ELECTRONIC STRUCTURE OF
URANIUM COMPOUNDS REVEALED BY
ANGLE RESOLVED PHOTOEMISSION SPECTROSCOPY

Actinide compounds exhibit a rich variety of electrical and magnetic properties such as heavy Fermion behaviors, a variety of superconductivity and magnetic ordering. Recently, "high-T_c" superconductivity at T_c =18 K was found in $PuCoGa_5$ [1], indicating that there remains an unexplored class of exotic materials in actinide compounds. In these compounds, the $5f$ electrons in actinide atoms are responsible for these properties. They have both atomic-like "localized" and band-like "itinerant" properties, and are difficult to treat theoretically. The most fundamental question is how the $5f$ states are involved in their band structure and Fermi surfaces (FSs), and what kind of theoretical treatment is appropriate for their description. To address this question, we have performed angle-resolved photoemission experiments on uranium compounds using the soft X-rays from beamline **BL23SU**. Angle-resolved photoemission spectroscopy (ARPES) is one of the most powerful experimental methods of determining the band structures and FSs of solids experimentally. By performing ARPES experiments in the soft X-ray region (SX-ARPES) [2], bulk-sensitive and $5f$-dominant band structures and FSs are obtained, and they can be directly compared with theoretical calculations. The present target material is the layered uranium compound $UFeGa_5$. $UFeGa_5$ is a paramagnetic uranium compound which has the same crystal structure as $PuCoGa_5$. Among the series of compounds with the same crystal structure, this compound is know as the "itinerant" U $5f$ compound.

Figures 1(a) and 1(b) show the experimental band structures of $UFeGa_5$ for the Z-R and Z-A directions of the Brillouin zone derived from SX-ARPES spectra measured at $h\nu$= 500 eV. The bright part in the image plot corresponds to the position of the band structure. In these plots, the contributions from U $5f$ states and Fe $3d$ states are dominant. For both directions, we could successfully observe the energy dispersion of the U $5f$ states. We compare these results with the energy band structure calculation, treating U $5f$ electrons as being itinerant states. Figures 1(c) and 1(d) show the results of the calculation for the Z-R and Z-A directions to be compared with Figs. 1(a) and 1(b), respectively. Contributions from the U $5f$ and Fe $3d$ states, which have large contributions in the spectra, are indicated on the color scale in each band. Although the overall agreement between experiment and calculation is not so complete, some calculated bands have a correspondence to the experimental bands. For the Z-R direction, there exist two or three bands around the Z point in the experimental band structure. In the band structure calculation, there are few bands in this energy region, and bands 1-3 seem to correspond to the experimental bands among them. Around the R point, the parabolic
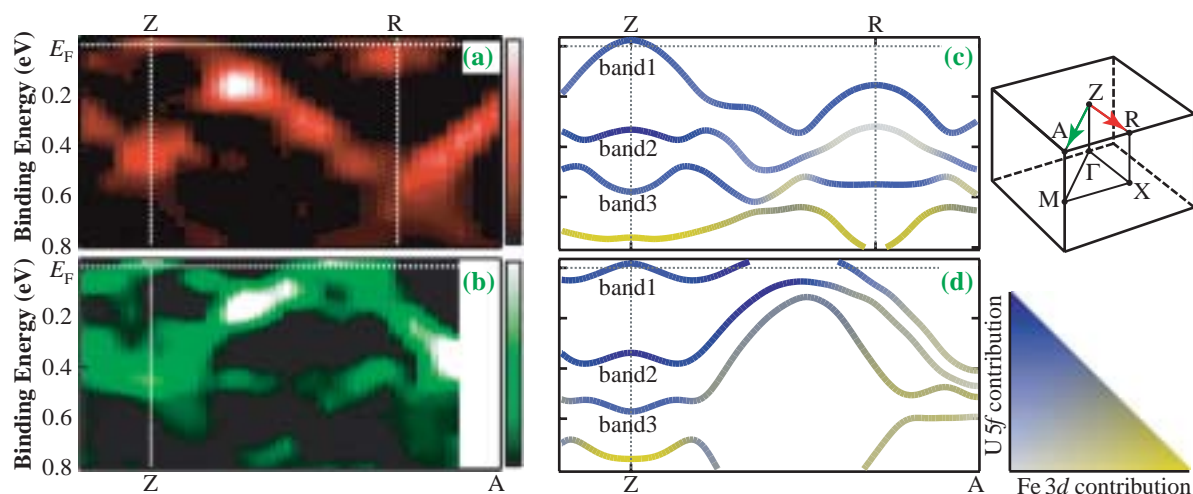

