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

Shinichiro HATTAT1,2*, Yukihiro HAYASHI1, Takashi NOMA1, Tetsuya ARUGA1,2

1Department of Chemistry, Graduate School of Science, Kyoto Univ., Kyoto 606-8502, Japan
2JST CREST, Saitama 330-0012, Japan

Introduction

Crystal surfaces and monolayers exhibiting large spin splitting due to the Rashba spin-orbit interaction (SOI) have been studied intensively in the last decade. Among them, semiconductor surfaces with metallic spin-split states are desired, because it allows us to address the issue of electric transport under the Rashba SOI. Recently, the Pb/Ge(111)-β-(√3×√3)R30˚ surface was found to have a metallic surface state with large Rashba-type spin splitting[1]. The superstructure consists of the dense Pb monolayer (4/3 ML) on the bulk-truncated Ge(111) substrate[2]. On the other hand, the strained Ge(111) thin film grows epitaxially on Si(111). In this study, we explore the electronic structure of the Pb-induced superstructure on Ge/Si(111) using angle-resolved photoemission spectroscopy (ARPES) and spin-resolved ARPES (SR-ARPES).

Experimental

The ARPES and SR-ARPES measurements were performed at BL-19A using the hemispherical electron analyzer (PHOIBOS 150, SPECS) and the very-low energy electron diffraction (VLEED) spin detector. A Si(111) substrate was cleaned by annealing at ~1050˚C. Ge was deposited on the room-temperature Si(111)-(7×7) surface followed by annealing at 900 K, yielding a sharp (5×5) low-energy electron diffraction (LEED) pattern. The superstructure is constructed of the single Ge bilayer with the well-known dimer-adatom-stacking-fault geometry. We deposited Pb of ~2 ML on the (5×5) surface. The (√3×√3)R30˚ superstructure appeared after post-annealing at 540 K.

Results and discussion

Figure 1(a) shows the (√3×√3) surface Brillouin zones. We measured the band dispersions along the Γ,M,Γ, Figure 1(b) shows the ARPES intensity map at M, measured at room temperature. It is found that a state, labeled S1, disperses from 0.7 eV to the Fermi level (EF) in the bulk band gap. The Fermi wavevector of the surface state was determined to be 0.41 Å⁻¹ from Γ1. In Fig. 1(b), two other bands, labeled S2 and S3, are seen. The observed band structure is very similar to that of Pb/Ge(111)-β, indicating that the Pb/Ge overlayer on Si(111) has the same atomic geometry of Pb/Ge(111)-β.

Comparing details of the band dispersions on the two (√3×√3) surfaces, it was found that the S1 dispersion on Pb/Ge/Si(111) is steeper than that of Pb/Ge(111)-β. According to the first-principles calculations, the S1 state is derived mainly from the in-plane Pb 6p orbitals. The increase of the dispersion may reflect the contraction of the Pb-Pb distances, since the unit cell of the single Ge(111) bilayer is smaller than that of bulk-truncated Ge(111) by 4%.

Another considerable difference was found on the spin splitting of S1. While the spin splitting on Pb/Ge(111)-β is 0.2 eV near EF, splitting was not identified in the ARPES spectra of Pb/Ge/Si(111). Figure 1(c) shows the SR-ARPES spectra of Pb/Ge/Si(111) measured at 100 K. While the S1 feature is seen above 0.4 eV, the spin splitting is not resolved, indicating that it is considerably smaller than that of Pb/Ge(111)-β.

References

* hatta@kuchem.kyoto-u.ac.jp