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Valence band of the surface of $Si(111)-\sqrt{21}\times\sqrt{21}-(Ag+Cs)$ formed at RT

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Introduction

Evaporating Cs atoms onto the $Si(111)-\sqrt{3}\times\sqrt{3}-Ag$ surface at room temperature (RT) has been found to form a $\sqrt{21}\times\sqrt{21}$ surface superstructure[1], which can be also found during evaporation of Au or Ag atoms onto the same substrate surface. These $\sqrt{21}\times\sqrt{21}$ surfaces seem to have some common characteristics including high two-dimensional electrical conductivity[1]. Especially in the cases of Au and Ag induced $\sqrt{21}\times\sqrt{21}$ surface, they are considered to have very similar atomic arrangements and electronic structures according to STM observations and PES measurements, and both of their high two-dimensional electrical conductivity is thought to due to surface-state bands[2].

For the Cs induced $\sqrt{21}\times\sqrt{21}$ surface, here for the first time we investigated the valence bands of the $\sqrt{21}-Cs$ surface, finding that there are also surface-state bands crossing the Fermi-Energy. We think the high two-dimensional electrical conductivity of $\sqrt{21}-Cs$ surface also results from these surface-state bands just like those of $\sqrt{21}-Ag$ and $\sqrt{21}-Au$ surfaces. But the dispersion of the surface-state bands of the $\sqrt{21}-Cs$ surface is quite different from those of the latter two.

Experiment

The substrate was a P-doped *n*-type Si(111) wafer with resistivity of 2-15 Ω·cm at RT, and its typical dimensions were 10×3×0.5 mm^3. Experiment was conducted in the ultrahigh vacuum (UHV) chamber set on BL-18A at Photon Factory of KEK.

A clear 7×7 surface was produced by flashing the sample several times at 1200°C. Then the $Si(111)-\sqrt{3}\times\sqrt{3}-Ag$ structure was formed at a substrate temperature of ~520 °C by depositing about one monolayer of Ag atoms. Finally, the wafer was cooled to RT and Cs atoms were evaporated from a thoroughly out-gassed commercial dispenser (SAES Getters Inc.) to the $Si(111)-\sqrt{3}\times\sqrt{3}-Ag$ surface until a $\sqrt{21}\times\sqrt{21}$ LEED pattern emerged. The formed $\sqrt{21}-Cs$ surface was cooled to about 120K for extending its lifetime and for ARPES measurement.

Results and Discussion

Figure 1(a) contains the ARPES spectra of the $\sqrt{21}-Cs$ surface, and Fig. 1(b) is its grey-scale band-dispersion diagram constructed from the second-derivatives of the spectra in (a) by using the measured work function of 2.53eV. It is very clear that there are two surface state bands near and crossing the Fermi-level; S1 is almost at Fermi energy with little dispersion while S2 is dispersing upwards crossing the Fermi level. The bottom of S2 band is located in between the $\bar{\Gamma}$ and $\bar{M}$ points in the second $\sqrt{3}\times\sqrt{3}$ -surface Brillouin zone.

From the dispersion of such valence bands of the $\sqrt{21}-Cs$ surface, it can be concluded that this is a metallic surface. The reported high surface conduction of the $\sqrt{21}-Cs$ surface is guessed to be due to the dispersing valence bands shown in the Fig. 1. But by comparing with the valence bands of the surfaces of $\sqrt{21}-Ag$ and $\sqrt{21}-Au$ [1,3], it is found that they are quite different, which indicates they belong to two different types of $\sqrt{21}\times\sqrt{21}$ surface superstructure.

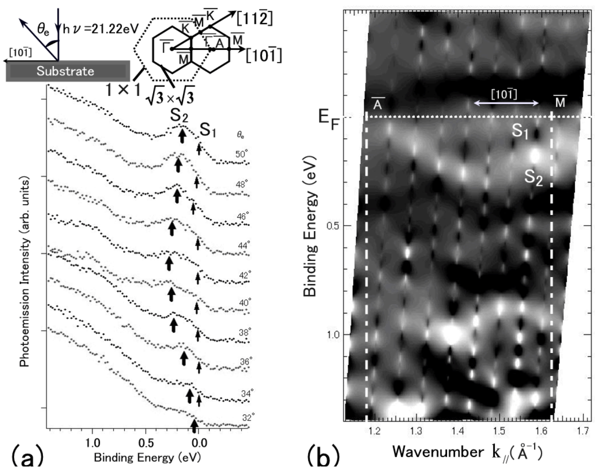

Figure 1: (a) ARPES spectra and (b) gray-scale band dispersion diagram for the $\sqrt{21}-Cs$ surface

References

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