3D Dynamic Probe Analysis of 1,4-Benzenediamine Single-Molecule Junction

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Single-molecule junctions have been extensively studied because of their high potential for future nanoscale device applications. A single molecular conductance is known to be strongly affected by the change of their conformational change. To clarify the effect, We have recently developed 3D dynamic probe system that enables to directly visualize the conformational dynamics in single-molecule junctions.

In this study, we have applied the 3D dynamic probe system to Au/1,4-Benzenediamine/Au single-molecule junction. Figure 1 schematically shows the 3D dynamic probe system. The current I was measured while the STM tip was moved back and forth in the z-direction in accordance with sinusoidal function and scanned two-dimensionally (x- and y-directions). Figure 2 shows the volume plots in the form of conductance maps as a function of the STM tip apex position which consist of the conductance [G/G_0] data obtained while the STM tip was retracted from Au surface. The cross sections corresponding to the frames indicated by the red lines in the volume plots and schematic illustrations of the high- and low-conductance states models, are shown together. A clear periodicity of Au(111) atomic structure observed in the xy cross section indicates high repeatability of site dependent conductance change. As shown in the yz cross section and G-z curve, conductance switching to higher state was observed during tip retraction. Our analysis and calculations revealed this change was caused by the conformational change of the end group on Au(111) surface. These results suggest that the conductance value is relevant to interactive key factors such as the bonding sites at an electrode and the bonding conformation.

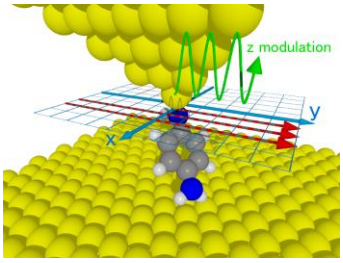

Figure 1. Schematic illustration of the 3D dynamic probe system.

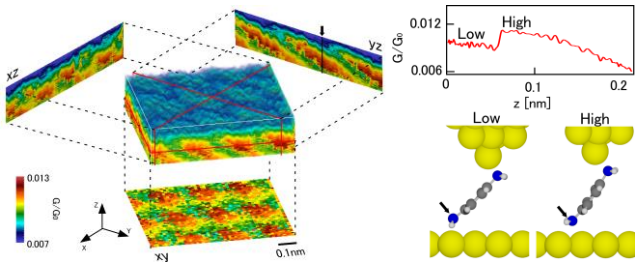

Figure 2. 3D volume plots, G-z curve and the high- and low-conductance states models.

[1] M. Nakamura et al, Nature Communications, 6, 8465 (2015)
[2] S. Yoshida et al, ACSnano, 2016, 10 (12), pp 11211–11218