Conductance of Single Molecules Chemically Bonded to Metal Electrodes

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SUMMARY:

We measured single molecular conductance by scanning tunnelling microscope (STM) point contact method. Here, we introduce our recent results on this issue.

INTRODUCTION:

Charge transport in a single molecule is one of the central issues of current molecular electronics. A metal/single-molecule/metal junction shows a broad conductance distribution and stochastic switching caused by the varieties of molecular conformations and interface geometries. Despite the importance of the phenomena for both fundamental and practical advances, the relationship between the characteristics of single molecular conductance and molecular junction geometries has not yet been clarified until now.

EXPERIMENTALS:

We used 3TS2(bisthio-terthiophene) and 3TSe2(biseleno-terthiophene) molecules as samples to study the influence of junction geometry on the single molecular conductance. Isolated 3TS2 or 3TSe2 molecules embedded in a SAM(self-assembled monolayer) of C8(octanethiol) molecules were prepared. Measurements were performed by STM point contact method[1)] under UHV at 77K. Schematic illustration for the measurement conformation is shown in Fig.1. And we changed the electrode gap space to modulate the molecular junction geometry during the I-V curve measurement.

RESULTS AND DISCUSSION:

After forming a molecular junction by approaching the STM tip (Au) to a target molecule, several hundreds of I-V curves were measured. Figure 2(a) shows a sequence of conductance values calculated from the I-V curves. Conductance switching and rupture of molecular junction can be seen. Figure 2(b) shows a conductance histogram obtained for 3TS2, under a fixed gap space condition. Several conductance peaks (indicated by arrows) can be observed due to the variety of adsorption sites of molecule on an Au surface. While, only a large single conductance peak (~170nS) remains (Fig. 2(c)) when the data of conductance measured just before the rupture of molecular junction (last conductance step) is plotted. Since the binding force of a thiol-Au bonding is stronger than that of an Au-Au bonding, the extensional strain exerted on a molecule induces the migration of the Au atom bound to the molecule and adsorption site hops to Au top site. Therefore, a narrower distribution can be obtained for the conductance measured in the last step.

CONCLUSIONS:

Precise measurement of single molecular conductance can be archived by controlling electrode-gap spacing. Further study using this method will clarify the relationship between conductance and interface geometry.

REFERENCES:

(1) Yasuda et al. *J.Am.Chem.Soc* **2006**, *128*, 7746-7747

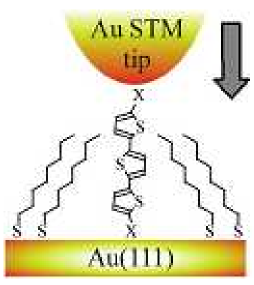

Fig.1 Schematic of measurement

(a)

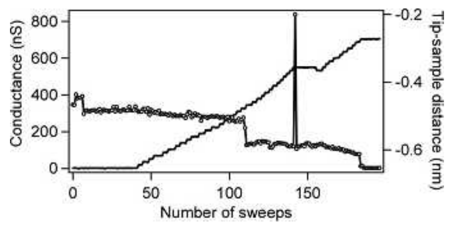

Fig.2 (a) Change in the conductance with increasing tip-sample distance. (b)Histogram of conductance obtained for a fixed tip-sample distance (c) Histogram of conductance measured for the last step.

(b)

(c)