FIRST-PRINCIPLES CALCULATION OF TRANSPORT PROPERTIES OF NANOSTRUCTURES

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In this presentation, we demonstrate the results of elaborate first-principles calculations with the incorporation of the overbridging boundary-matching (OBM) formalism [1] to elucidate a relationship between the geometrical structure and electronic conductance in which the nanostructures are suspended between two semi-infinite electrodes.

(1) Na wire [2]

The single-row sodium nanowires exhibit conductance oscillation and bunching of high electron density with two atom-lengths in the channel density distribution. The relationship between the period of the conductance oscillation and the length of the bunches is interpreted using a simplified model. The difference in the penetration parameters between the incident Bloch wave and the reflected one inside the nanowire is closely related to the period of the conductance oscillation and the length of the bunches.

(2) Helical gold nanowire [3]

Multishell helical gold nanowires (HGNs) suspended between semi-infinite electrodes are found to exhibit peculiar electron-conduction properties. Our results that the numbers of conduction channels in the HGNs and their conductances are smaller than those expected from a single-atom row nanowire verify the recent experiment. In addition, we obtained a more striking result that, in the cases of thin HGNs, distinct magnetic fields are induced by the electronic current helically flowing around the shells. This finding indicates that the HGNs can be good candidates for nanometer-scale solenoids.

(3) Thin SiO_2 film

It is now technologically possible to fabricate metal oxide semiconductor field effect transistors with SiO_2 gate oxides less than 1.3 nm thick. In such a thin film, conduction of electron becomes ballistic and its property is described by the quantum dynamics. Under such a condition, the understanding and control of structural and quantum electronic properties of the SiO_2 are the key subjects, therefore intensive studies have been made both experimentally and theoretically. However, interactions of interface are hardly revealed on by experiments because of the difficulty in reproducibility. In order to interpret these phenomena, theoretical study is also important and efficient. We present here theoretical study on the electron conduction properties of a very thin silicon oxide film. The electronic structure, local density of states (LDOS) of this film, and leakage tunneling current are explored. From the LDOS, we found that there are no electronic states near the Fermi level. Furthermore, leakage current increased in the case of the compressed films, while leakage current decreased in the model of stretched films. It is interpreted by the change of LDOS around Fermi level.

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] Y. Egami, T. Ono, and K. Hirose, Phys. Rev. B, to be published.
[3] T. Ono and K. Hirose, Phys. Rev. Lett. **94**, 206806 (2005).