Effect of defective connection to electrodes in atomic scale conductors

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INTRODUCTION

Owing to development of fabrication technologies, atomic scale conductors have been realized. Although electrodes are necessary in utilizing such conductors for electronic devices, it is difficult to create the electrodes with a conventional way such as metal heat bonding. If interface between the device and electrodes is defective, characteristics of the atomic scale device would be rectified or washed out due to large contact resistance.

In this study, we investigate how current-voltage characteristics of a small two-dimensional conductor change when connection between the device and the electrode is malfunction.

MODEL

Figure 1 shows the structure of the model we study. A two-dimensional conductor, which is depicted as the dark shaded region, is cladded by electrodes. By applying the effective mass approximation, the device is discretized by 10 mesh points in the longitudinal direction. We consider two structures with different width which are divided by 3 or 6 mesh points, respectively. We refer the 3×10 and 6×10 structures as (A) and (B), respectively. The mesh points, which have energy $\varepsilon + V_i$ (V_i: potential due to applied voltage), are connected by the nearest neighbor hopping integral t. To model the malfunction in connection to the electrodes, we set some of the hopping integrals between the device and electrodes to zero. We evaluated current through the device at 300 K by using the non-equilibrium Green's function method.

RESULTS

In Fig. 2, we show current-voltage characteristics of the structure (A). The solid curve shows the current for the case of perfect connection to the electrode. The dashed curve denotes the current with defect at the edge of the interface. The dot-dashed curve denotes the current with defect at the center of the interface. Position of the defect is schematically shown by the crosses in the insets. We observe that the defective connection reduces the current. Reduction of current due to defect located at the center of the interface is larger than that due to defect at the edge.

Fig. 3 shows current-voltage characteristics of the structure (B). The defective connection also reduces the current, however, in this case, effect of disconnection at the edge of the interface is larger than that at the center.

In Fig. 4, we show electron densities for the two structures. For both cases, the defect is located at the middle of the interface between the device and cathode. We observe that the electron distributions are quite different for the two samples.

DISCUSSION

Such difference in the effect of the position of the defect in the connection would be explained by difference in relevant lateral modes which are schematically shown in Fig. 5. In the structure (A), current flows mainly through the lowest mode. The current is largely affected by the defect at the center because it locates on the belly of the lowest mode. Whereas in the wider structure (B), the second mode is dominant for the current. In this case, the defect at the center of the interface, which locates at the node of the mode, has small effect on current.

REFERENCES

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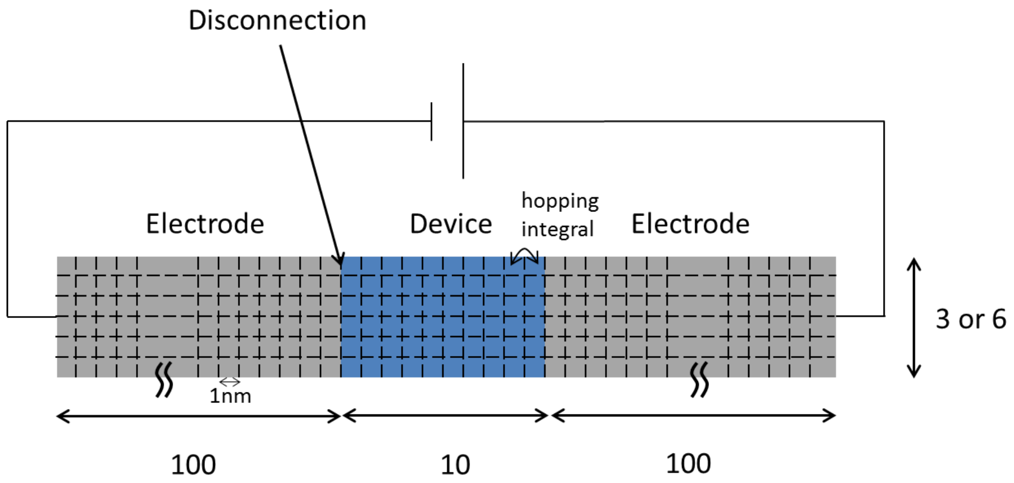

Fig. 1. Schematic structure of the device we studied. Discretized mesh points are connected by hopping integral, and there are disconnection between the electrode (cathode) and device.

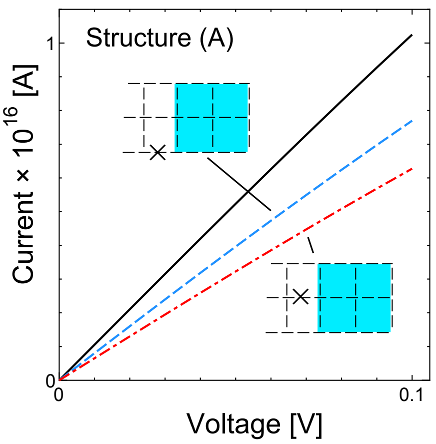

Fig. 2. Current-Voltage characteristics of the 3×10 device.

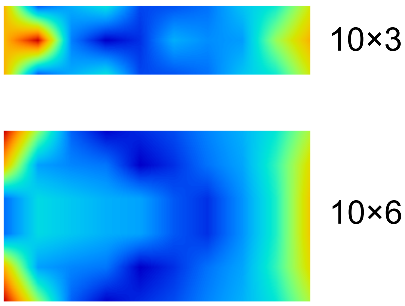

Fig. 4. Electron density when the connection was lost in the middle of the device

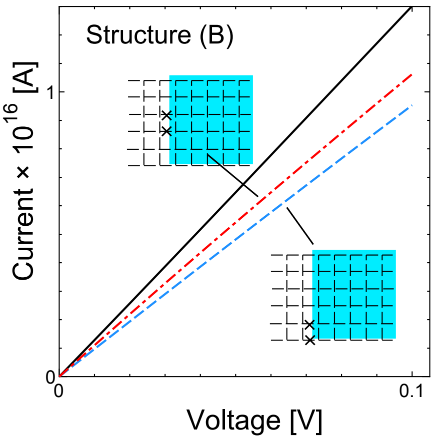

Fig. 3. Current-Voltage characteristics of the 6×10 device.

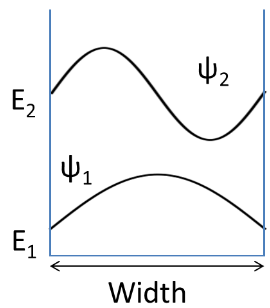

Fig. 5. Wave functions in the lateral direction are schematically shown.