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Investigation on nanotube-metal contacts under different contact types

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ABSTRACT

The contacts of the metallic or semiconducting carbon nanotubes (CNTs) and the Ti (side-contacted type) or TiC (end-contacted type) have been investigated by non-equilibrium Green's function approach. The transmission coefficient and resistance of the contacts are calculated. The study shows the contact resistance between TiC and metallic or semiconducting CNT is 2 and 4 orders of magnitude lower than that between Ti and metallic or semiconducting CNT, respectively. The contact resistance between TiC and metallic CNT can be low down to ~6.8 kΩ. The contact characteristics are illustrated by the wave-vector conservation of electron transportation between CNT and metal.

1. Introduction

Carbon nanotubes (CNTs) are ideal blocks of next-generation nanoelectronic devices and integrated circuit. The CNT-metal contact plays a critical role in CNT-based electronic devices, such as the CNT field-effect transistor (CNTFET). The low contact resistance is a key to achieve high device performance for the scaled-down devices and meet the international technology roadmap for semiconductors [1]. The contact resistance is large when the CNT is placed on and contacted to the metal by the Van der Waals force [2]. The origin of the large contact resistance between CNT and metal had been studied based on the first-principles quantum mechanical density functional and matrix Green's function methods [3]. To improve the CNT/metal contact, many methods had been attempted to treat the contact of CNT and metal. The high-temperature annealing [4–7] and ultrasonic nanowelding [8–9] had been demonstrated to be able to effectively improve the CNT/electrode contact performance by forming the carbide at contacts and thereby changing the contact configuration. For a Titanium (Ti)-contacted CNTFET, the titanium carbide (TiC) could be formed at the contact after the high-temperature annealing or ultrasonic nanowelding. More recent studies also implied that the contact configuration could significantly affect the electrical characteristics in CNT/metal interconnection [10] and the device performance [9] in CNT photovoltaic cell. The first-principle calculation based on the density functional theory [11] had been reported to study the Ti–TiC–CNT heterojunction. However, the effect of the contact configuration on the contact characteristics had not been considered in previous theoretical studies, which is assumed to play an important role in the contact characteristics.

In this paper, we study the contacts between both the metallic or semiconductuing CNT and the Ti or TiC electrode using a non-equilibrium Green's function (NEGF) method with the tight-binding approximation. The CNT/Ti and CNT/TiC contacts are modeled as the side-contacted and end-contacted configurations, respectively. The contact characteristics are explained by the *k*-vector conservation of electron transportation.

2. Modeling

To calculating the transmission and current–voltage characteristics of the CNT/Ti and CNT/TiC contacts, the side-contacted and end-contacted configurations are used in the modeling for the CNT/Ti and CNT/TiC contacts respectively (Fig. 1), which are consistent with the results of previous experimental studies [4,8]. In the side-contacted case (Fig. 1a), a cylindrical nanotube lies on the metal electrode (*M*). In the modeling, the contact region between the carbon nanotube and metal is assumed as a narrow cylindrical surface along the axis direction.

The Green's function of the device in the side-contact case is

$$G^r(E) = [(E - eU)I - H_D - \Sigma_R^r - \Sigma_M^r]^{-1}, \quad (1)$$

where E is the energy, e is the electronic charge, U is the

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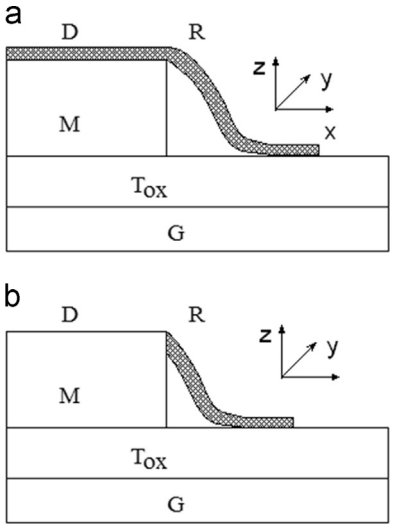

Fig. 1. The schematic of the side-contacted CNT-Ti configuration (a) and the end-contacted CNT-TiC configuration (b). *M* represents the Ti or TiC electrode; *D* represents the CNT segment contacted by the Ti or TiC electrode and *R* represents the CNT segment outside the electrode; T_{ox} is the oxide (gate insulator) layer; *G* is the gate.

electrostatic potential of the nanotube, H_D is the π-electron tight-binding Halmitonian of the nanotube with the on-site potential (0 eV) and the hopping potential between nearest-neighbor carbon atoms (3.1 eV). The self-energy$\Sigma_R$represents the interaction of *R* and *D*, which can be expressed as $\Sigma_R = V_{DR} g_R^r V_{RD}$, where $V_{DR}(V_{RD})$ is the coupling between *D* and *R* (*R* and *D*) and $g_R^r$is the surface Green's function of the *R*. For the semiconductor and metallic CNTs, the g_R^r are obtained respectively as the methods in Ref. [12,13] and Ref. [14].

