11th International Workshop on Computational Electronics
TU Wien, 25-27 May 2006

Computational Study of the Schottky Barrier at the Metal-Carbon Nanotube Contact

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INTRODUCTION

Nano scale electronic devices utilizing material properties of the carbon nanotube (CNT) have been widely investigated recent years [1]. In this field of study the Schottky barrier at the metal-carbon nanotube contact has been a prime issue [2]. Here we use ***ab initio*** density-functional method [3,4] to investigate the electronic structure and the Fermi level alignment at the metal-carbon nanotube contact. The dependency of the Schottky barrier on the metal work function as well as on the detailed atomic structures at the contact is addressed with an accurate electronic structure calculations [5,6]. We find that, in such a contact between metal and nano-sized semiconductor, the interface atomic geometry could be far more important than the simple electrostatic effect of the metal surfaces.

CALCULATION AND DISCUSSION

We use the standard density-functional method to investigate the metal-nanotube contact [3]. The total energy of the system and the energy band structures are obtained by the self-consistent solution of the Kohn-Sham equation, as described in the Eq. (1) and (2). Throughout this work, the Vienna ***Ab initio*** Simulation Package is used [4].

$$E_{tot} = T_0[n(\boldsymbol{r})] + \tfrac{1}{2}\iint d\boldsymbol{r}d\boldsymbol{r}' \frac{n(\boldsymbol{r})n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|} + E_{xc}[n] + \int d\boldsymbol{r} v_{ext}(\boldsymbol{r})n(\boldsymbol{r}) + \tfrac{1}{2}\sum_{\mu\nu}\frac{z_\mu z_\nu}{|\boldsymbol{R}_\mu - \boldsymbol{R}_\nu|} \quad (1)$$

$$\left[-\tfrac{1}{2}\nabla^2 + \hat{v}_{ion} + \mathrm{v}_{\mathrm{H}} + \mathrm{v}_{\mathrm{xc}}\right]\psi_i = \varepsilon_i \psi_i \quad (2)$$

Figure 1 is an illustration of the prototypical back-gated carbon nanotube field effect transistor (CNFET). Noting previous suggestions that the CNFET may operate as a Schottky barrier transistor (SBFET) [2] we focus on the metal-nanotube contact, as indicated by the arrow in Fig. 1.

We first investigate the effect of metal work function, calculating the projected densities of states (PDOS) for the semiconducting nanotube on the Al, oxidated Al, and Au surfaces, as shown in Figs. 2(a), 2(b), and 2(c), respectively. The Fermi level of the aluminum surface sits at the conduction band edge of the semiconducting (10,0) nanotube, while that of oxidized aluminum surface and that of gold surface are aligned at the valence band edge of the nantoube. This clearly indicates that, when the CNT is side-contacted without metal-carbon bond formation, the work function of the metal surface would be a governing factor whether the Schottky barrier favors either the hole transport or electron transport.

However, such Schottky barrier could not be solely determined by a simple difference between the metal work function and the electron affinity of the carbon nanotube. Here we show one example that a detailed local atomic structure substantially affect the Schottky barrier height. Following usual experimental prcedure to form the source and drain electrode, there are likely to be a substantial pressure on the carbon nanotube surface imbeded under the metal layers [7]. Figure 3 shows that such a pressure between the metal layer and carbon nanotube surface could result in a significant modification in the Schottky barrier height. When the CNT is simply in contact with gold surface, as shown in Fig. 2(c), the Fermi level is aligned at the

ISBN 3-901578-16-1

valence band edge. However, as the CNT is compressed between the metal layers, the metal Fermi level is found to shift up toward the conduction band edge of the nanotube, as shown in Figs. 3(a) and 3(b). This means the simple Au-CNT contact favors the hole transport, while the compressed Au-CNT contact favors the electron transport.

CONCLUSION

We investigated the Schottky barrier formation at the metal-carbon nanotube contact, with ***ab initio*** electronic structure calculations. We found that not only the metal work function but the local atomic configuration as well significantly affects the height of the Schottky barrier at the metal-CNT contact

ACKNOWLEDGEMENT

We would like to acknowledge the support from KISTI under "Grand Challenge Support Program" with Dr. S. Lee as the technical supporter. The use of the computing system of the Supercomputing Center is also greatly appreciated.

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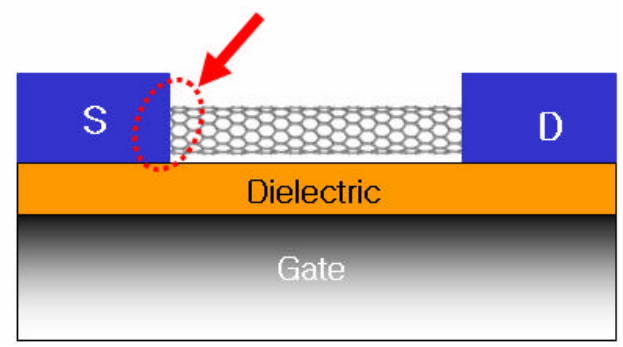

Fig. 1. Prototypical back-gated nanotube field effect transistor

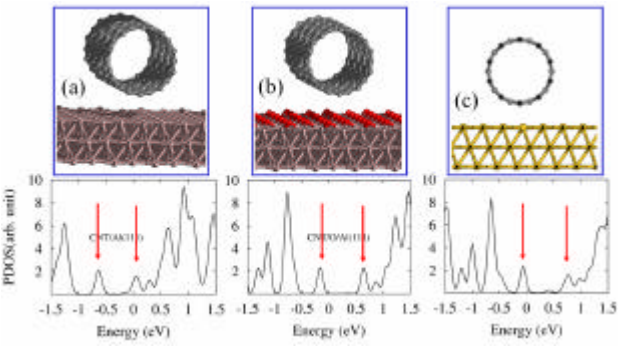

Fig. 2. Electronic structures of the carbon nanotube in contact with (a) Al, (b) oxidized Al, and (c)Au surfaces, respectively. Down-ward arrows in the lower panels indicate valence band and conduction band edges of the nanotube.

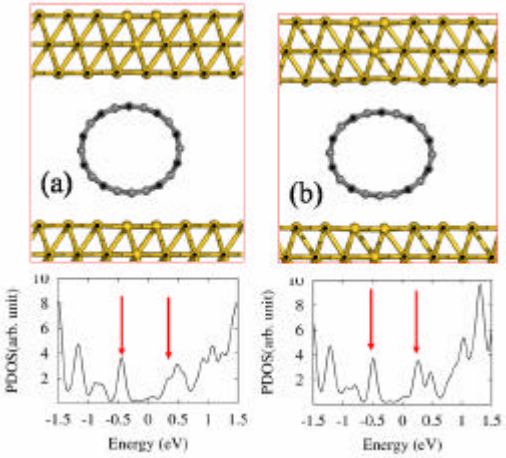

Fig. 3. Electronic structures of the semiconducting carbon nanotube compressed between two gold layers.