Poster

First-Principles Study on Electron Transport Property through Nanostructures

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Within the last several years, a large number of experiments concerning metallic wire contacts have been carried out using a scanning tunneling microscope and a mechanically controllable break junction. Recently, the unique phenomena of ballistic electron transport through nanoscale junctions such as quantized conductance have been observed experimentally and theoretically. In this situation, 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) Al wire between Al electrodes[1-3]
The 3-aluminum-atom wire, which is shown in Fig. 1, has a conductance of ~ 1 G_0, and there is only one channel that gives a dominant contribution to the electron conduction at the Fermi level (see Fig. 2). The conductance trace as a function of electrode spacing decreases in the early stage of the elongation process and shows a minimum; with an increase in electrode spacing, the conductance reduces. When electrode spacing is still further increased, the wire forms into a straight structure with a one-dimensional character, which contributes to the enhancement of electron transmission. As a result, the curve of the conductance trace is convex downward before the wire breaks, and subsequently the conduction channels between the two electrodes disappear. This result is in consistent with the experimental result.

(2) Gold helical wire between Au electrodes
The conductance of the 7-1 gold helical wire suspended between electrodes is studied (see Fig. 3). Since the single-row atomic wire suspended between electrodes exhibits the conductance of 1 G_0, the conductance of the 7-1 helical wire consisting of eight atomic row is expected to be 8 G_0. Surprisingly, the first-principles calculation predicts that the helical wire has only six conduction channel and posses the conductance of ~ 5 G_0.

(3) C_{20} molecules between Au electrodes[4]
The conduction properties of the C_{20} molecules between electrodes are examined (see Fig. 4). The conductance is largely depends on the number of C_{20} molecules between electrodes. The conductances of C_{20} *monomers* between electrodes are more than 1 G_0, and on the other hand those of *dimers* are dramatically smaller. Electron currents follow the C-C bonds, and do not cross inside the C_{20} cages. Reflection of the incident electrons occurs at the C_{20}-electrodes interfaces and the C_{20}-C_{20} junctions of the dimers, though it does not take place on the C_{20} molecules.

References:
[1] T. Ono, S. Tsukamoto, and K. Hirose, Appl. Phys. Lett. **82**, 4570, (2003).
[2] T. Ono and K. Hirose, Phys. Rev. B **68**, 045409, (2003).
[3] T. Ono and K. Hirose, cond-mat/0307684.
[4] M. Otani, T. Ono, and K. Hirose, Phys. Rev. B **69**, 121408(R), (2004).

Figures:

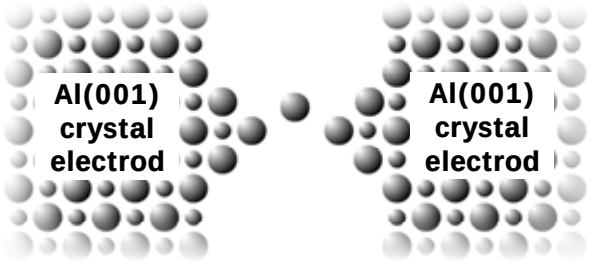

Fig. 1: Schematic representation of the aluminum nanowire model.

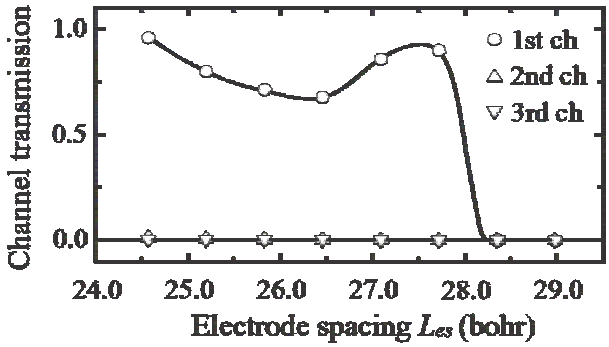

Fig. 2: Channel transmission at the Fermi level for the optimized three-aluminum-atom wire as a function of electrode spacing.

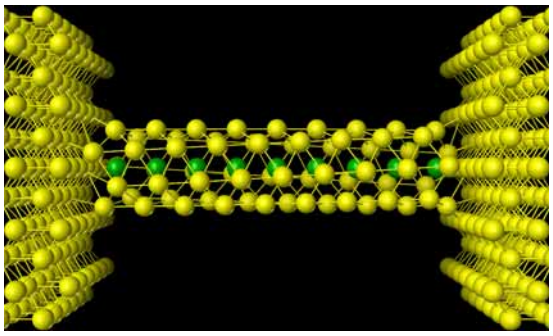

Fig. 3: Schematic image of the helical gold nanowire model.

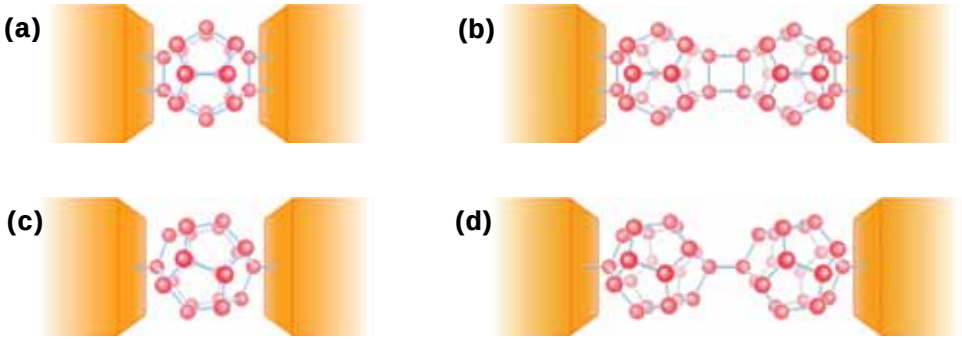

Fig. 4: Schematic descriptions of the scattering region of C_{20} suspended between Au electrodes: (a) double-bonded monomer, (b) single-bonded monomer, (c) double-bonded dimer, and (d) single-bonded dimer models.