FIRST-PRINCIPLES STUDY ON ELECTRON TRANSPORT PROPERTIES OF NANOSCALE STRUCTURES

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Recently, the unique phenomena of ballistic electron transport through nanoscale junctions such as quantized conductance have been observed experimentally and theoretically. Future research on transport properties can be expected to lead to new discoveries of nanoscience and novel fabrications of electronic devices. In this presentation, we demonstrate the results of first-principles calculations with the incorporation of the overbridging boundary matching formalism to elucidate a relationship between the geometrical structure and electron transport property in which the nanostructures are suspended between two semi-infinite electrodes[1,2].

(I) Helical gold nanowire between Au electrodes[3-5].

The tip-suspended multishell helical gold nanowires (HGNs) of ~1 nm diameter and ~5 nm length are found by Kondo and Takayanagi [6] using transmission electron microscopy. We examined the electron-conduction properties of HGNs suspended between semi-infinite gold electrodes. Computational model is depicted in Fig. 1. Our findings are that the numbers of conduction channels of the HGNs do not coincide with the numbers of atom rows in the HGNs, while the number of conduction channels in a single-atom-row nanowire is one. In addition, some channels of the HGNs are not fully open, whereas the channel transmission of the single-atom-row nanowire is close to one. As a consequence, the conductances of the HGNs are not quantized and become much smaller than those expected from a single-atom-row nanowire. More intriguingly, in the thin HGNs, electronic currents rotate around the nanowire axis so as to induce a magnetic field, while no distinct magnetic fields are observed in the thick HGNs because there are no channel density distributions twisting sensibly around the nanowire axis (see Fig. 2).

(II) Tunneling Current Image of H-Adsorbed Si(001) in Scanning Tunneling Microscopy

The tunneling current flowing between the tip and H-adsorbed Si(001) surface in scanning tunneling microscopy (STM) is investigated. The resultant current map shown in Fig. 3 is consistent with the STM image in which H-adsorbed dimer looks geometrically lower than the bare dimer; although the isosurface of the local density of states above the H-terminated Si dimer, which are mainly attributed by the Si-H bonding states, locate itself higher than that above the bare Si buckled dimer, these bonding states do not contribute to the tunneling current. On the other hand, many electrons tunnel from π bond of the unreacted dimer into the tip. Accordingly, the H-adsorbed dimer appears geometrically lower than the bare dimer in the STM, since the tip must approach closer to the sample surface in order to achieve the constant tunneling current.

References:

[1] K. Hirose, T. Ono, Y. Fujimoto and S. Tsukamoto, First-Principles Calculations in Real-Space Formalism, Electronic Configurations and Transport Properties of Nanostructures, (Imperial College Press, London, 2005).
[2] T. Ono and K. Hirose, Phys. Rev. Lett. **82**, 5016 (1999); cond-mat/0412571 (2004).
[3] T. Ono and K. Hirose, Phys. Rev. Lett., accepted.
[4] M. Otani, T. Ono, and K. Hirose, Phys. Rev. B, **69**, 121408(R) (2004).
[5] T. Ono and K. Hirose, Phys. Rev. B, **70**, 033403 (2004).
[6] Y. Kondo and K. Takayanagi, Science **289**, 606 (2000).

Figures:

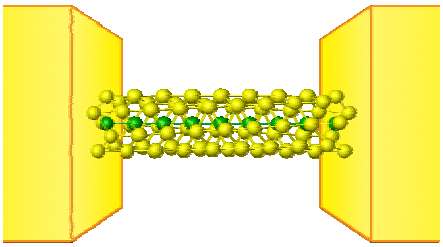

Fig. 1: Schematic image of the helical gold nanowire model.

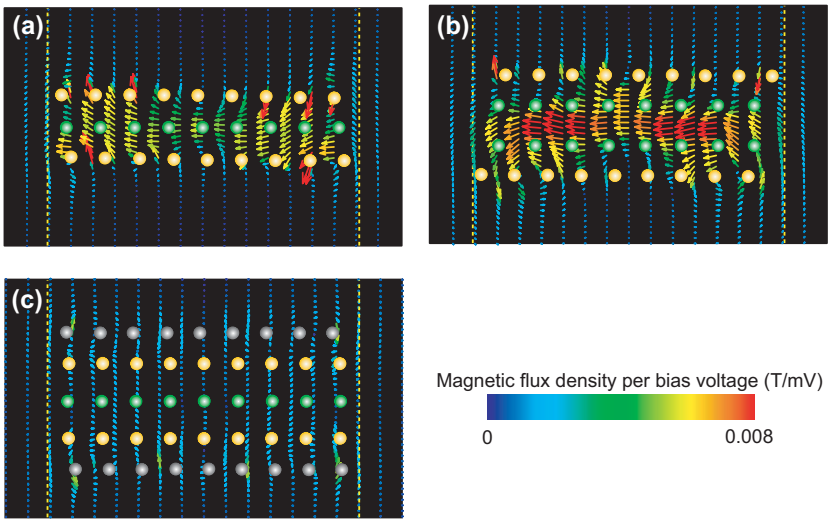

Fig. 2: Induced magnetic flux density per bias voltage. (a) 7-1 nanowire, (b) 11-4, and (c) 15-8-1 nanowire. The green, yellow and gray spheres represent the atoms in the innermost, second, and third shells, respectively. The broken lines are the edges of the jellium electrodes. Definition of the nanowires is the same as that in Ref. 6.

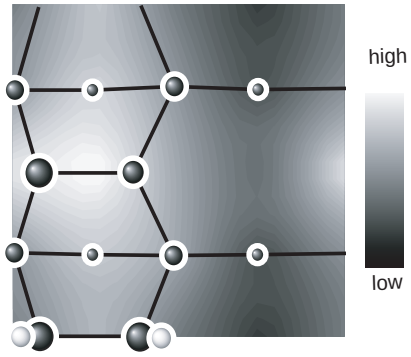

Fig. 3: Theoretical constant-height STM image of a Si(001) surface. In order to compare with STM images, positions with high tunneling current are shaded lighter than those with low tunneling current. White and black balls represent H and Si atoms, respectively. Si atoms are denoted by larger and smaller balls according to the distance from the surface.