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Electronic Evidence of the Inequivalent Triangle Structure on Si(111) √3x√3-Ag

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Introduction

The determination of surface (electronic) structure of Si(111) √3x√3-Ag has been the center of the arguments in surface science. Among so many structure models proposed through the past two decades, the surface structure once seemed to be explained by honeycomb-chained-triangle (HCT) model [1]. However, recent low-temperature scanning tunneling microscope study with the first principles calculations found that the ground state structure of this system is not the HCT structure but the inequivalent triangle (IET) structure [2]. Both the HCT and IET models are characterized by the Ag trimers arranged on the honeycomb lattice. The difference is that, while these trimers are equivalent with each other in the HCT model, one of the Ag trimer in the unit cell is larger than the other in the IET model. Such a geometric distinction is reflected in electronic structure. The band calculations have shown that two surface states of Si(111) √3x√3-Ag are degenerate at the $\bar{K}$ point in the HCT model and the two states are energetically separated for 0.15 eV at the point in the IET model [2].While, up to now, there are also several surface structure studies confirming the IET structure [3], on the other hand, all the reported electronic structure studies have supported the HCT model [4].

In this research, we have performed angle-resolved photoemission spectroscopy (ARPES) experiments using synchrotron radiation in order to settle the controversy between the geometric and electronic structures of Si(111) √3x√3-Ag.

Experiments

The experiments were done at the VUV-beamline at ELETTRA, Trieste, ITALY and BL-18A at PF-KEK, Tsukuba, JAPAN. Well-optimized samples were prepared by monitoring the Si 2p core-level spectra [5] and ARPES measurement conditions. The ARPES spectra were taken at 120 K.

Results and Discussion

Figure shows ARPES spectra taken along the surface Brillouin zone line $\bar{\Gamma}$–$\bar{K}$. Two surface states of Si(111) √3x√3-Ag, S_2 and S_3, are identified at binding energy of ~ 1 eV [4]. Through detailed ARPES measurements with various measurement geometries [4], these two surface states obviously show an energy gap of 0.22 +/- 0.07 eV at the $\bar{K}$ point, corresponding to an emission angle (θ_e) of 20°. A close match of the energy gap with the theoretical prediction [2] firmly supports that the surface has the IET structure at 120 K, not the HCT. No previous work of ARPES studies on the electronic structure of this surface [4] reported this band splitting.

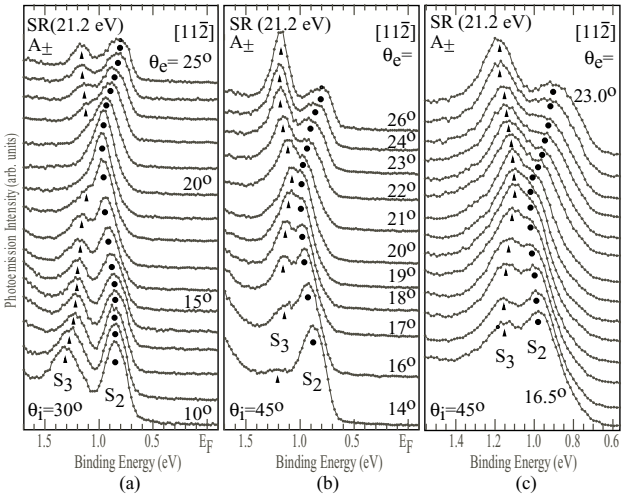

Figure Normalized ARPES spectra for the Si(111) √3x√3-Ag surface taken along the surface Brillouin zone line $\bar{\Gamma}$–$\bar{K}$ ([11$\bar{2}$] axis) at 120 K. The photon energy used is 21.22 eV and the photon incident angles θ_i are (a) 30°, (b) 45 °, and (c) 45 °. The measurement geometry is given in Ref. [4].

References:

[1] S. Hasegawa *et al.,* Prog. Surf. Sci. **60**, 89 (1999).
[2] H. Aizawa *et al.,* Surf. Sci. **429**, L509 (1999).
[3] N. Sasaki *et al.,*Surf. Sci.**493**, 188 (2001).
[4] L. S. O. Johansson *et al.*, Phys. Rev. Lett. **63**, 2092 (1989).
[5] R. I. G. Uhrberg *et al.,* Phys. Rev. B **65**, 081305.

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