermore, in the present case, where the transmission functions $T_{ij}(E)$ are bias-voltage independent, self-gating effect[10] can be excluded as a possible reason for the observed rectification and switching properties found in the symmetric Y junctions. Also, doping effects,[9] absent in our case, cannot account for the observed properties. The present results, however, support that the findings of Treboux *et al.*[12] (who showed the existence of interference effects in Y junctions) can be a major reason for the observed properties.

In conclusion, we have shown that symmetric Y junctions consisting of semiconducting branches can support both BR and BS operating modes. Although structural symmetry of the Y junction is found to be a necessary condition for rectification, it may not be sufficient in all cases. This finding may be important in finding fabrication pathways for future functioning devices and switches. Investigations are underway to examine other constraints.

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