The self-energy $\Sigma_M = V_{DM} g_M^r V_{MD}$ represents the interaction between *D* and *M*. $V_{DM}(V_{MD})$ is the coupling between *D* and *M* (*M* and *D*). The g_M^r is the surface Green's function of metal. The g_M^r is calculated within the free-electron approximation using the procedure outlined below. The metal electrode has a rectangular cross section of dimensions L_x and L_z in the *x* and *z* directions respectively and is infinitely long in the *y* direction. While the (*y*,*z*) coordinates are assumed to be continuous, the *x* coordinate is assumed to be discrete with lattice spacing $a = L_x/(N_x+1)$,where N_x is the number of lattice points. According to the calculation method in Ref. [18], we obtain the g_M^r expression

$$g_M^r(E) = -\frac{im_0}{\hbar^2}\frac{1}{L_x L_z}\sum_{m,n}\frac{1}{k_l}\sin^2\left(\frac{m\pi x}{L_x}\right)\times \sin\left(\frac{n\pi z}{L_z}\right)\sin\left(\frac{n\pi z'}{L_z}\right), \quad (2)$$

where,

$$k_l = \left\{k^2 - \left(\frac{n\pi}{L_z}\right)^2 - \frac{1}{a^2}\left[1 - \cos\left(\frac{m\pi}{N_x+1}\right)\right] + i\eta\right\}^{1/2}, \quad (3)$$

where $k = \sqrt{2m_0E/\hbar^2 + k_f^2}$, k_f is the Fermi wave vector of the metal.

The transmission probability between *M* and *R* is given by

$$T_{MR}(E) = Tr[\Gamma_M(E) G^r(E) \Gamma_R(E) G^a(E)], \quad (4)$$

where $\Gamma_M = 2\pi V_{DM}\rho_M(E)V_{MD}$, thereinto $\rho_M(E) = -(1/\pi)\mathrm{Im}[g_M^r(E)]$ is the surface density of states of lead *M*.

In the case that the TiC is formed at the metal/CNT contact, the CNT is end-contacted to the TiC. For this case, the Green's function of the device is

$$G^r(E) = [(E - eU)I - H_D - \Sigma_R^r]^{-1} \quad (5)$$

The transmission probability between TiC and *R* is given by

$$T_{MR}(E) = Tr[\Gamma_R(E) G^a(E)], \quad (6)$$

where $\Gamma_R = i[\Sigma_R^r - \Sigma_R^a]$.

The obtained transmission probability was then used in the Landuar–Buttiker formula to calculate the current through the contact shown as follows:

$$I = 4e/h \int [f(E + eV_M) - f(E + eV_R)] T_{MR} dE \quad (7)$$

Finally, the contact resistances between the CNT and the electrode can be obtained from the current-bias characteristics

In the calculation, the work functions of CNT, Ti and TiC are taken as 4.5 eV[15], 3.9 eV[16] and 4.6 eV[17,18], respectively. A suitable gate voltage was applied to make the contact be in the On state when calculating the *I*–*V* characteristics and contact resistance.

3. Results and discussion

Fig. 2 shows the transmission function near the Fermi energy when metallic and semiconducting CNTs are contacted to Ti and TiC respectively. It is shown that the transmission coefficient (*T*) between Ti and metallic CNT is larger than that between Ti and semiconducting CNT as shown in Fig. 2. The *T* between TiC and metallic CNT is the largest in the most of energy range among four kinds of contact configurations.

Fig. 3 shows that the *I*–*V* characteristics (Fig. 3a and Fig. 3c) and the corresponding contact resistance (Fig. 3b and Fig. 3d) for four kinds of contact cases. In the end-contacted geometry with CNT contacted to TiC, a lower contact resistance is observed than that in the side-contacted geometry with CNT contacted to Ti. For the metallic CNT, the lowest contact resistance is reduced from 647 kΩ in the Ti-contacted case to 6.8 kΩ in the TiC-contacted case, which is reduced by 2 orders of magnitude. The calculated contact resistance (6.8 kΩ) between the metallic CNT and TiC is a little higher than the theoretical minimum contact resistance (3.2 kΩ), which is about half of the theoretical minimum resistance (6.45 kΩ) of a ballistic conducting metallic SWCNT with ideal contacts and derives from the electron scattering at CNT/metal interface. For the semiconducting CNT, the lowest contact resistances are 112 *M*Ω and 12.7 *k*Ω for Ti-contacted case and TiC-contacted case respectively, varying by about 4 orders of magnitude. The calculated result is consistent with that in the experimental reports [8,19]. Previous experimental study showed that the contact resistance could be reduced by more than three orders of magnitude using a ultrasonic nanowelding method to convert the Ti-CNT contact into TiC-CNT contact [8]. It was also

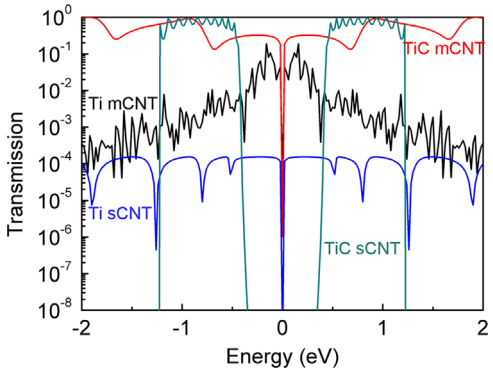

Fig. 2. The transmission coefficient (*T*) of the contacts in the cases that the metallic and semiconducting CNT are contacted to Ti and TiC, respectively.