Conductance measurement of single molecule with Si electrode toward explore novel function of molecule junction

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We have succeeded in investigating the I-V characteristics of Si based single molecular junction and the influence of molecular conformation using STM point contact method [1]. Rigid Si-C bonding formed between the electrode and the molecule not only provides robust single molecular junction with long-time stable I-V characteristics, but also allows us to manipulate the molecular conformation without breaking junction. Therefore we were enabled to measure transport property of molecule junction while changing electrode separation. STM tip and substrate surface made of a same n-type Si(001) wafer were used as electrodes. We used diethinylbenzene (DEB) molecules, whose triple bonds react covalently with Si electrodes. A single molecular junction was formed by approaching a Si-STM tip toward an isolated DEB molecule adsorbed on a H-Si(001) substrate (Fig.1). Figure 2 shows the change in tunneling current at positive (+1.8V) sample bias voltage as a function of the electrode distance. A binary-conductance switching was reproducibly observed, showing hysteresis characteristics. From the reversible characteristics, it is considered to be caused by the transformation between cis- and trans-conformations, DEB molecular isomerizes, while changing the distance between the electrodes. To understand the mechanism in more detail, we carried out theoretical calculation, and the observed transformation was supported by the electrode-distance dependent structure energy (Fig. 3). These results demonstrate a possibility of mechanical controllability of carrier transport in a single molecular junction. Details will be discussed at the conference.

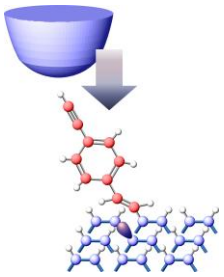

Fig.1 Formation of a single molecule junction

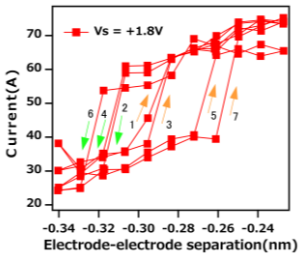

Fig.2 Change in tunneling currents at +1.8 V as a function of electrode distance

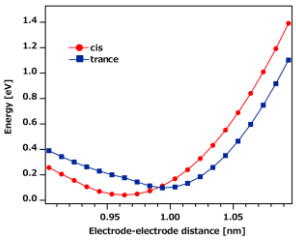

Fig.3 Structural energies of cis and trans conformations

[1] Yasuda et al. J. Am.Chem.Soc.128, 2006,7746-7747 E-mail address at speaker: mikipuyu@yahoo.co.jp