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

M. Nakamura¹, S. Yoshida¹, Y. Mera², O. Takeuchi¹, and, H. Shigekawa¹
¹Faculty of pure and applied sciences, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan
²Shiga University of Medical Science, Otsu, Shiga, 520-2121, Japan

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.