Modeling of kink-shaped carbon-nanotube Schottky diode with gate bias modulation

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A model is proposed for the recent gate voltage $V_G$ modulation experiment of a kink-shaped carbon nanotube (NT) Schottky diode [Z. Yao, H. Postma, L. Balents, and C. Dekker, Nature (London) 402, 273 (1999)]. Since larger $V_G$ increases both the forward and the reverse turn-on voltages of the diode, we show that: (1) the rectification must occur at the kink where the metallic and the semiconducting NTs meet, and not at the electrode contact, and (2) the semiconducting NT must be $n$ type. The turn-on voltages are derived analytically as a function of $V_G$ considering the electrode contact contribution and a good agreement is obtained with the experimental data. © 2002 American Institute of Physics. [DOI: 10.1063/1.1481213]

Recently, the Delft group has observed rectifying current–voltage characteristics for a fused kink-shaped carbon nanotube (NT) metal–semiconductor (MS) diode.¹ They applied the gate voltage $V_G$ to change the carrier density in the semiconducting NT and modulated the diode characteristics. Previous analysis focused on the two-terminal properties with a one-dimensional (1D) coherent transport model in a self-consistent field.² In this letter, we will emphasize the three-terminal properties, i.e., how $V_G$ modulates the diode characteristics. From this $V_G$ dependence, we show that: (1) the rectification occurred at the NT MS junction and not at the electrode contact, and (2) the carriers involved in the transport must be electrons rather than holes, unlike commonly observed $p$-type NTs.

In Ref. 1, they placed NTs on TiAu electrodes on a SiO$_2$/doped-Si substrate (backgate) as in Fig. 1(a) and applied $V_G$ to the backgate with electrode 3 grounded under a low temperature environment of 100 K. The circuit between electrodes 0 and 1 showed linear characteristics (110 kΩ) without noticeable $V_G$ dependence. Thus, the left NT was metallic. However, the circuit between electrodes 1 and 3 across 2 showed rectifying characteristics with appreciable $V_G$ dependence as in Fig. 1(b). Therefore, the right NT had to be semiconducting. We introduce an equivalent circuit with drain current $I_D$ and voltage $V_D$ at electrode 1. A linear resistor $R_1$ represents contact 1. $V_G$ modulates the carrier density in the semiconducting NT and a capacitor $C_{NT}$ represents the capacitance with respect to the substrate. The metallic and the semiconducting NTs meet at kink 2, and a MS junction $J_2$ is formed. The semiconducting NT reaches electrode 3 and a semiconductor–metal (SM) junction $J_3$ is formed. For rectification to take place, either $J_2$ or $J_3$ should be a Schottky diode and the other should be a resistive element. In fact, if both are Schottky diodes, then $J_2$ and $J_3$ are either front-to-front $(+|>|<|)$ or back-to-back $(+|<|>|<|)$ connected by sharing the semiconducting NT and will allow only negligible current through them. If both are resistive elements allowing current in both polarities, then there is no mechanism for rectification.

The forward direction occurred when $V_D>0$.¹ Thus, two equivalent circuits are possible: $J_2$ is a Schottky diode with an $n$-type NT and $J_3$ is a resistor as in Fig. 2(a), or $J_2$ is a resistor and $J_3$ is a Schottky diode with a $p$-type NT as in Fig. 2(b). We introduce forward and reverse turn-on voltages for a diode, $V_{onF}$ and $V_{onR}$, respectively,³ corresponding to the onset of $I_D$. The experimental $V_G$ dependence is such that: if $V_G < V'_G$, then $0 < V_{onF} < V'_{onF}$ and $V_{onR} < V'_{onR} < 0$ as in Fig. 1(b), where a prime indicates a quantity at $V'_G$. Or increasing $V_G$ shifts both $V_{onF}$ and $V_{onR}$ in the positive $V_D$ direction.

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Schottky barriers for electrons at voltages shown in Figs. 2 and 3 of selected Si NTs. Energy band diagrams for Si NT–electrode SM cases are examined, thus, $\mid V_{bi} \mid < \mid V'_{bi} \mid$ and $V_{onR} < V'_{onR}$. This is also consistent with the experiment.

However, neither trends for $V_{onF}$ and $V_{onR}$ are explained by the $p$-NT scenario with D₃ as in Fig. 2(b). Increasing $V_{G}$ results in lower hole density and $\xi$ increases. Thus, again $\xi < \xi'$. However, $V_{bi} > V_{bi}'$ for holes as shown in Figs. 2(i) and 2(j). Thus, $V_{onF} > V'_{onF}$ in the forward direction, but this is contrary to the experiment. In the reverse direction, the effective doping is smaller for larger $V_{G}$ and the Schottky barrier is thicker. Thus, $\mid V_{bi} \mid < \mid V_{bi}' \mid$ and $V_{onR} > V'_{onR}$. This is again contrary to the experiment. Therefore, we conclude that: (1) the rectification occurred at $D_2$, and (2) the NT must be $n$ type.

