

**COMMENTS****Comment on "Intrinsic electron transport properties of carbon nanotube Y- junctions" [Appl. Phys. Lett. 81, 5234 (2002)]**Antonios N. Andriotis<sup>a)</sup>*Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1527, 71110 Heraklio, Crete, Greece*Deepak Srivastava<sup>b)</sup>*NASA Ames Research Center, CSC, Mail Stop T27-A1, Moffett Field, California 94035-1000*Madhu Menon<sup>c)</sup>*Department of Physics and Astronomy and Center for Computational Sciences, University of Kentucky, Lexington, Kentucky 40506-0055*

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Carbon nanotubes have received much attention recently for molecular electronic device applications due to their ability to form both metallic and semiconducting type nanotubes in experiments.<sup>1,2</sup> Two- and three-terminal junctions of different type of nanotubes were first proposed in simulations<sup>3–10</sup> and later fabricated in experiments.<sup>11–19</sup> The importance of three terminal *T*- and *Y*- junction nanotubes arises from the fact that these can provide the framework on which simple nanoscale carbon based transistor, power amplification, or analog logic devices could be designed and fabricated. Initial investigations and proposals, in this case, also were primarily through theoretical modeling and computer simulation based studies.<sup>7–10</sup> Structural stability, role of topological defects in connecting nanotubes of different chirality, and the electronic structure have been investigated and reported in detail.<sup>9,10</sup> Studies of electronic transport and possible device applications of nanotube *T*- and *Y* junctions have taken on urgency because it is now feasible to fabricate multiterminal junctions of single-wall carbon nanotubes (SWCNs) via the electron or ion-beam irradiation induced nano-welding at the location of the junction.<sup>20</sup>

Recently, in a series of papers we have reported the structure and electron transport properties of SWCN *Y* junctions.<sup>21–23</sup> Our calculations were based on a Green's function embedding scheme for conductivity.<sup>24</sup> According to our results SWCN *Y* junctions, when biased as a two terminal current carrying devices with metallic contacts, exhibit (a) asymmetric current–voltage characteristics in general and (b) perfect rectification in certain cases where a semiconducting nanotube forms the stem or base of the symmetric *Y* junction. Based on these studies, we concluded that the above two characteristics are intrinsic properties of the carbon nanotube *Y* junctions.<sup>23</sup>

In a recent letter, Meunier *et al.*,<sup>25</sup> make a claim that the

rectification effect is entirely due to metallic contacts and that three-terminal geometry is not necessary for rectification. This is based on their calculation and comparison of a threefold symmetric (10,0) SWCN *Y* junction (with and without metallic electrodes) case with a straight (10,0) carbon nanotube (with and without metallic electrodes). Transmission functions and local densities of states (LDOS) in the two cases were computed and compared. Meunier *et al.* find no rectification if the symmetric (10,0) *Y* junction is seamlessly extended by three semi-infinite nanotubes acting as leads (system 1, denoted as  $S_1$ ). In the case of the metal-terminated SWCN *Y* junction consisting of finite length branches (system 2, denoted as  $S_2$ ), however, they obtain asymmetric transmission function and LDOS.

Searching for the qualitative differences between  $S_1$  and  $S_2$  and the effect these can have on the resonance transmission, and therefore, on the conductance of the *Y* junction, we point out the following

(1) In  $S_1$ , the allowed energy-levels are common to the whole system (i.e., to the three branches and node of the system); the node (*Y* junction) cannot behave as a quantum dot.

(2) By making the system finite in  $S_2$ , inherently we redefine the zero-energy level of the node (*Y* junction) with respect to the vacuum. This means that the occupied energy levels of the finite *Y* junction relevant to the resonance tunneling are relatively shifted to lower energies as compared to the vacuum level as specified by the metallic leads. This is a simple consequence of the stability of the system. In other words, if the Fermi level is at the  $E=0$ , the active resonance levels should appear more(less) dense for the negative (positive) energies as a consequence of the finiteness of the *Y* junction (as a finite quantum well at the node). This automatically leads to an asymmetry in  $T(E)$  and hence to rectification.

