Three-dimensional visualization of molecular conformation effect on single molecular conductance

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With the development of various techniques to fabricate single molecular junctions, tremendous effort has been devoted to elucidate the transport properties of single molecules. We have advanced the "STM point contact method", which we previously developed, to realize three-dimensional analysis of the influence of molecular conformation on the carrier transport in a Si-based single molecular junction. STM tip and substrate surface made of a same n-type Si (001) wafer were used as electrodes. We used diethinylbenzene (DEB) molecule, whose triple bonds react covalently with Si electrodes. A single molecular junction was formed with a Si-STM tip approached toward an isolated DEB molecule adsorbed on a H-Si (001) substrate (Fig.1). After the molecular junction being formed, current flowing through a single molecular junction was measured with a fixed bias voltage while the STM tip, which was moved back and forth in the Z direction, was scanned two-dimensionally (X- and Y-directions), as the scheme is shown in Fig.2. The single molecular conductance of the DEB molecule modulated by the 3-D conformational change was visualized by mapping the measured current as a function of the STM tip position. Figure 3 shows a result. An abrupt change in conductance due to the conformational change of molecule caused by the STM tip movement in Z-direction is shown by the change in color between blue and yellow in Fig. 3 (X-Z plane). The switching position gradually changes with X-directional scan. The obtained results clearly demonstrate the high-degree usefulness of this technique. Details will be discussed at the conference.

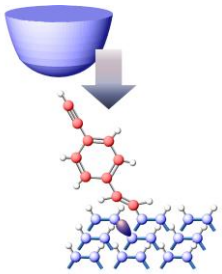

Fig.1 Schematic of measurement.

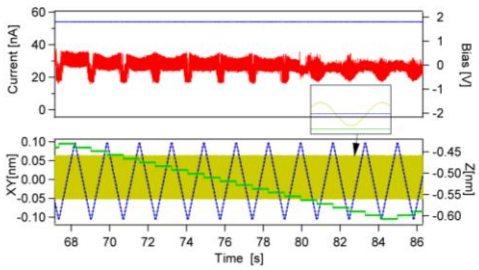

Fig.2 Tunneling current measured with 3D change in the STM tip positions (upper graph, red: current, blue: bias voltage, and lower graph, blue: x, green: y, yarrow: z positions).

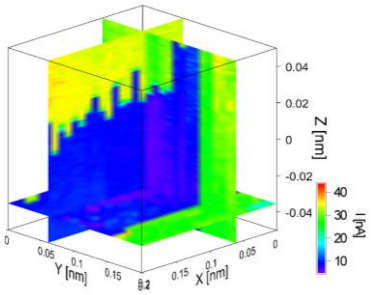

Fig.3 2D cross sections of the 3D measurement of conductance.