We will express $V_{onF}$ and $V_{onR}$ as a function of $V_{G}$ based on this view. Since the onset of $I_D$ is our present interest, we do not solve the transport problem but identify the diode turn-on voltages. This is practically enough for many electronics applications. V₃ attracts or repels electrons through contact 3 (electrodes are infinite charge reservoirs), and causes a linear change in $\xi$, such that $\xi(V_{bi}) = \xi(0) + \alpha V_{bi}$. The coefficient $\alpha$ is related to the NT state density and $C_{NT}$, and thus depends on the quasi-1D NT band structure as well as the detailed device geometry including the SiO₂ layer. The NT specific information is embedded in $\alpha$. By inspecting the band diagram in Fig. 2(c), we have $eV_{bi} = \phi_{NT} - \phi_{Au} - [E_G - \xi(V_{G})]$. The forward turn on is achieved by applying $V_{D2} = V_{bi}$. Thus, the forward turn-on modulation by $V_{G}$ is given by $\Delta V_{bi}(V_{G}) = \alpha \Delta V_{G}$.

The reverse turn on for a different $V_{G}$ occurs when the Schottky barrier has the same slope (electric field) at the junction. In this case, transport electrons see the same Schottky barrier height and the width since $\phi_{NT}$ is independent of $V_{G}$. The electric field at the junction is proportional to $[(V_{bi} + |V_{bi}'|)N_d]^{1/2}$ based on the planar junction theory. By equating $V_{bi} + |V_{bi}'| = N_d'$ for finite and zero $V_{G}$ cases with an ionized donor density $N_d'$, we have $(V_{bi} + |V_{bi}'| - \alpha V_{G})(N_d' + N_d'V_{bi}/(V_{bi} + |V_{bi}'|)) = (V_{bi} + |V_{bi}'|)N_d'$, where the subscript 0 refers to $V_G=0$. $V_{bi} = -\beta (\leq 0)$ is a voltage such that the electrons are repelled completely, and the NT becomes intrinsic. The reverse turn on is achieved by applying $V_{D2} = V_{bi}$. Therefore, the modulation is given by $\Delta V_{bi}(V_{G}) = -(\mid V_{bi} \mid - \mid V_{bi}' \mid) = \alpha \Delta V_{G} - \Delta(V_{bi} + |V_{bi}'|)$. 

$E_c$ and $E_v$ are conduction and valence band edges with a band gap $E_g$. $\xi$ is a chemical potential $E_{FS} - E_v$ and $\chi$ is an electron affinity. $V_{bi} (>0)$ is a built-in voltage and $V_{bi} (<0)$ is a breakdown voltage. $e (>0)$ is the unit charge.

We examine the $n$-NT scenario with $D_2$ as in Fig. 2(a) and compare the influences of $V_{G}$. Increasing $V_{G}$ results in higher electron density, and $\xi$ increases. Thus, $\xi < \xi'$ and we may think that the doping is effectively increased. Since $\phi_{NT}$ is independent of $V_{G}$, $V_{bi} > V_{bi}'$ as shown in Figs. 2(c) and 2(d). In the thermionic emission $^3$ (Ref. 2 estimated a thick Schottky barrier of several nanometers), the forward turn-on occurs when $V_D - V_{bi}$. Therefore, $V_{onF} < V'_{onF}$, as in Figs. 2(e) and 2(f). This is consistent with the experiment. The reverse turn on occurs when the gradient and the width of the Schottky barrier exceed certain thresholds or $V_D - V_{bi}$. This is the beginning of the tunneling breakdown. The effective doping is larger for larger $V_{G}$, leading to the thinner Schottky barrier as in Figs. 2(g) and 2(h).

Thus, $\mid V_{bi} \mid < \mid V_{bi}' \mid$ and $V_{onR} < V'_{onR}$. This is also consistent with the experiment.

Such $V_{G}$ dependence is possible with an $n$-NT, but not with a $p$-NT. The band diagrams for Schottky diode $D_2$ of $n$ type in Fig. 2(a) are shown in Figs. 2(c)–2(h) for selected $D_2$ voltages $V_{D2}$, and those for $D_3$ of $p$ type in Fig. 2(b) are shown in Figs. 2(i)–2(j) for null $D_3$ voltage $V_{D3}$, respectively. We compare small $V_{G}$ (left) and large $V_{G}$ (right) cases. $\phi_M$ is a metallic NT work function. $\phi_{NT}$ and $\phi_{Au}$ are Schottky barriers for electrons at $D_2$ and holes at $D_3$, respectively. $E_{FM}$ and $E_{FS}$ are electrochemical potentials, $\xi$ is a chemical potential, $E_v$ and $E_c$ are conduction and valence band edges with a band gap $E_g$. $V_{bi}$ and $V_{bi}'$ are built-in and breakdown voltages, and $\chi$ is an electron affinity.