Photoemission study of the Si (111) 3×1-Ba surface

Taichi OKUDA[1*], Ki-Seok AN[2], Hidenori ASHIMA[3], Hideo TAKEDA[3],
Ayumi HARASAWA[1], AND Toyohiko KINOSHITA[1]
[1] Institute for Solid State Physics, The University of Tokyo, Kashiwa 277-8581, Japan
[2] Korea Research Institute of Chemical Technology, Taejon 305-600, Korea
[3] Department of Physics, Graduate School of Science, Tohoku University, Sendai,980-8578, Japan

Introduction

The geometrical and electronic structures of the alkali metal(AM) or alkali earth metal(AEM) induced Si(111)3×1 surface have not reached to consensus in spite of the extensive investigation more than a decade. One of the most interesting issue of the surface is the semiconducting character of the AEM induced 3×1 surface despite the odd number of surface electrons with 1/3ML coverage[1]. In order to solve the problem, we have performed the detailed investigation of the surface core level shift(SCLS) and surface-state band structure of the single domain Si(111)3×1-Ba surface by means of the Si 2p core level photoemission and the angle-resolved photoelectron spectroscopy(ARPES) using synchrotron radiation.

Experimental

SCLS and ARPES measurements have been done at the beamlines BL-16B and 18A. The single domain surface was obtained by depositing Ba onto the vicinal n-type Si(111) wafer (20-30 Ωcm) from getter source. As for the ARPES measurement we used the different photon energies(hν = 12.5, 21.2, and 27.0 eV) and experimental geometry($A_{//}$ and $A_{\perp}$, see inset of the figure). In the SCLS measurement, we recorded the Si 2p core level spectra in different surface sensitivity using different photon energies (hν = 110-140 eV).

Results and Discussion

Figure 1 shows the experimental band dispersion of the prominent surface states (circles and squares with solid curves) obtained by the ARPES measurement as well as that of the calculated ones (dashed curves) for the honeycomb chained channel(HCC) model by Erwin and Weitering[2]. Nearly perfect agreement of the experimental surface states(S_1 , S_2 , and S_3) with the calculated ones (S_2^-, S_2^+, and S_1^+) suggests that the HCC model is one of the promising model for the Si structure of the 3×1 surface. However, the theoretically predicted metal state (S_1^- in the figure) resulting from the odd number of electrons with the 1/3ML Ba on the 3×1 surface is hardly observed in our ARPES measurement.

Figure 2 shows the surface sensitive Si 2p core level spectrum measured at hν=130 eV. The fitting results of the spectrum is also in good agreement with the calculated SCLS for the HCC model by Kang *et al.*[3]. The shape of Si 2p core level spectrum without asymmetric tails also suggest the semiconducting character of the surface.

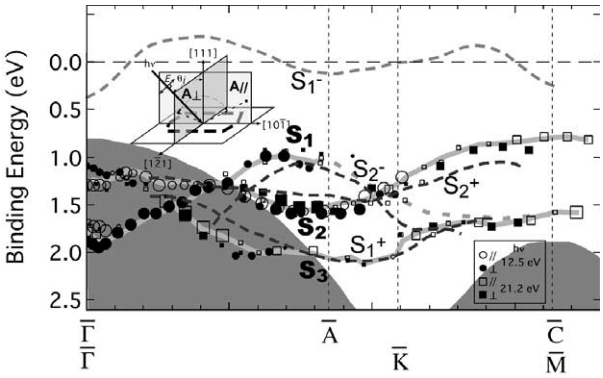

Fig.1 Summary of the band dispersion of the surface states(circles and squares with solid curves) as well as those of calculation (dashed curves from ref.[2]). Dark shaded area is bulk band projection and inset is the experimental geometry.

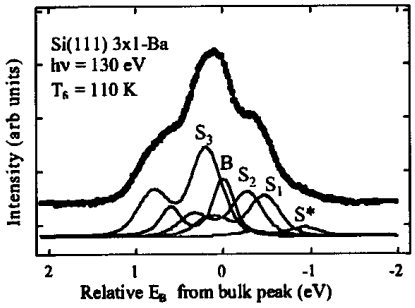

Fig.2 Surface sensitive Si 2p spectrum measured at hν=130 eV and Ts=110 K. Experimental spectrum (filled circle) is well fitted by the one bulk (B) and three surface components(S_1, S_2, S_3).

Thus, the surface Si structure of the Si(111)3×1-Ba should have almost the same structure(=HCC model) to that of alkali metal induced 3×1 surfaces. The inconsistency of electronic property between experiment and theory can be explained by the idea that the coverage of AEM is half of that of AM on the 3×1 surface, *i.e.* 1/6 ML.

References

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*okudat@issp.u-tokyo.ac.jp