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Phase transition of the Ag/Si(111)-($\sqrt{3}\times\sqrt{3}$) surface studied by photoelectron diffraction

Toshihiro SUZUKI[1], Keisuke KOBAYASHI[1], Kazuyuki SAKAMOTO[1], Satoshi TOYODA[2], Jun OKABAYASHI[2], Kanta ONO[3], Masaharu OSHIMA[2]
[1]Department of Physics, Tohoku University, Sendai, Miyagi 980-8578, Japan
[2]Department of Applied Chemistry, the University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan
[3]KEK-PF, Tsukuba, Ibaraki 305-0801, Japan

One- and two-dimensional superstructures, which are formed on semiconductor surfaces by the adsorption of metal atoms, have been a topic of experimental investigation for the creation of nanoscale quantum structures with high perfection. These nanoscale structures are quite nice systems for the study of low-dimensional physics, e.g., phase-transitions in one- or two-dimensional systems [1], and they are also of a profound interest from the technological point of view. Among the great number of metal induced surface reconstructions, the Ag/Si(111) –($\sqrt{3}\times\sqrt{3}$) surface is one of the most well known. Based on the STM image and theoretical calculation [2], different structural models have been proposed for the room temperature (RT) phase and the low temperature (LT) phase, i.e., the models called a "honeycomb-chained triangle" (HCT) and an "inequivalent triangle" (IET) model (Fig. 1). However, it was reported that the RT phase is not a static HCT structure but rather a thermally fluctuating structure between IET(+) and IET(-) structure in a recent photoemission study [3]. In order to determine the origin of the transition observed on the Ag/Si(111) –($\sqrt{3}\times\sqrt{3}$) surface, we have performed Si *2p* photoelectron diffraction (PED) measurements at different temperatures.

PED measurements were performed at BL-1C KEK-PF at RT and 10 K. The temperature was measured by thermocouples fixed on the sample holder close to the sample. The Si(111) sample was cleaned *in situ* by direct current heating up to 1520 K. The Ag/Si(111)–($\sqrt{3}\times\sqrt{3}$) surface was prepared by evaporating approximately 1 ML of Ag on the Si(111)-(7×7) clean surface at a sample temperature of 823 K, followed by further annealing at 873 K. The quality of the surface was ascertained by the observation of a sharp $\sqrt{3}\times\sqrt{3}$ LEED pattern and the valence-band photoemission spectra. Incident photon energies from 130 eV to 280 eV were used in the present study.

The Si *2p* core-level spectrum of the Ag/Si(111)–($\sqrt{3}\times\sqrt{3}$) surface is composed by one bulk component and two surface components [4]. By analyzing all the spectra obtained in the present study by a standard least-squares-fitting method using spin-orbit split Voigt functions, and using the relative binding energy of the three components reported in Ref. 4, we have obtained the kinetic energy-dependent intensity for each Si *2p* component. Figure 2 shows the kinetic energy dependence of the Si *2p* core-level intensity from Si atoms bonded to Ag, measured at RT (open circles) and 10 K (filled circles). The similar energy-dependent intensity suggests that the geometric structure of the Ag/Si(111) –($\sqrt{3}\times\sqrt{3}$) surface is the same at RT and 10 K, and thus that the origin of the phase transition of this surface is an order-disorder transition.

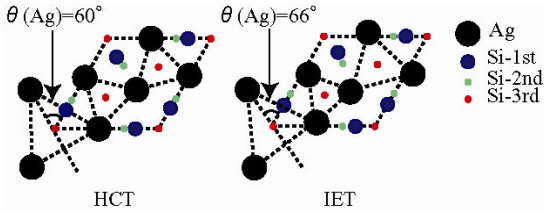

Fig.1; HCT and IET models proposed for the Ag/Si(111) –($\sqrt{3}\times\sqrt{3}$) surface.

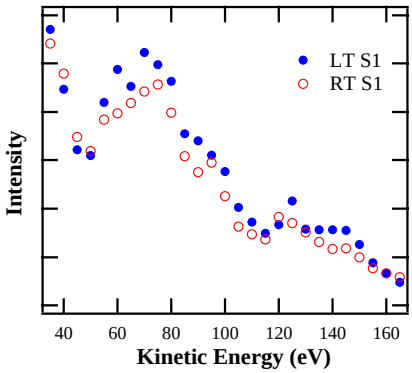

Fig. 2; Kinetic energy dependence of the Si *2p* core-level intensity from Si atoms bonded to Ag, measured at RT (open circles) and LT (10 K; filled circles).

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sakamoto@surface.phys.tohoku.ac.jp