Fig. 1. Band structure of $UFeGa_5$ measured along **(a)** Z-R and **(b)** Z-A directions. Calculated energy band dispersions to be compared with the experiment along **(c)** Z-R and **(d)** Z-A directions are shown.

band dispersion was observed in the experiment, but it does not exist in the calculation. Instead, there exist bands 1-3 in the calculation, and the experimental band seems to correspond to the trace of these calculated bands. For the Z-A direction, while the positions of E_F-crossing are different between the calculation and experiment, the experimental band near E_F shows a good correspondence to the calculations. At the Z point, a hole-like FS is observed in both the experiment and calculation. In addition, the hole-pocket, which is observed in the middle of the Z-A line, also exists in the calculated energy band dispersion.

To obtain more information about the FSs, we have made a 2D mapping of the photoemission intensity at EF. Figure 2(a) shows the mapping as a function of k_x and k_y. A bright part corresponds to higher intensity and a dark part to lower intensity. The most prominent feature in this image is the large round-shaped high intensity part centered at the point A. Its inner and outer boundaries correspond to the hole-like and electron-like FS centered at the point A, respectively. The calculated FSs of UFeGa$_5$ for the Z-R-A plane are also shown in Fig. 2(b). In the band

structure calculation, there exist two large quasi-2D cylindrical FSs centered at the A-M line as indicated in Fig. 2(c). These cylindrical FSs have large contributions from the U 5f states. The comparison of the experimental FSs with those of the calculation shows that although their sizes and shapes are different between the experiment and the calculation, these FSs exist in the experiment also. Hence, we have obtained a qualitative agreement between experimental FS and the result of the band structure calculation. Meanwhile, an important point to note is that the high intensity part persists from the outer hole-like FS to the inner electron FS as indicated in Fig. 2(b). This indicates the renormalization of bands around E_F. This result shows an existence of the electron correlation effect in this compound.

Accordingly, we conclude that although the agreement between the calculation and the experiment is not complete, the essential band structure and morphology of FS of UFeGa$_5$ are explained by the band structure calculation. At the same time, we have observed that the bands near E_F are renormalized, suggesting the importance of electron correlation effects even in itinerant uranium compounds.
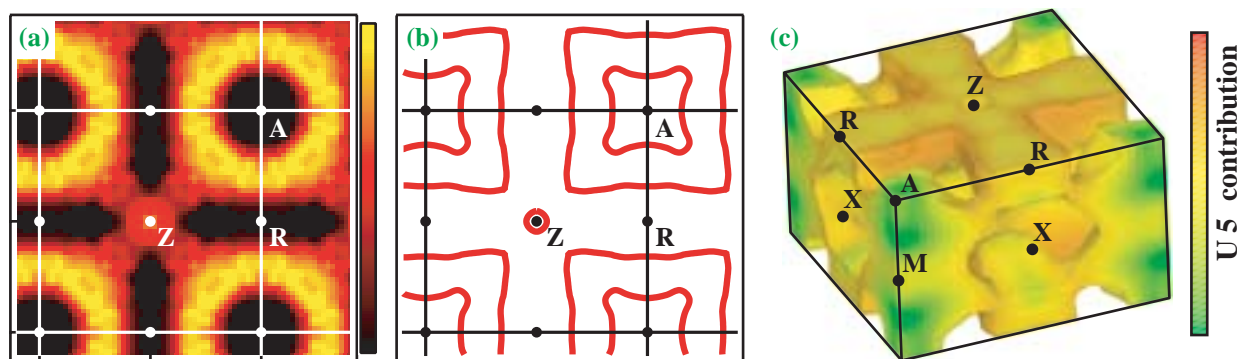

Fig. 2. **(a)** Experimental Fermi surface of UFeGa$_5$ **(b)** Calculated Fermi surface of UFeGa$_5$ in Z-R-A plane. **(c)** Calculated three-dimensional Fermi surface of UFeGa$_5$.

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References

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