Fermi surface of the filled skutterudite $LaOs_4Sb_{12}$

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Abstract

The electronic band structure and Fermi surface are calculated for $LaOs_4Sb_{12}$, which is a reference material of a new heavy fermion superconductor $PrOs_4Sb_{12}$. The calculated Fermi surfaces consist of two closed hole surfaces around the Γ point and a multiply connected one. The topology of the Fermi surface is different from that in $LaFe_4P_{12}$ due to the larger hybridisation between Os-*d* and Sb-*p* bands.

Key words: Fermi surface; $LaOs_4Sb_{12}$; band structure ; skutterudite

The Pr-compounds belonging to a family of the filled skutterudites have shown a variety of interesting physical properties. $PrRu_4P_{12}$ shows a metal-insulator (M-I) transition at $T_{MI} = 60$ K [1], and $PrFe_4P_{12}$ undergoes a non-magnetic ordering showing heavy fermion behaviour under magnetic fields [2–4]. Very recently, a new class of heavy fermion superconductivity has been reported in $PrOs_4Sb_{12}$ [5,6]. $PrOs_4Sb_{12}$ shows superconductivity below T_C=1.85K where the large specific heat jump $\Delta C/T_C \sim 500\mathrm{mJ}/K^2$ indicates the heavy electrons contribute the superconductivity. Furthermore, the recent measurement of the longitudinal relaxation rates $1/T_1$ of NQR at Sb site shows very unusual temperature dependence both below and above T_C [7]. In many other heavy fermion superconductor, *i.e.* $CeCoIn_5$ [8] or UPt_3 [9], it has been widely accepted that the f-electrons participate to form Fermi surface, where the itinerant f-electron model is applicable. Now, in the new heavy fermion superconductor, there arises a question whether the $4f^2$-electrons in Pr are itinerant or not. In this contribution, the electronic band structure and Fermi surface are calculated for $LaOs_4Sb_{12}$, to reveal the Fermi surface of the f^0 reference system.

A band structure is calculated by using an FLAPW method with the local density approximation for the exchange correlation potential. $PrOs_4Sb_{12}$ crystallises in a unique body-centered cubic structure of a space group $Im\bar{3}$ (T_h^5, # 204). The atomic parameters are obtained as a=9.30807 Å for the lattice constant and $u = 0.3414$, $v = 0.1566$ for 24*g*-site occupied by Sb [10]. The details of the method follows the previous calculation for $LaFe_4P_{12}$ [11].

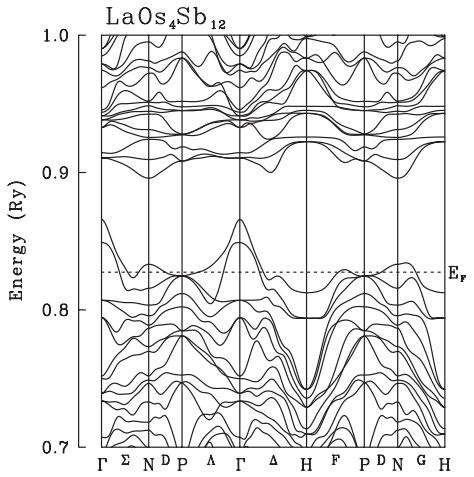

Fig. 1. The calculated band structure of $LaOs_4Sb_{12}$ in the vicinity of the Fermi level denoted by E_F.

The band structure is obtained as shown in Fig. 1. The Fermi level is situated around the sharp peak in

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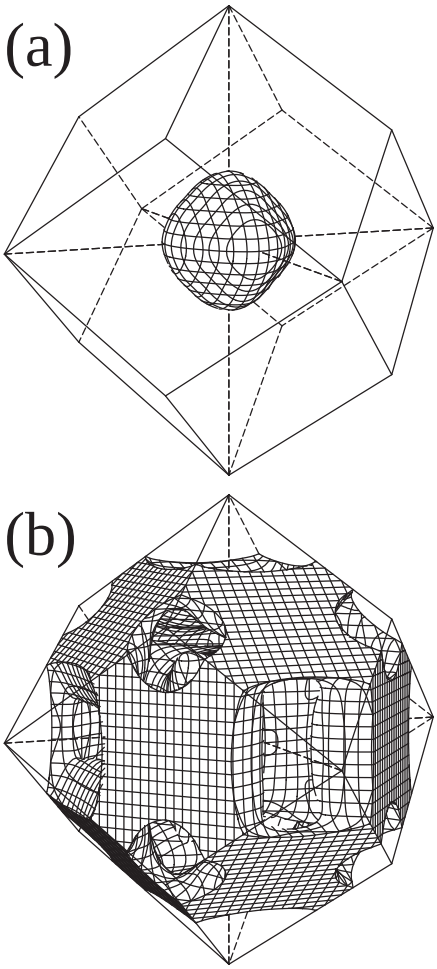

Fig. 2. The calculated Fermi surface of $LaOs_4Sb_{12}$ consisting of (a) the closed hole surface from the 47th band and (b) the closed and multiply connected hole surfaces from 48th band.

the density of states, as in $LaFe_4P_{12}$ [11], resulting in 35.9 mJ/mol K^2 for the specific heat coefficient γ value. As in $LaFe_4P_{12}$, two bands (the 47th and the 48th) cross the Fermi level, then Fermi surfaces appear in two Brillouin zone, as shown in Fig. 2. The 47th Fermi surfaces in both compounds are the closed hole surfaces around the Γ point. The 48th Fermi surface in $LaFe_4P_{12}$ is multiply connected one showing a good nesting property with $q = (1, 0, 0)$. The Fermi surface consists, in principle, of X-p molecular orbital, which symmetry is xyz. However, the corresponding Fermi surface in $LaOs_4Sb_{12}$ is split to two parts, one of which is a closed hole surface around the Γ point and the other is a multiply connected one. The hybridisation between T-d bands and X-p bands is larger in $LaOs_4Sb_{12}$ than that in $LaFe_4P_{12}$, then the shape of the Fermi surface is modified in $LaOs_4Sb_{12}$.

The nesting property in the main Fermi surface is significant for the metal-insulator transition in $PrRu_4P_{12}$ [12] and for the antiquadrupole ordering in $PrFe_4P_{12}$ [13,14]. In $LaOs_4Sb_{12}$, it is not expected such the nesting property with $q = (1, 0, 0)$. Very recently, the superconductivity in $PrOs_4Sb_{12}$ has been discussed in the basis of the topology of the Fermi surface [15].

Recently the dHvA measurements have been performed for $LaOs_4Sb_{12}$ and $PrOs_4Sb_{12}$ [16], then it has been revealed they have very similar topology. The calculated dHvA frequencies agree quite well with the measured values. The cyclotron masses are found to be enhanced in the measured value by up to 3 times in $LaOs_4Sb_{12}$ and by up to 8 times in $PrOs_4Sb_{12}$. The detailed results including the LDA+U calculation for $PrOs_4Sb_{12}$ will be published in a separate paper.

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