FIRST-PRINCIPLES STUDY ON CONDUCTION PROPERTIES OF NANOSTRUCTURE

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In the recent semiconductor device industry, electronic devices are highly integrated and miniaturized, and the device in which the size of elements are smaller than the electron mean free path is expected be put in practical use. However, it is known that the electronic properties in minute systems whose dimensions are approximately equal to the Fermi wavelength can be different from those in the bulk and the conductance is quantized in the unit of $G_0=2e^2/h$, where e is the electron charge and h is the Planck constant.

We study on the conduction properties of the nanostructure having atomic scale dimension in order to explore the possibility of such new devices. So far, a lot of experimental researches for the electron-conduction properties through nanostructures have found that quantized conductance appears in single-row wires consisting of Na, Cu, Ag and Au, which are experimentally made using a scanning tunneling microscope and a mechanically controllable break junction. On the theoretical side, it is indicated that the conductance of the single-row wire made of Au and Na suspended between electrodes is quantized. Furthermore, an even-odd behavior, which is the oscillation of the conductance with the varying of the wire length, is found. These results are consistent with the experiment that the conductance trace of the Au wire oscillates during elongation, which is reported by Sim *et al.* [1].

In this study, we perform the first-principles calculations to examine electron conduction of the closed packed structure and single-row wires consisting of sodium atoms sandwiched between semi-infinite crystalline electrodes (Fig. 1), employing the overbridging boundary-matching method [2]. We find that the conductance of the closed packed structure and that of the single-row wires are ~3 G_0 and ~1 G_0, respectively, and the result that the conductance of 2 G_0 is never manifested for the single-row wire is in agreement with the results of the experiment (Fig. 2). In addition, the even-odd behavior of the conductance occurs for the single-row wire [3]. We also study the conductance of the cylindrical wire suspended semi-infinite electrodes using the continuum structure made of jellium in order to explore the origin of the even-odd behavior. As shown in Fig. 3, the conductance is periodically varied according to the length of the wire. Consequently, we find that there is a bunch of the electron density of the length almost equal to the z component of the Fermi wavelength, λ_z, in a sodium crystal. In the case that the distance between electrodes is integral multiple of λ_z, the conductance is ~1 G_0, and low conductance appears in the other cases. From above results, we conclude that the even-odd behavior of the conductance is associated with the relationship between the Fermi wavelength in the bulk and the distance from between electrodes.

References:

[1] R. H. Smit *et al.*, Phys. Lett. **91**, 076805 (2003)]
[2] Y. Fujimoto and K. Hirose, Phys. Rev. B **67**, 195315 (2003).
[3] Y. Egami et al., Materials Transactions, JIM, in printing.

Figures:

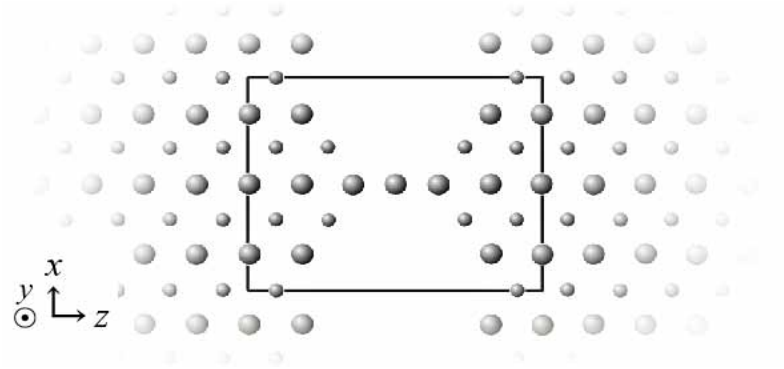

Fig. 1 Calculation model.

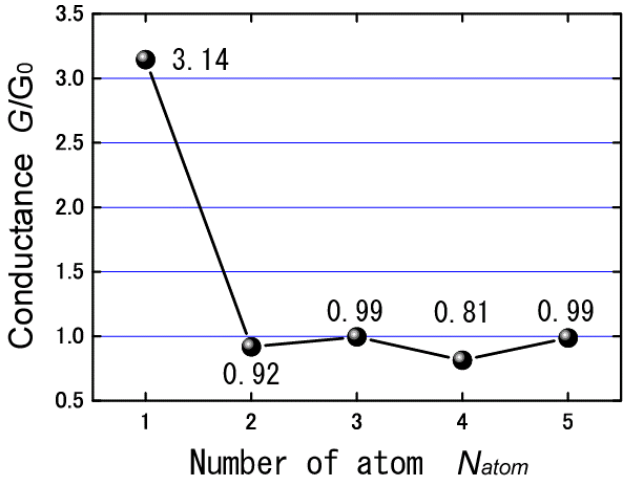

Fig. 2 Conductance of sodium single-row wires.

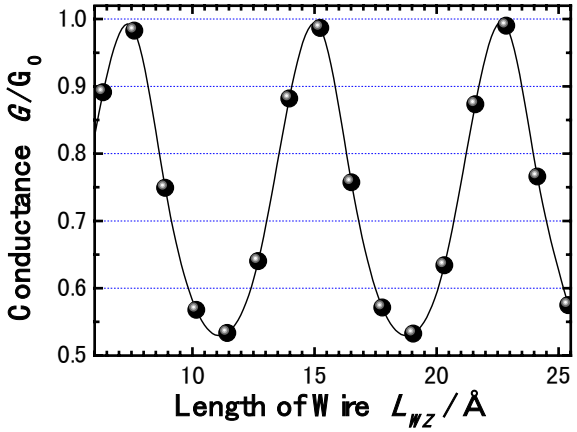

Fig. 3 Conductance of cylindrical wire made of jellium.