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ARPES study of the Tl/Ge(111)-3×1 surface

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Introduction

Reconstructed semiconductor surfaces induced by metal adsorption have gained much attention because of interesting physical properties particular to low-dimensional systems. Adsorption of thallium onto the Ge(111) surface induces two phases at room temperature [1]. The (3×1) surface at 1/3 ML has a one-dimensional chain structure, as observed on the alkali-metal induced (3×1) surfaces. A scanning tunneling spectroscopy (STS) measurement on this surface implies that this surface has a very narrow gap or a metallic character. We investigated the electronic structures of the single-domain Tl/Ge(111)-3×1 surface by angle-resolved photoelectron spectroscopy (ARPES).

Experimental

The ARPES measurements were performed at beam line 18A. For the preparation of the single-domain (3×1) surfaces, we used a vicinal Ge(111) substrate tilted from [111] by 1.5° toward the $[\bar{1}\bar{1}2]$ direction. The substrate was cleaned by Ar-ion sputtering and annealing (<950 K) by direct current heating. Tl was deposited on the substrate at room temperature and then the surface was annealed to ~550 K for a few minutes. Low-energy electron diffraction (LEED) showed the single-domain (3×1) diffraction pattern. The ARPES spectra were taken at room temperature.

Results and discussion

Figure1 shows a set of spectra along $\bar{\Gamma}_{1\times1} - \bar{K}_{1\times1}$ for the Tl/Ge(111)-(3×1) surface, taken at $h\nu$=40 eV. Two bands dispersing over gap regions of the projected bulk bands are seen. In the spectra taken at $h\nu$=16 eV, these states were observed at almost the same binding energies. Therefore we consider these bands to be surface bands. They are labeled S1 and S2, as shown in Fig. 1. S1 moderately disperses from a minimum binding energy of ~1.0 eV near the $\bar{A}_{3\times1}$ point to a binding energy of ~0.5 eV near the $\bar{C}_{3\times1}$ point. S2 does not display a distinct dispersion.

Figure2 shows the atomic structure model of the Tl/Ge(111)-(3×1) surface proposed from the STM studies on this surface [1] and on the Na/Ge(111)-(3×1) surface [2]. First-principle band calculations were performed in our laboratory using this structure model. Comparing the experimental results with the calculations, we tentatively assign S1 to the dangling bond states on the Ge adatom labeled "4" in Fig. 2 and S2 to the dangling bond states on the Ge adatom labeled "3".

For a more thorough understanding of the electronic properties, especially the metallicity, of this surface, further analyses of the ARPES data are now in progress.
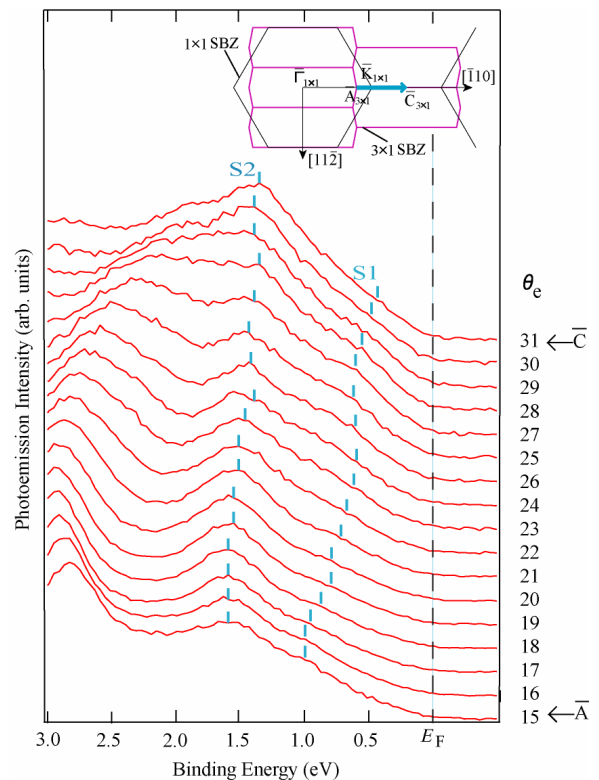

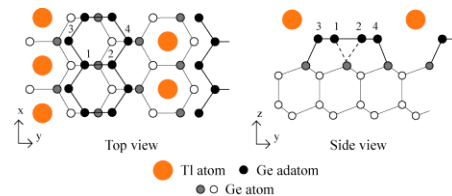Fig. 1. ARPES spectra along $\bar{\Gamma}_{1\times1} - \bar{K}_{1\times1}$ for the Tl/Ge(111)-(3×1) surface.

Fig. 2. The modified HCC structure model of the Tl/Ge(111)-(3×1) surface.

References
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