As a consequence of (1) and (2), some level or amount of asymmetry should be and is expected for any nanotube (straight or *Y* shaped) of finite size. This is not necessarily

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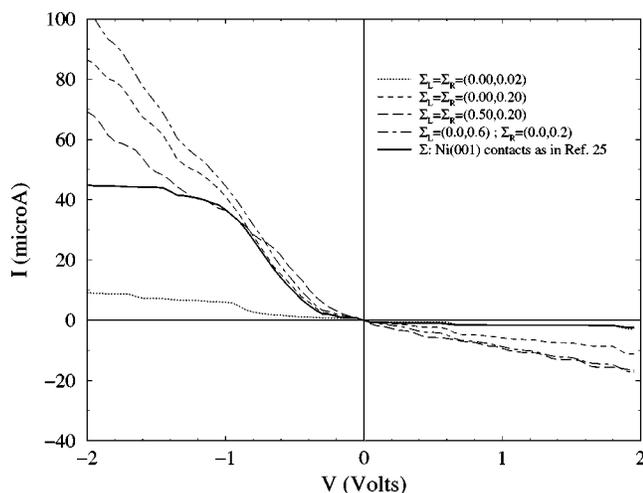


FIG. 1. The  $I$ - $V$  (current vs applied bias voltage) characteristics of a 500-atom (5,5)-SWCN in contact with metal leads made of Ni(001) under asymmetric bias. Only the carbon atoms at both ends of the tube are in contact with the metal leads. The effect of this contact is represented by self-energy terms ( $\Sigma_L$  and  $\Sigma_R$  for left and right ends, respectively) of the Hamiltonian of the system (tube plus metal contacts, Ref. 24). The effect of the strength of the metal-tube coupling is simulated by changing the value of the self-energy as indicated in the legend.

enough to cause rectification in a straight tube with metallic leads. However, the level of asymmetry (i.e., location of allowed energy levels with respect to  $E=0$ ) and, therefore, the rectification properties of the quantum well at the node or  $Y$  junction are the inherent property of the structure at the junction. The asymmetry and amount of rectification is determined from the structural characteristics of the quantum well at the junction (i.e., straight,  $Y$  shaped, tube chirality, and symmetry) and also the strength of the contact-lead interactions.

In a straight nanotube of finite length, this point can be emphasized by examining the effect of the bias or gate voltage on the nature of asymmetry imposed on the  $I$ - $V$  characteristics and the rectification characteristics of such tube. As shown in Fig. 1, we note that the asymmetric  $I$ - $V$  characteristics in a finite length straight tube are manifested only if the applied bias is asymmetric i.e., when  $\eta=0$  [see Eqs. (19) and (20) in Ref. 24]. For a symmetric bias [ $\eta=0.5$  in Eqs. (19) and (20) in Ref. 24] there is no rectification.

From the discussion earlier, it is apparent that the asymmetric nature of the  $I$ - $V$  characteristics of SWCNs is a consequence of the finite size of the nanotubes with or without leads. In case of  $Y$  junction nanotubes, the rectification is determined by four factors: (a) formation of a quantum dot at the location of the  $Y$  junctions, (b) finite length of the stem and branches going out to the metallic leads, (c) the strength of SWCN-metal lead interactions and, (d) the asymmetry of the bias. Attributing the overall rectification effect to only the SWCN-metal lead interactions, and to the Schottky barrier, as concluded by Meunier *et al.*, is neither correct nor complete. We have shown in our recent paper<sup>23</sup> that the intrinsic symmetry of the structural nature at the junction and the external asymmetric conditions imposed by the bias voltage play a significant role in deciding the rectification behavior

of the junction. This is why the asymmetric  $I$ - $V$  characteristics and the rectification at the junction is found to be sensitive to (a) the chirality of the underlying carbon nanotube and (b) the intrinsic structural symmetry at the junction. Rectification does not occur uniformly for all  $Y$  junctions. In a wide variety of junctions examined, perfect rectification was achieved only if the stem (or  $S$  branch) was made of a zig-zag nanotube and the branches were structurally symmetric with respect to the junction. Significant leakage current was observed in all other cases. Our overall conclusion, that the rectification behavior depends on the intrinsic structural nature of the junction, still stands. The Schottky barrier formation at the SWCN-metal lead interface may have additional effects in the case of doped SWCNs and will be investigated in future.

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