

# Adsorption mechanism of C<sub>60</sub> on Au/Si(111) surfaces

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## 1. Introduction

Understanding of adsorption mechanism and its electronic character between organic molecule and inorganic substrate is important for organic-inorganic hetero-junction devices. Surface structure of silicon can be controlled in various ways by metal atom adsorption and annealing. In the case of gold adsorption on Si(111) surface, many types of surface superstructures such as Si(111)5×2-Au, Si(111)√3×√3-Au, and Si(111)6×6-Au have been reported. We have been studying about the adsorption of organic molecules on the various Si(111)-Au surface superstructures. For example, we found that L-tyrosine molecules are adsorbed on the Si(111)5×2-Au surface and tend to align along Au one-dimensional rows via formation of chemical bonds between molecules and Si dangling bonds [1]. On the other hand, we revealed that no benzenethiol exists on the Si(111)√3×√3-Au surface contrary to the expectation of well-known covalent bond formation between thiol molecules having mercapto-group (-SH) and Au surface. Chemical property of Au monolayer film on the Si surfaces is quite different from bulk Au. Mechanism of molecular adsorption on such surface is nontrivial, indeed. In this study, we focused on C<sub>60</sub> which act as a good electron acceptor.

## 2. Experimental Details

Sample preparation and all measurements were carried out under ultra-high vacuum (UHV) condition. Au/Si(111) surface superstructures were prepared by reacted deposition epitaxy (RDE) method. Clean Si(111) surface with 7×7 structure was kept at 850 K during Au deposition. Dosage of Au was carefully controlled by using RHEED and LEED. Pure Si(111) 5×2-Au, pure √3×√3-Au, and their coexisting surfaces were prepared. C<sub>60</sub> adsorption sites and dynamics were investigated by STM and *in situ* RHEED. C<sub>60</sub> adsorbate electronic structure was investigated by photoelectron spectroscopy using the Display-type analyzer (DIANA) installed at BL-7.

### 3. Results and Discussion

Figure 1 shows RHEED spot intensity change during  $C_{60}$  deposition. As  $C_{60}$  is deposited, the intensities of the diffraction spot from two superstructures decreased and diminished at the same time. This indicates that  $C_{60}$  are adsorbed on the both surface and the sticking probability is similar. This is different compared to the case of thiol and amino acid molecules which the sticking coefficient is much smaller on the  $\sqrt{3} \times \sqrt{3}$ -Au surface.

Figure 2 shows STM images of the  $5 \times 2$ -Au surface before and after  $C_{60}$  deposition. At the first layer of the  $5 \times 2$ -Au surface, Si dangling bonds form one-dimensional arrays. Density of bright protrusions corresponding to  $C_{60}$  adsorbates are about the same as that of Si dangling bonds on the  $5 \times 2$ -Au surface. This suggests the strong interaction between  $C_{60}$  and Si dangling bonds.

Figure 3 shows photoelectron spectra. Molecular orbital peaks of  $C_{60}$  on the  $5 \times 2$ -Au surface shift to lower binding energy compared to those of  $C_{60}$  multilayer indicating that the adsorption is accompanied by charge transfer from  $5 \times 2$ -Au substrate to  $C_{60}$  adsorbates. On the other hand, the peaks in the  $C_{60}/\sqrt{3} \times \sqrt{3}$ -Au spectra appeared at the same position as those of multilayers.  $C_{60}$  molecules are physisorbed on the  $\sqrt{3} \times \sqrt{3}$ -Au surface without charge redistribution by bond formation.

Furthermore,  $C_{60}$  was deposited on the  $5 \times 2$ -Au and  $\sqrt{3} \times \sqrt{3}$ -Au coexisting surface and annealed at  $550^\circ\text{C}$  subsequently. From the surface structure analysis by RHEED and STM observation, the  $\sqrt{3} \times \sqrt{3}$ -Au domains reappeared after annealing. This is another indication supporting that  $C_{60}$  molecules are chemisorbed on the  $5 \times 2$ -Au surface, while they are physisorbed on the  $\sqrt{3} \times \sqrt{3}$ -Au surface.

### 4. Conclusion

Adsorption of  $C_{60}$  molecules on the  $5 \times 2$ -Au and  $\sqrt{3} \times \sqrt{3}$ -Au surfaces was compared using *in situ* RHEED, STM and photoelectron spectroscopy.  $C_{60}$  molecules were found to be physisorbed on the  $\sqrt{3} \times \sqrt{3}$ -Au surface while they were chemisorbed and aligned along Au row on the  $5 \times 2$ -Au surface. Monolayer Au atoms on the Si surface passivate Si dangling bonds and prevent formation of chemical bond between substrate and  $C_{60}$  molecules.

### References

[1] M. Yoshimura et al., e-J. Surf. Sci. Nanotech. Vol. **8**, 303 (2010).

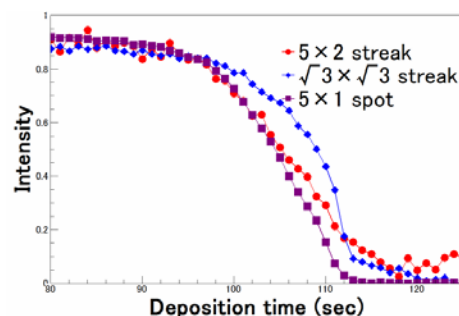


Fig.1 RHEED spot intensity change during  $C_{60}$  deposition on the Si(111)  $5 \times 2 + \sqrt{3} \times \sqrt{3}$ -Au surface.

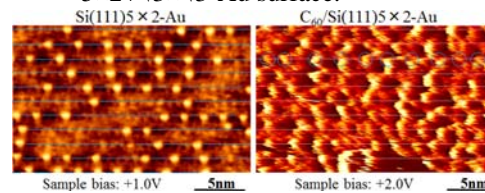


Fig.2 STM image of the clean and  $C_{60}$  adsorbed Si(111)  $5 \times 2$ -Au surface.

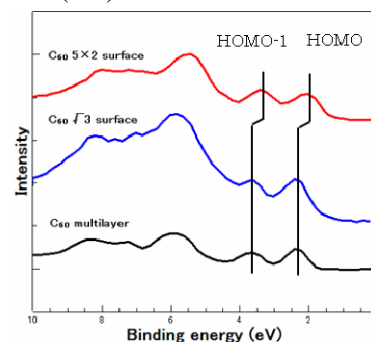


Fig.3 Photoelectron spectra from  $C_{60}$  adsorbed Au/Si(111) surfaces.