Electronic structure of the Pb-covered bilayer Ge film on Si(111)

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Introduction

Much attention has been paid to spin-orbit interaction (SOI) and spin splitting on crystal surfaces. The Rashba SOI is caused by the structural inversion asymmetry at a surface and induces wavevector-dependent spin splitting with the polarization perpendicular to the wavevector and the surface normal. The magnitude of surface-state spin splitting is closely related to atomic SOI of topmost atoms or adatoms. Indeed, most of large spin splittings of surface bands have been observed on surfaces containing heavy elements belonging to the sixth row in the periodic table. Among them, the Pb-covered Ge(111) surface is interesting because it has a metallic surface state with the large spin splitting of ~200 meV at the Fermi level (E_F)[1]. On the other hand, recently, the spin polarization of the electronic states localized in the subsurface region was found on Bi/Ge(111)[2] and Br/Ge(111)[3]. These studies demonstrate that SOI of the Ge atoms can derive measurable spin splitting.

It is well known that the Ge(111) thin film grows epitaxially on the Si(111) substrate. Due to the lattice mismatch, the Ge(111) thin film has the in-plane compressive strain. Besides, some adsorbed metals act as surfactant to promote the layer-by-layer growth. The electronic structure of the Ge thin film terminated by metal adatoms is expected to be quite different from the bulk Ge(111) surface. From this point of view, we investigated the electronic structure of the Pb-covered bilayer Ge film using angle-resolved photoelectron spectroscopy (ARPES) and spin-resolved ARPES.

Experimental

The ARPES and spin-resolved ARPES experiments were performed at KEK-PF BL-19A. We used a PHOIBOS 150 spectrometer (SPECS) and a very-low energy electron diffraction (VLEED) spin detector. A clean Si(111)-(7×7) surface was obtained by annealing at ~1320 K. The deposition of Ge was done from a graphite crucible heated by electron beam onto the room temperature Si(111) substrate. The post-annealing at 920 K yielded a sharp (5×5) low-energy electron diffraction (LEED) pattern[4], as shown in Fig. 1(a). The (5×5) superstructure is constructed of the dimer-adatom-stacking-fault (DAS) geometry on bulk-truncated Si(111). The nominal coverage of Ge is 2 ML, where 1 ML is defined as the atom density of Si(111). We deposited Pb from an alumina crucible onto the Ge/Si(111)-(5×5) surface at room temperature. A (√3×√3)R30° LEED pattern appeared by annealing above ~450 K. The annealing at 540 K yielded a (√3×√3)R30° pattern with low background intensity, as shown in Fig. 1(b).

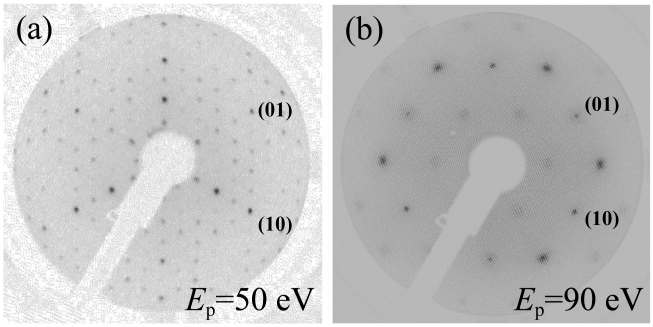

Figure 1: LEED patterns of (a) Ge/Si(111)-(5×5) and (b) Pb/Ge/Si(111)-(√3×√3)R30° measured at room temperature.

