Photoemission study of CeMIn$_5$ (M=Rh, Ir) : nearly localized nature of f electrons

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Abstract

We have performed $4d$-$4f$ ($h\nu = 122$ eV) and $3d$-$4f$ ($h\nu = 881$ eV) resonant photoemission spectroscopy studies on the heavy-fermion cerium compounds CeMIn$_5$ (M=Rh and Ir), which show competition between superconductivity and antiferromagnetism. The results suggest that the Ce $4f$ electrons in both compounds are nearly localized. We have also found that although the Ce $4f$ electrons in the superconducting CeIrIn$_5$ are more delocalized than those in the antiferromagnetic CeRhIn$_5$, their electronic structures are very similar to each other.

Key words: photoemission spectroscopy; CeRhIn$_5$; CeIrIn$_5$

In recent years, relationship between magnetism and superconductivity has attracted much attention. Especially, some magnetic f-electron compounds show superconductivity under high pressure, suggesting that magnetic interactions may play essential roles in the superconductivity[1,2]. CeMIn$_5$ (M=Rh and Ir) are recently synthesized this class of Ce-based compounds. They are thought to be located near the quantum critical point (QCP) in Doniach's phase diagram, and are good target materials to study how the magnetic interactions are involved in the pairing mechanism. The CeMIn$_5$ compounds crystallize in the tetragonal HoCoGa$_5$-type structure, which can be viewed as an alternating stack of the CeIn$_3$ and MIn$_2$ layers. Therefore, they can be regarded as a quasi-two-dimenstional version of CeIn$_3$. CeRhIn$_5$ is a heavy fermion (HF) antiferromagnet with T_{N}=3.8 K at ambient pressure. According to their lattice constants, the CeIn$_3$ layers experience a chemical pressure of ~14 kbar relative to bulk CeIn$_3$. Hegger *et al.*[3] have discovered that CeRhIn$_5$ undergoes a superconducting transition at $P_{\mathrm{C}} \sim 16.3$ kbar and T_{C}=2 K. This P_{C} is actually lower than that of CeIn$_3$, supporting that CeRhIn$_5$ corresponds to CeIn$_3$ under high pressure. On the other hand, CeIrIn$_5$ has a small lattice constant along the c axis compared with that of CeRhIn$_5$, and corresponds to CeRhIn$_5$ under pressure. CeIrIn$_5$ is a HF superconductor with T_{C}=0.4 K at ambient pressure, which is again consistent with the picture that the CeIn$_3$ layers in CeIrIn$_5$ experience a high chemical pressure compared with those in CeRhIn$_5$.

In the present study, we have performed $4d$-$4f$ ($h\nu = 122$ eV) and $3d$-$4f$ ($h\nu = 881$ eV) resonant photoemission spectroscopy (RPES) measurements to study

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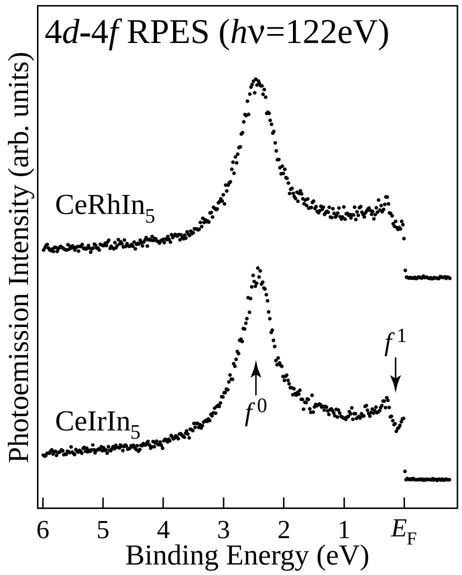

Fig. 1. $4d$-$4f$ resonant photoemission spectra of CeMIn$_5$.

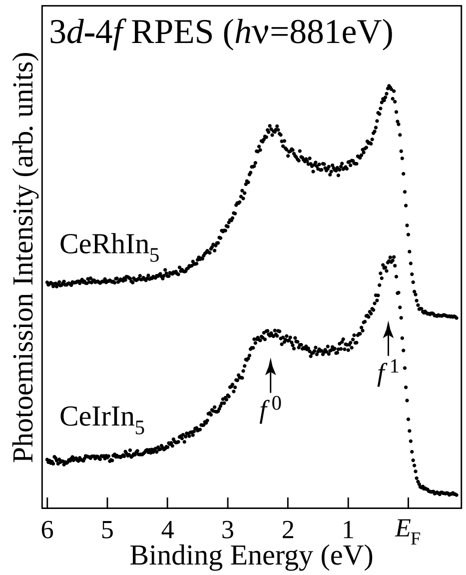

Fig. 2. $3d$-$4f$ resonant photoemission spectra of CeMIn$_5$.

their electronic structures.

Single crystals of CeRhIn$_5$ and CeIrIn$_5$ were grown by the self-flux method described in Ref [3]. The $3d$-$4f$ resonant photoemission experiments ($h\nu$ = 881.2 eV) were performed at BL23SU of SPring-8. The sample temperature was kept at 15 K during the course of measurements, and overall energy resolution was set to about 200 meV. The $4d$-$4f$ resonant photoemission experiments ($h\nu$ = 122 eV) were performed at BL1 of Hiroshima Synchrotron Radiation Center (HiSOR). The sample temperature was kept at 10 K during the course of measurements, and overall energy resolution was set to about 20 meV

Figure 1 shows $4d$-$4f$ RPES spectra ($h\nu$ = 122 eV) of CeMIn$_5$. The spectra consist of the f^1 final-state peak located just below the Fermi level and the f^0 final-state peak at about 2.4 eV. These spectral features have been observed in other Ce-based compounds, and understood within the framework of the single impurity Anderson model (SIAM)[4]. According to SIAM, the stronger the f electrons hybridize with conduction electrons, the stronger the f^1 peak becomes. Here, the intensity of f^0 final state peak, located at about 2.4 eV, is very strong, suggesting that the Ce $4f$ electrons are strongly localized.

Figure 2 shows the $3d$-$4f$ RPES spectra ($h\nu$ = 881 eV) of CeMIn$_5$. The spectra consist of the f^1 and f^0 final-state peaks, same as $4d$-$4f$ RPES spectra, but their relative intensities are different from those in $4d$-$4f$ RPES spectra. The intensity of f^1 final state peak is much stronger than those in $4d$-$4f$ RPES spectra. This is considered to be due to the surface insensitivities in the $3d$-$4f$ RPES experiments, compared with those in the $4d$-$4f$ RPES experiments[5]. In these spectra, the intensity of f^0 final state peak is still large even it is compared with those of the low T_K HF Ce-based compounds, such as CeRu$_2$Si$_2$ (T_K = 22 K)[5]. This again argues that Ce $4f$ electrons in these compounds are nearly localized. We also note that although both spectra are very similar, the f^1 to f^0 intensity ratio is somewhat large in CeIrIn$_5$ compared with that of CeRhIn$_5$. This indicates that the hybridization between the conduction electrons and the Ce $4f$ electrons in CeIrIn$_5$ is slightly larger than that in CeRhIn$_5$. This is consistent with the fact that CeIrIn$_5$ corresponds to CeRhIn$_5$ under pressure.

To summarize, we have found that Ce $4f$ electrons in CeMIn$_5$ (M=Rh, Ir) are nearly localized. Although the Ce $4f$ electrons in CeIrIn$_5$ are more delocalized than those in CeRhIn$_5$, they are more localized than low T_K compound like CeRu$_2$Si$_2$.

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