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Soft x-ray energy-dependent angle-resolved photoemission study of $CeIrIn_5$

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Abstract

Soft x-ray energy-dependent angle-resolved photoemission measurements are performed on the heavy-fermion superconductor $CeIrIn_5$ to study the Fermi surface (FS) and the electronic structure near the Fermi level in the ΓMZA plane. The non-dispersive band designated as the Ce $4f^1_{7/2}$ final state is found at 280 meV along with the main body of the valence band consisting of highly dispersive In 5p bands, which are in good qualitative agreement with the band structure calculation based on the itinerant 4f electron model. Furthermore, we found two electron-like and one hole-like cylindrical FSs at the M (A) and Γ (Z) points. The Fermi momenta of the observed FSs are consistent with the de Haas–van Alphen experiment, while they contradict the stronger anisotropy of the FS along the k_z direction predicted by the band calculation. The results suggest stronger two-dimensionality of the electronic structure of $CeIrIn_5$ and point to the need for its theoretical verification.

(Some figures in this article are in colour only in the electronic version)

$CeIrIn_5$ has recently attracted much attention because of its anomalous physical properties, especially an ambient pressure superconductivity at $T_c = 0.4$ K [1–3]. A large electronic specific heat coefficient ($\gamma = 750$ mJ mol^{-1} K^{-2}) and a power law temperature dependence of thermodynamic properties below T_c have revealed its unconventional superconductivity with an anisotropic superconducting gap, correlating with spin and/or valence fluctuations [1, 3]. These observed anomalous physical properties, which are reminiscent of the high-T_c superconductors, are believed to originate in the low dimensionality of the electronic (magnetic) structure. In fact, the recent de Haas–van Alphen (dHvA) experiment reported quasi-two-dimensional Fermi surfaces (FSs) with undulations along the k_z direction in $CeIrIn_5$ from the comparison with the

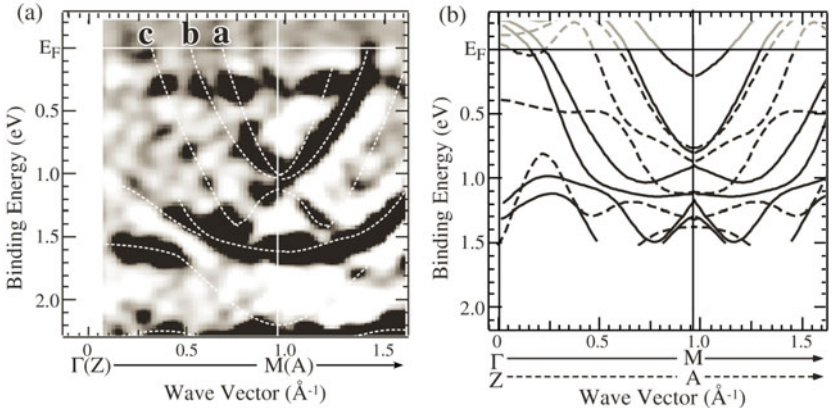

Figure 1. (a) Experimental band structure of $CeIrIn_5$ along the ΓM high-symmetry line. White dashed curves are guides for the eyes. (b) The band structure calculation based on the RLAPW method along the ΓM (solid curves) and ZA (dashed curves) high-symmetry lines [7].

band calculation based on the itinerant 4f electron model [1, 2]. On the other hand, a significant localized nature of Ce 4f electrons in $CeIrIn_5$ is expected from the recent thermodynamic experiments on $CeRh_{1-x}Ir_xIn_5$ [4]. Thus the starting point in understanding the electronic structure of $CeIrIn_5$ based on the assumption of an itinerant 4f electron model is still questioned. In order to clarify the electronic structure as well as the intrinsic nature of Ce 4f electrons in $CeIrIn_5$, we have performed soft x-ray energy-dependent angle-resolved photoemission spectroscopy (ARPES).

$CeIrIn_5$ single crystals were grown by the self-flux method. The x-ray diffraction, electrical resistivity, magnetic susceptibility and specific heat measurements have been performed for characterization, and are in good agreement with previous reports [1–3]. ARPES measurements were performed at the beam line BL27SU in SPring-8 using a SCIENTA SES-2002 analyser. The energy resolution was set at 130 meV and an energy range of 200–300 eV was used. The angular resolution was set at 0.5° which corresponds to a momentum resolution of about 0.1 $Å^{-1}$ along $k_{x,y}$ ($k_\parallel$) at the selected photon energy. The mean free path of photoelectrons of 10 ± 4 Å for the kinetic energy 200–300 eV give a momentum broadening of 0.13 ± 0.06 $Å^{-1}$ along k_z ($k_\perp$) [5]. Since the Brillouin zone sizes along $k_\parallel$ and $k_\perp$ are about 0.96 $Å^{-1}$ (|ΓM|) and 0.46 $Å^{-1}$ (|ΓZ|), respectively, the present momentum resolution should be enough to observe band dispersion and the $k_\perp$ broadening does not average the FS. Single crystals were cleaved *in situ* at 30 K just before the measurement under ultra-high vacuum of 3×10^{-10} Torr to obtain clean mirror-like (001) surfaces with the ΓM–ZA photoemission plane in the probe. The Fermi level (E_F) of samples was referenced to that of a gold film on the sample substrate.

