Electron transport through alkanethiol molecules in single and double tunneling junctions

Norio Okabayashi[a,b,*], Tadahiro Komeda[c], Yutaka Majima[a,b]

[a]Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, 226-8503, Japan
[b]CREST, Japan Science and Technology Agency (JST), Saitama 332-0012, Japan,
[c]Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai, 980-8577, Japan
*E-mail: norio@msl.titech.ac.jp

Alkanethiol molecules are known to form self-assembled monolayer (SAM) on a metal surface only by dipping the sample into the solution containing the alkanethiol molecules. The formed SAM is stable against adsorption of contaminations even in the ambient atmosphere. Because of these advantages, alkanethiol SAM is frequently investigated as a bench mark sample in the research of molecular electronics. In our presentation, we will discuss electron tunneling processes for alkanethiol molecules in a single tunneling junction by using scanning tunnelng microscope (STM) [1-3] and those for a double tunneling junction constituted by a gold nanoparticle (NP) and a nano-gap electrodes.

Figure 1(a) shows current voltage relationship of the alkanethiol SAM measured by STM. We can see approximately Ohmic behavior around Fermi level. However, in the first derivation (Fig. 1(b)) and second derivation (Fig. 1(c)) of *IV* curve, we can see the small increase of the conductance and peak/dip at some sample biases, respectively [1]. These sample biases are identical to the vibrational energy of the alkanethiol molecules. By using the isotope labeling of alkanethiol molecule and by employing the density functional theory combing combined with non-equilibrium Green's function, we found the vibrational mode containing substantial displacement of C-C bond dominantly contribute to these conductance changes [2-3].

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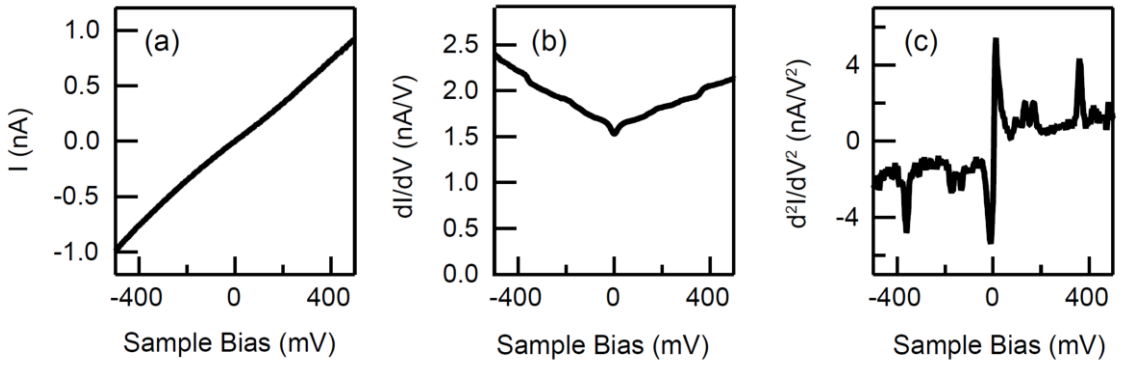

Figure 1. (a) IV curve, dI/dV and d^2I/dV^2 for alkanethiol SAM on the Au(111) surface .

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