Continuous and Simultaneous Measurement of Electrical Conductance and SERS for the Single Molecular Junction

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[Introduction] Single molecular junctions have been envisioned as components for miniaturized electronic circuits since the first theoretical proposal of a molecular diode. Electrical conductance of the junction changes upon the stretching process. Conductance jump, gradual change, and steps are observed in the conductance traces. The conductance fluctuation of the single molecular junction is explained by the transition between the different molecular adsorption sites, change in molecular orientation and metal-molecule distance by theoretical calculations. In this study, we have investigated the conductance and electronic structure of the BDT single molecular junction as a function of stretching length of the junction. The electronic structure was investigated by the simultaneous measurement of current-voltage (*I*-*V*) characteristics and surface-enhanced Raman scattering (SERS).

[Experiment] We used mechanically controllable break junction (MCBJ) techniques to study the electronic structure of the single molecular junction. The high stability of the junction is required for the stretching length dependence measurement. The stability of the single molecular junction depends on the length of the free standing nano bridge part of the Au electrodes. Therefore, the Au electrodes were fabricated with the nano fabrication techniques. A drop of a BDT solution (0.97 mM in EtOH) was dropped on the Au electrode. A self-assembled monolayer (SAM) film was formed on the surface of the Au electrode. The free standing Au nano bridge was mechanically broken by bending the substrate using a piezoelectric push-rod. We analyzed the obtained I-V curves based on the single channel model.

[Result and Discussion] Figure 1 shows the relationship between stretch length and G, Γ where G and Γ are the electronic conductance and coupling strength between molecular orbital and metal orbital. The conductance of the BDT single molecular junction gradually decreased with the stretching length of the junction. The sign of the slope of G and Γ were negative. The energy difference between molecular orbital and metal orbital showed little stretching length dependence. The present experimental result showed that the decrease in conductance was mainly caused by the decreases in the metal-molecule coupling.

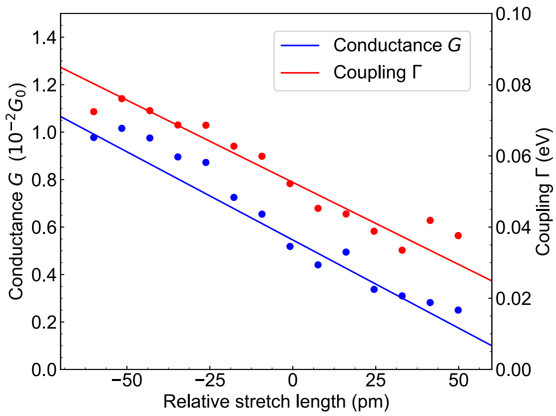

Fig.1. The relationship between stretch length and G, Γ of the BDT single molecular junction.