Results and discussion

Figure 2(a) shows the surface Brillouin zones (SBZs) of Si(111)-(1×1) and the (√3×√3)R30°. The surface band structure of Pb/Ge/Si(111)-(√3×√3)R30° was measured along the $\Gamma M_{\sqrt{3}}$ direction. Figure 2(b) shows the ARPES intensity map as a function of emission angle and binding energy. Three features labeled S1–3 are clearly seen. The S1 band disperses in the Si bulk band gap and crosses E_F at 19° ($k_{||}$=0.40 Å^{-1} from the second Γ point). It was found that the band dispersions of S1–3 are very similar to those observed on Pb/Ge(111). According to the first-principles calculation of Pb/Ge(111), these bands are closely related to the bonding of Pb-Pb and between Pb and topmost Ge. Therefore the similarity in band structure indicates that Pb/Ge/Si(111) has a same atomic geometry as Pb/Ge(111). On the other hand, the band effective mass of S1 on Pb/Ge/Si(111) was slightly larger than that on Pb/Ge(111). This may be attributed to the decrease of the Pb-Pb distances due to the compressive strain of the Ge(111) film. For Ge-derived states, we have not yet obtained clear evidence. The observed (√3×√3) LEED spots in Fig. 1(b) have larger widths than the (1×1) spots. The insufficient order of the Pb/Ge film may make the feature of Ge-derived state obscure.

Figure 2(c) shows the spin-resolved ARPES spectra of Pb/Ge/Si(111) for the in-plane spin polarization perpendicular to the $\Gamma M_{\sqrt{3}}$ direction. Whereas the large spin polarization was observed for S2 and S3, the spin splitting of S1 was not confirmed. This indicates the smaller spin splitting of the S1 band compared to Pb/Ge(111). The relation between the spin splitting and the compressive strain is an intriguing issue. We are proceeding with further analysis with the first-principles band calculation.

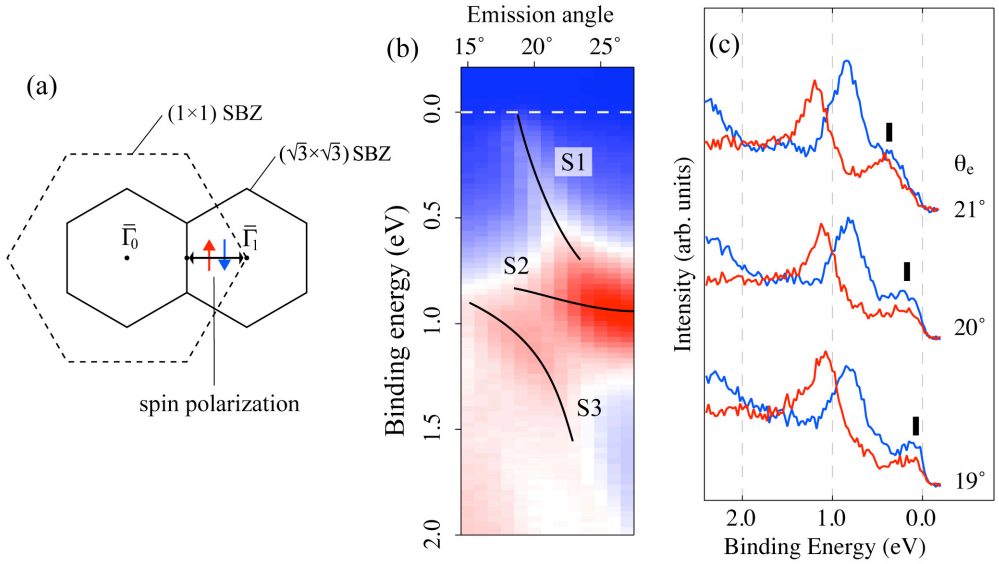

Figure 2: (a) Surface Brillouin zones of Si(111)-(1×1) and (√3×√3)R30°. (b) The measured band structure of Pb/Ge/Si(111) along $\Gamma M_{\sqrt{3}}$. The two-headed arrow in (a) represents the measured $k_{||}$ region. (c) Spin-resolved ARPES spectra at the emission angles of 19–21°.

References

[1] K. Yaji *et al*., Nat. Commun. 1, 17 (2010); K. Yaji *et al*. Phys. Rev. B 86, 235317 (2012).
[2] Y. Ohtsubo *et al*., Phys. Rev. B 82, 201307 (2010).
[3] Y. Ohtsubo *et al*., Phys. Rev. B 86, 165325 (2012).
[4] K. Shoji *et al*., Jpn. J. Appl. Phys., 22, L200 (1983).