Transition matrix effect in ZrB_2 valence photoelectron angular distribution patterns

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1. Introduction

Zirconium diboride (ZrB_2) is an attractive material for wide applications. It has a high melting point, high electric conductivity, and high corrosion resistance. ZrB_2(0001) surface is a promising substrate for the GaN(0001) epitaxial thin film growth too. Moreover, MgB_2 is a novel superconductor at exceptionally high critical temperature (39 K) [1], which has the same crystal structure as ZrB_2, but ZrB_2 has no superconductivity at such a high temperature. Therefore, to understand the difference on the electronic structure between ZrB_2 and MgB_2 is very important to figure out the property of superconductors. Therefore, the understanding of the surface electronic structure of ZrB_2 is significant for both basic knowledge and application. Although it has been studied by using angle-resolved ultraviolet photoelectron spectroscopy [2], the orbital character of the energy band has not been studied. In this study, we have measured two-dimensional photoelectron intensity angular distributions (PIADs) by utilizing a horizontally linearly-polarized synchrotron radiation (SR) and a display-type spherical mirror analyzer (DIANA) [3]. The purpose of this research is to analyze the atomic orbitals constituting each band from these PIADs which contain transition matrix effect.

2. Experiment

The experiment was done at BL-7 of SR center, Ritsumeikan University [4]. The sample was heated up to 1000℃ at first for degassing in the preparation chamber. After recovery of the vacuum, the sample was flash-annealed at 1500℃ several times. The surface quality was checked by low energy electron diffraction and Auger electron spectroscopy. The two-dimensional photoelectron spectroscopy (2D-PES) measurements were performed at
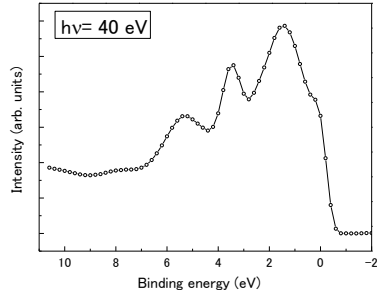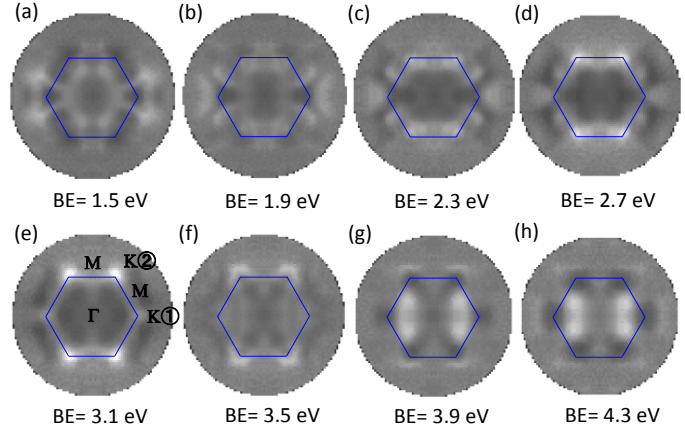
Fig. 1 Angle-integrated PES spectrum of ZrB$_2$.

Fig. 2 PIADs of ZrB$_2$(0001) valence band excited by a horizontally linearly-polarized light.

room temperature under the ultrahigh vacuum of ~1×10^{-8} Pa by using DIANA. The photon energy of SR was 40 eV. The total energy resolution was about 400 meV and the angular resolution was about 1°.

3. Results and discussion

Figure 1 shows the angle-integrated photoelectron spectrum of ZrB$_2$. Fig.2 (a)-(h) are the PIAD patterns of ZrB$_2$(0001). The original patterns were averaged by horizontal and vertical mirror symmetry operation considering the symmetry of the crystal and excitation light. Hexagons in Fig. 2 indicate the first Brillouin zone (BZ) of ZrB$_2$. These patterns indicate the cross-sections of valence band excited by a horizontally linearly-polarized light. The bright areas correspond to the cross-sections of the band structures in these patterns, and their shapes change with the binding energy. The hexagon like structure inside BZ in Fig.2 (a) spreads toward outside of BZ with increasing the binding energy in Fig.2 (b)-(h). When we focus on Fig.2 (e), we can see the transition matrix element effect in this 2D-PIAD pattern. That is, at K points in Fig.2 (e), the intensity of photoelectron at K② is stronger than that at K①. This difference is the transition-matrix-element effect when the atomic orbitals consisting of each band are excited by a linearly-polarized light. Thus, we have obtained the useful data to analyze the atomic orbital.

4. Conclusions

We have succeeded in three-dimensional band structure (E, k_x, k_y) measurements of ZrB$_2$(0001). The patterns obtained by using 2D-PES contain the transition matrix element effect that enables us to analyze the atomic orbitals composing each band.

References

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