

## Transport modeling for metallic electrode - semiconducting nanotube systems

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Recently, current-voltage ( $I$ - $V$ ) characteristics have been reported by Collins *et al.* for a system with a scanning tunneling microscope (STM) tip and a carbon nanotube [1]. The STM tip was driven forward into a film of many entangled nanotubes on a substrate, and then was retracted, so that one of nanotubes bridged the STM and the film.  $I$ - $V$  characteristics had two different patterns as shown in Figs. 1(a) and 1(b) for different heights. One showed large  $dI/dV$  with  $V > 0$ , small  $dI/dV$  with  $V < 0$ , and  $I = 0$  near  $V = 0$  (type-I), while the other showed rectification, i.e.,  $I \neq 0$  only with  $V < 0$  (type-II), with the tip grounded. We propose a physical mechanism to explain the observed  $I$ - $V$  patterns.

We consider that the observed characteristics strongly reflected the nature of the tip (metal) - nanotube (semiconductor) contact [2]. The other end of the nanotube was entangled well in the film, and simply provided a good Ohmic contact. We will argue that there are two different contact modes - vacuum gap (left) and touching (right) modes as in Fig. 1(c), depending on the presence or absence of a tiny vacuum gap  $d \sim 0.1$ - $0.2$  nm at the junction. These modes may be related to physisorption and chemisorption, respectively. Once admitting their existence, it is naturally shown that  $I$ - $V$  characteristics are type-I in the vacuum gap mode, and type-II in the touching mode. We argue that the nanotube had to be an  $n$ -type semiconductor judging from the  $I$ - $V$  characteristics, contrary to often observed  $p$ -type in the transistor applications [3], where  $p$ -type is probably due to the oxidation in air or the trapped charges in the silicon-dioxide.

The band diagrams are shown in Fig. 1: (d) - (f) for type-I (left) and (g) - (i) for type-II (right). In the metal,  $E_{FM}$  is the Fermi energy and  $\phi_M$  is the work function. In the semiconductor,  $\chi$  is the electron affinity,  $E_{FS}$  is the Fermi energy, and  $E_G$  is the band gap.  $E_c$  and  $E_v$  are conduction and valence band edges, respectively, and depend on the applied voltage  $V$  after the tip is grounded.  $\phi_n$  and  $\phi_p$  are Schottky barriers and  $\xi = E_{FS} - E_v$ . At (d), valence-band electrons tunnel to the tip with  $V < 0$ , resulting in smaller  $dI/dV$ . (e) is a thermal equilibrium with  $V = 0$ . At (f), tip electrons tunnel to the conduction band with  $V > 0$ , resulting in larger  $dI/dV$ . The vacuum gap provides flexibility for  $E_c$  and  $E_v$  to align freely with  $E_{FM}$  by absorbing the necessary voltage drop for given  $V$ . In the touching mode,  $\phi_n$  and  $\phi_p$  are fixed regardless of  $V$ . The Schottky forward transport occurred at the same bias polarity as the *valence*-band tunneling of (d). Thus, (g) follows with  $V > 0$ , and the nanotube has to be  $n$ -type. (h) is a thermal equilibrium. (i) is a reverse condition with  $V > 0$  with negligible current. We note that for  $p$ -nanotubes, the entire  $I$ - $V$  pattern simply shifts to the positive  $V$  direction in the vacuum gap mode, while it rotates by  $\pi$  in the touching mode. Thus, if the Schottky forward transport had occurred at the same polarity as the *conduction*-band tunneling of (f) ( $V > 0$ ), then the nanotube should have been  $p$ -type, but this was not the case.

We have performed numerical calculations based on either the tunneling formula [4] or the familiar Schottky

formula assuming a (17,0) semiconducting nanotube, and results are compared to the experimental data of Ref. 1. Reasonable agreement is obtained.

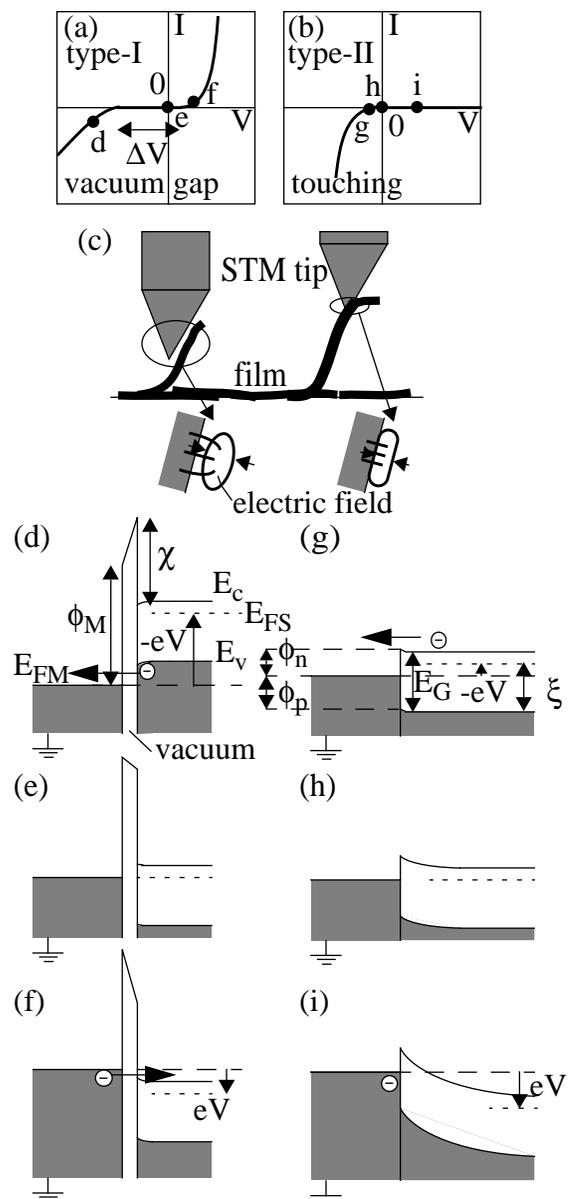


Fig. 1 (a) and (b)  $I$ - $V$  characteristics; (c) two contact modes; (d)-(i) band diagrams.

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