Figure 1(a) shows the experimental band structure along the ΓM high-symmetry line of $CeIrIn_5$ at 30 K obtained from the present ARPES measurement with an excitation energy of 259 eV. We have mapped out the band dispersions by plotting the combined intensity of the ARPES (energy distribution curve (EDC)) and MDC (momentum distribution curve) spectra with gradual shading as a function of wavevector and binding energy after taking second derivatives of each spectrum. Dark areas correspond to 'bands'. We find in figure 1(a) highly dispersive bands at E_F-2.5 eV and a non-dispersive 'band' around 280 meV, being roughly consistent with the previous ARPES study performed with the He I resonance line (21.2 eV) [6]. It is clear that some of the parabolic dispersions around the M (A) point cross E_F and form FSs.

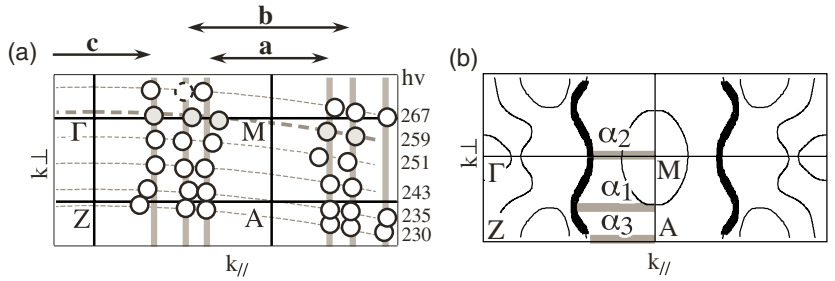

Figure 2. FSs in the ΓZ–MA plane of $CeIrIn_5$ determined by the present ARPES experiment (a) and the band calculation (b) [7]. Dashed curves correspond to the $k_{\parallel}$–$k_{\perp}$ slice for a selected photon energy from 230 to 267 eV by assuming an inner potential of 15 eV. Open circles correspond to experimental Fermi momenta. Thick lines in (a) are guide for the eyes. Thick lines in (b) indicate the corresponding dHvA frequencies expected in the calculation [1, 2].

From the peak position of the MDC spectra at E_F, we estimate the Fermi momenta of each of FS a, b and c as 0.35, 0.45 and 0.63 Å^{-1} from the M (A) point, respectively. A good qualitative agreement of experimental FS-forming highly dispersive bands with In 5p bands in the calculation based on the relativistic linearized augmented plane wave (RLAPW) method (figure 1(b)) [7] allows us to ascribe FSs a, b and c (figure 1(a)) to two electron pockets at the M point and one of two hole pockets at the Γ point, respectively. This qualitative agreement between experiment and calculation substantiates the validity of the itinerant 4f electron model to understand the overall valence electronic structure of $CeIrIn_5$.

On the other hand, there are some quantitative discrepancies between experiment and calculation. The bottom of the In 5p bands are located at higher binding energy than in the calculation, indicative of a strong hybridization effect between In 5p and Ce 4f electrons near E_F. Furthermore, in figure 1(b), there is no flat band near E_F corresponding to the experimental 'band' at 280 meV where the strong Ce 4f character has also been observed in the 3d–4f resonant photoemission spectra (not shown). The absence of the Ce 4f state in the calculation has also been reported on the PES spectra of many heavy-fermion Ce compounds, where the Ce $4f^1_{7/2}$ final state is located at 280 meV originating in hybridization between a 'localized' 4f electron and conduction electrons [8]. These observed differences suggest the importance of the p–f hybridization effect in understanding essential electronic properties in $CeIrIn_5$.

In figure 2, we have mapped out the FS of $CeIrIn_5$ along the ΓZ–MA plane to study the FS topology in detail. A $k_{\parallel}$–$k_{\perp}$ slice of FS in the ΓZ–MA plane has been obtained by plotting the peak position of MDC spectra at E_F as a function of photon energy according to the free-electron final-state model [9]. To determine $k_{\perp}$, we have assumed an inner potential of 15 eV (symmetry in the $h\nu$ dependence allows us to determine the inner potential of 15 eV), slightly larger than the usual value in other heavy-fermion compounds [10, 11]. In figure 2(a), we show at least three cylindrical FSs without sizable anisotropy along the $k_{\perp}$ direction, reflecting strong two-dimensionality in the electronic properties of $CeIrIn_5$ as expected from thermodynamic experiments [1, 3]. When we compare the Fermi momentum between ARPES and dHvA experiments [1, 2], we find that the Fermi momenta of two electron-like FSs a, b around the M point and a hole-like FS c around the Γ point in the ARPES experiment (0.45, 0.35 and 0.32 Å^{-1}) agree well with the dHvA frequencies α_1, α_2 and α_3 (0.52, 0.35 and 0.45 Å^{-1}) which show $1/\cos\theta$ dependence. On the other hand, the dHvA frequencies have been attributed to extreme cross sections of single cylindrical electron-like FSs at the M(A)

point in the band calculation (see figure 2 (b)) [1, 2, 7]. The origin of this substantial difference between experiment and calculation is not clear at present. The large momentum broadening along the $k_\perp$ direction in the ARPES measurement is one possible reason, since the projection of the singularities in the calculated single anisotropic FS may reflect as a few cylindrical FSs. However, the $h\nu$ dependence of the ARPES peak with broad symmetry around 259 eV has been unambiguously observed, assuring the intrinsic $k_\perp$ independence of the FSs reported here. Furthermore, the expected undulation of the calculated FS is large enough compared to the present momentum resolution. Thus, the discrepancy in the FS topology between ARPES and calculation demands a theoretical check for the existence of additional cylindrical FSs as well as the stronger two-dimensionality of the electronic structure of $CeIrIn_5$.

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