# Au 5d dispersion on Si(111)5×2-Au studied by Two-dimensional Photoelectron Spectrometer DELMA (Display-type Ellipsoidal Mesh Analyzer)

Hiromi Nakajima[a], Makoto Morita[a], Satoshi Kitagawa[a], Hiroyuki Matsuda[a], Fumihiko Matsui[a], Ryo Ishii[a], Masayoshi Fujita[a], Kaoru Yasuda[a], Takuya Ota[a], Tomohiro Matsushita[b], Laszlo Toth[a], Hiroshi Daimon[a]

[a]*Nara Institute of Science and Technology (NAIST), 8916-5 Takayama, Ikoma, Nara 630-0192, Japan*
[b]*Japan Synchrotron Radiation Research Institute (JASRI), SPring-8, 1-1-1 Koto, Sayo, Hyogo 679-5198, Japan*

1. Introduction

The character of *d* electron is important in molecular adsorption phenomena at surface. Because the radiui of *d* electron wavefunction is small, *d* electron has a localized feature and shows a spin-orbital splitting to $d_{3/2}$ and $d_{5/2}$. On the other hand *d* electrons in valence band has delocalized feature due to some overlap with nearest neighbor atoms and shows a dispersion of energy band although the width of the *d* band is narrow.

A strange behavior of *d* band was found in the valence band of Si(111)5×2-Au surface [1], where one of the spin-orbit split band had a dispersion whereas the other had no dispersion. Hence we investigated here the *d* band dispersion of Si(111)5×2-Au surface by two-dimensional photoelectron spectroscopy (2D-PES) using a new apparatus called DELMA.

2. Experimental apparatus DELMA(Display-type Ellipsoidal Mesh Analyzer)

Two-dimensional photoelectron spectroscopy (2D-PES) is an important tool to investigate electronic and atomic structure of materials. It is necessary to measure electronic structure within one Brillouin zone which corresponds to ±30° for usual crystal at kinetic energy of 20 eV. Recently ±30° analyzer is commercially available, but this angular range is not enough for atomic structure analysis. Three-dimensional atomic structure of bulk, surface or around impurity can be studied using photoelectron diffraction technique [2], which includes recent technique of atomic stereophotograph[3] and new photoelectron holography[4]. Many crystals have fcc, bcc and diamond structure, hence more than ±45° is necessary to detect important strong forward focusing peaks from nearest or second nearest neighbor atoms in these crystals.

Efficient measurement of two-dimensional photoelectron intensity angular distribution (2D-PIAD) has been made by a display-type spherical mirror analyzer [5]. This apparatus can measure angular distributions over the angular cone of ±60° at a time and has been used to measure photoelectron diffraction and atomic stereophotograph effectively. However its energy resolution is about 5 eV at kinetic energy around 500 eV, which is not enough for valence band analysis.

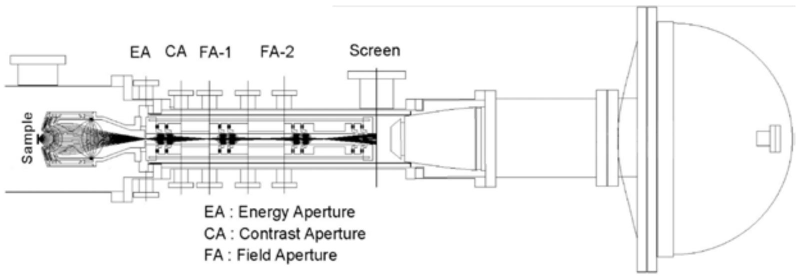


Fig. 1 Display-type Ellipsoidal Mesh Analyzer (DELMA).

On the other hand photoelectron emission microscope (PEEM) can also measure wide angle 2D-PIAD at kinetic energies of around 30 eV, but it cannot measure wide angle 2D-PIAD at several hundred eV because the acceptance angular cone decreases to about ±15° at several hundred eV.

Therefore, we have developed a new system called DELMA which contains a wide acceptance angle electron lens (WAAEL) [6], a lens system, and a concentric hemispherical analyzer (CHA) as shown in Fig. 1. WAAEL utilizes an ellipsoid mesh electrode to remove the spherical aberration, and it can accept the electrons in angular cone of up to ±60°. WAAEL was utilized for hard X-ray photoelectron spectroscopy (HAXPES) to cancel the small photoionization cross-section in the hard- x-ray photon energy region [7]. This apparatus can display a magnified sample image and the angular distribution from a selected area on the screen in Fig. 1 [8]. The lens system controls the image formation (imaging mode and diffraction mode) by changing the lens voltages with a combination of energy aperture EA, contrast aperture CA, and field aperture FA in Fig. 1. This new spectrometer has been tested [9-11] at the free port of BL07LSU in SPring-8.

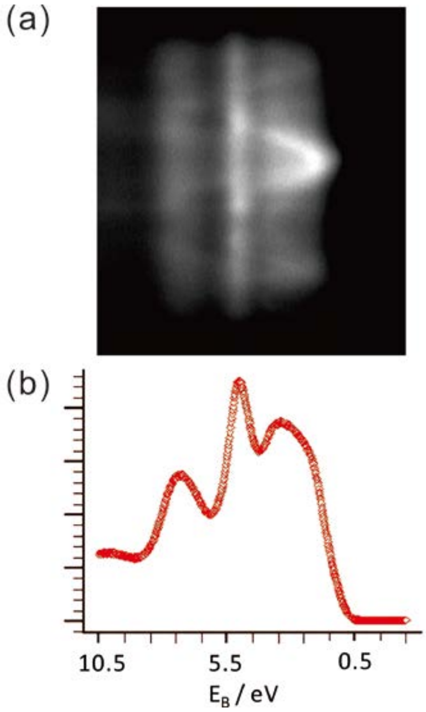


Fig. 2 (a) angle resolved ($E_B$-angle) mapping and (b) angle integrated spectrum of Si(111)5×2-Au surface.

3. Results and discussions

Si(111)5×2-Au surface was produced by depositing 0.45ML Au on clean Si(111)7×7 and annealing. The 5×2 superstructure was confirmed by RHEED. Photons of 500 eV are focused to 30 $\mu$m on the surface. Figure 2(a) shows angle resolved ($E_B$-angle) mapping and (b) its angle integrated spectrum taken by Scienta R4000 in Fig. 1.

Two spin-orbit split peaks, $d_{3/2}$ and $d_{5/2}$, are seen at binding energies $E_B$ at 7.5 and 5.0 eV, respectively. We can confirm the localized feature of the *d* electron from the flat dispersion of these two peaks in Fig. 2(a). The peak width of $d_{3/2}$ band is wider than that of $d_{5/2}$ and a resonant band with Si 3p looks strong. Hence the origin of the dispersion in only one spin-orbit split component band was found to be (1) the resonance with the Si 3p band and (2) the wide band width which enables to show the dispersion.

## References

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