Electronic structure and the Fermi surface of ThRhIn$_5$ in comparison with uranium and transuranium compounds

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Abstract

By using a relativistic linear augmented-plane-wave method, we clarify energy band structure and the Fermi surfaces of recently synthesized thorium compound ThRhIn$_5$. We find several cylindrical Fermi surface sheets, which are similar to those of CeTIn$_5$ (T=Ir and Co), PuTGa$_5$ (T=Co and Rh), and AmCoGa$_5$. We discuss such similarity among the compounds including rare-earth or actinide ions with different f electron numbers.

Key words: Relativistic linear APW method, Fermi surface, Thorium compounds

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In order to clarify 5f electron properties, it is useful to investigate thorium compounds both from experimental and theoretical viewpoints, since it is possible to extract pure 5f-electron properties by subtracting the 5f contributions of thorium compounds from those of uranium and transuranium materials. In fact, the electronic structure of thorium compounds has been investigated by band theory as proper reference for the study of 5f electronic states of actinide compounds.

In this paper, we calculate energy band structure and Fermi surface for ThRhIn$_5$ [1] by applying a relativistic linear augmented plane wave (RLAPW) method. It belongs to the material group with HoCoGa$_5$-type crystal structure, frequently referred to as “115”. We compare the present result with those for Ce- [2], Pu- [3,4], and Am-115 compounds [5].

Here we calculate the energy band structure by using the RLAPW method with the exchange and correlation potential in the local density approximation. The muffin-tin approximation is adopted for the spatial shape of one-electron potential and self-consistent calculations are carried out for experimental lattice constants. Note that all 5f electrons are assumed to be itinerant in our calculations. The energy band structure for ThRhIn$_5$ is shown in Fig. 1. The Fermi level, $E_F$, is located at 0.428 Ryd. and shown by a solid line in Fig. 1. Since 13th, 14th, 15th, and 16th bands are partially occupied, these four bands construct the Fermi surface. The number of the valence electrons in the APW sphere is partitioned according to the sites and the angular momenta as 0.42(s), 6.13(p), 2.41(d) and 0.55(f) in the Th sphere. There are 8.74 valence electrons outside the APW sphere in the primitive cell.

Here we note a significant amount of f component due to large hybridization between 5f and 5p electron states. The value of the f component is a little larger than that of fcc-Th, obtained by the RAPW calculation [6], in which the value of 0.41 was reported for the f component. The density of states (DOS) at $E_F$ is evaluated as 56.6 states/Ryd.cell. The contribution from the f states to the DOS at $E_F$ amounts to 14.8% of the total. Above $E_F$ near the M point, flat 5f bands split into two groups, specified by $j=5/2$ for lower and 7/2 for upper bands, respectively, where $j$ is the total angular momentum. The magnitude of the splitting in 5f states corresponds to the spin-orbit coupling, estimated as 0.048 Ryd. As shown in Fig. 1, the main part
of the $f$ bands exist just above $E_F$.

In Fig. 2, we show the Fermi surfaces of ThRhIn$_5$. The Fermi surfaces from the 13th band have one sheet centered at the $\Gamma$ point, two equivalent sheets centered at the X points. The 14th band constructs a large cylindrical hole sheet centered at the $\Gamma$ point, which exhibits a complex network consisting of big “arms” along the edges of the Brillouin zone, as observed in Fig. 2(b). The 15th band has a cylindrical electron sheet centered at the M point. The Fermi surface from the 16th band consists of one hole sheet centered at the M point. The number of carriers contained in these Fermi-surface sheets are 0.051 holes/cell, 0.603 holes/cell, 0.581 electrons/cell, and 0.073 electrons/cell in the 13th, 14th, 15th, and 16th bands, respectively. The total number of holes is equal to that of electrons, since ThRhIn$_5$ is a compensated metal.

We remark that the Fermi surfaces of ThRhIn$_5$ look similar to those of CeTIn$_5$ ($T=$Ir and Co) [2], PuTGa$_5$ ($T=$Co and Rh) [3,4], and AmCoGa$_5$ [5]. If we assume the trivalent rare-earth or actinide ion in 115 structure, we find zero, one, five, and six electrons per ion for Th-, Ce-, Pu-, and Am-115 compounds, respectively. In the $j$-$j$ coupling scheme, we accommodate $n$ electrons in the $j=5/2$ sextet and thus, the electron-hole relation is expected [7]. In this sense, it seems to be natural to observe similar Fermi-surface structure for the cases of $n$ and $6-n$ electrons. Namely, it is enough to discuss the similarity between the cases of $n=0$ and 1. The Fermi surfaces of ThRhIn$_5$ constructed from the four bands contain the $f$ components appreciably due to the large hybridization between $f$ and $p$ electrons near the Fermi level. In fact, in our band-calculation results, we have found 0.55 $5f$ electrons in Th atom. Then, the Fermi-surface structure of Th-115 becomes similar to that of Ce-115.

In summary, we have performed the band calculation for ThRhIn$_5$ by using the RLAPW method. The similarity in the Fermi-surface structure among Th-, Ce-, Pu-, and Am-115 compounds are understood by the electron-hole relation in the $j$-$j$ coupling scheme and the large hybridization between $f$- and $5p$-electron states in the vicinity of $E_F$.

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