Comprehensive Photoelectron Diffraction and Spectroscopy for Surface Science

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Visualization of three-dimensional atomic arrangements of surfaces, interfaces, nanostructures, and molecular adsorbates is essential in materials science and engineering. This is accomplished by holographic reconstruction of element-specific photoelectron diffraction from the localized core level. Furthermore, the electronic properties and chemical reactivity of materials are closely related to the behavior of valence electrons near the Fermi level. Momentum-resolved valence-band (VB) photoelectron spectroscopy is a powerful technique to characterize such electrons. We have been working on the development of wide-acceptance-angle electron energy analyzers for photoelectron angular distribution measurement. In order to establish the reliability of these methods, comprehensive measurement and understanding of the photoelectron emission process are important.[1)]

1. Valence Band Atomic Orbital Analysis of Layered Compounds

BL6U at UVSOR is a beamline dedicated to VB dispersion mapping with a practical photon energy range of 45 to 600 eV. Wide-acceptance-angle acquisition system enables measurement of full set of VB dispersion data over several Brillouin zones.[2)] The cross sections of VB from $MoSe_2$ along the $\Gamma_{00\ 11}$M and $\Gamma_{00\ 12}$M directions are shown in Figure 1(a) and (b), respectively, together with the ab initio simulations. The interlayer interaction induces the splitting of the band degenerated at A point into two at Γ point. Band A, B, and C appeared intense at the $\Gamma_{00\ 11}$M plane, while their counterparts, Band A', B', and C' appeared intense at the $\Gamma_{00\ 12}$ M plane. We found that the two split bands appear alternatively in the Brillouin zones along the k_z direction. This 4π-periodic k_z oscillation was also observed for graphite[3)] and was explained by considering the photoelectron interference from atomic orbitals within the unit cell, *i.e.* photoelectron structure factor. We expanded this concept to the layered compound and investigated the bonding characters of these bands.

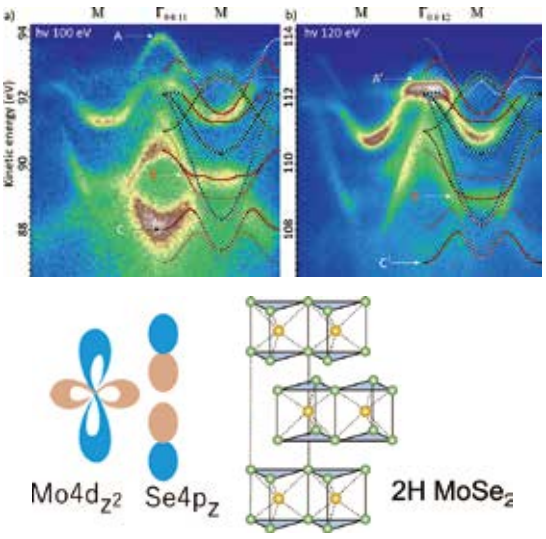

Figure 1. Cross section of $MoSe_2$ VB along the (a) $\Gamma_{00\ 11}$M and (b) $\Gamma_{00\ 12}$M directions together with ab initio simulation. Pairs of black and red dotted curves appear alternatively in the Brillouin zones along the k_z direction. Mo4d$_{z^2}$ is the key-player orbital.

2. Momentum Microscope & PESCATORA

Conventionally, azimuthal and polar scans of sample orientation were required for the angle-resolved photoelectron spectroscopy and diffraction measurements. Aforementioned wide-acceptance-angle acquisition system combines a special mesh for gathering photoelectrons emitted into wide solid angle and a mechanical lens deflector for two-dimensional data acquisition. Alternatively, display-type analyzers enable the direct observation of wide-solid-angle photoelectron intensity distribution from a selected point without changing the angles of incident light or the sample orientation. By combining a photoelectron emission microscope column and two hemispherical deflection analyzers, *i.e. momentum microscope*, iso-energy photoelectron intensity k_x–k_y distribution can be obtained with high-momentum, energy, and spatial resolutions. My mission is to install state-of-the-art momentum microscope to UVSOR and establish a comprehensive photoemission experimental station.

Furthermore, we have recently invented a new type of display-type analyzer called **P**rojector for **ESCA to R**eal space **A**nalysis (PESCATORA) using an electrostatic lens making the trajectory of photoelectrons emitted within 1π steradian into parallel rays and a fine tube array plate as a collimator for energy and angular distribution analysis, realizing the detection of photoelectron diffraction with a high angle resolution.[4)]

References

1) F. Matsui, T. Matsushita and H. Daimon, *J. Phys. Soc. Jpn.* **87**, 061004 (2018).
2) H. Yamane *et al.*, in preparation.
3) F. Matsui, H. Nishikawa, H. Daimon, M. Muntwiler, M. Takizawa, H. Namba and T. Greber, *Phys. Rev. B* **97**, 045430 (2018).
4) F. Matsui and H. Matsuda, Patent PCT/JP2016/070744.