FERMI SURFACE OF ANTIFERROMAGNET $UPtGa_5$ IN RELATIVISTIC SPIN-POLARIZED BAND THEORY*

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A first-principle study of Fermi surface and magnetism for antiferromagnet $UPtGa_5$ is done by all-electron band calculations using fully-relativistic spin-polarized LAPW method in a local spin-density approximation. The Fermi surfaces, mainly having cylinder-like shapes with open structure along the [001] direction, explain well the angular-dependence of de Haas-van Alphen frequencies. In a picture of $5f$-band antiferromagnet, the local magnetic moment at U site is in good agreement with the observed moment.

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1. Introduction

$UPtGa_5$ shows an antiferromagnetic ordering below 25K, and the local magnetic moments at the U site are arranged with the wave vector $Q = (0, 0, 1/2)$ and the easy axis along the [001] direction [1]. The crystal structure belongs to $HoCoGa_5$-type tetragonal structure with a symmetry of $P4/mmm$ [2]. Recent de Haas-van Alphen (dHvA) measurements clarify that the Fermi surfaces of $UPtGa_5$ are basically cylindrical along the [001] direction [3,4]. The topology of Fermi surface is found to be different from that of $UNiGa_5$ [5] with the same crystal structure, but a different magnetic structure of $Q = (1/2, 1/2, 1/2)$ [1]. The angular dependence of dHvA frequencies in $UNiGa_5$ has been explained from the band theory together with magnetic moments [6].

In the paper a first-principle study of Fermi surface and magnetism for antiferromagnet $UPtGa_5$ is performed by all-electron band calculations using a fully-relativistic spin-polarized LAPW method [7] within exchange-corre-

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lation potentials in a local spin-density approximation [8]. Accordingly we obtain a theoretical evidence to show that the antiferromagnetic structure directly controls the topology of Fermi surfaces for $UNiGa_5$ and $UPtGa_5$.

2. Calculated results and discussion

In the self-consistent calculations the $5f$, $6p$, $6d$ and $7s$ electrons in the U site, the $5d$ and $7s$ in the Pt site and the $3d$, $4s$ and $4p$ in the Ga site are treated as valence electrons. The densities and potentials are constructed in the muffin-tin approximation. The magnetic moments at the U site are oriented antiferromagnetically along the [001] direction using a local spin-rotation technique [7] and the magnetic directions around the Pt atoms are set along the [001] direction so as to hold a magnetic symmetry. The lattice constants are set to experimental values of $a = 4.3426\,\text{Å}$ and $c = 6.8120\,\text{Å}$.

Fig. 1 show total and partial density of state (DOS) for antiferromagnet $UPtGa_5$, where the dashed lines presents the Fermi energy (E_F). The Ga(1) and Ga(2) denote two different positions of the Ga atom in $UPtGa_5$: those are Ga(1)=(1/2,1/2,0) and Ga(2)=(0,1/2,z) with $z = 0.295$ in the unit cell. The $5f$ bands around E_F are hybridized mainly with the U-$6d$ bands and the Ga(2)-$4p$ bands. The theoretical electronic specific heat coefficient γ_b is estimated as $22.52\,\text{mJ/K}^2$ mole from the total DOS at E_F. The experimental

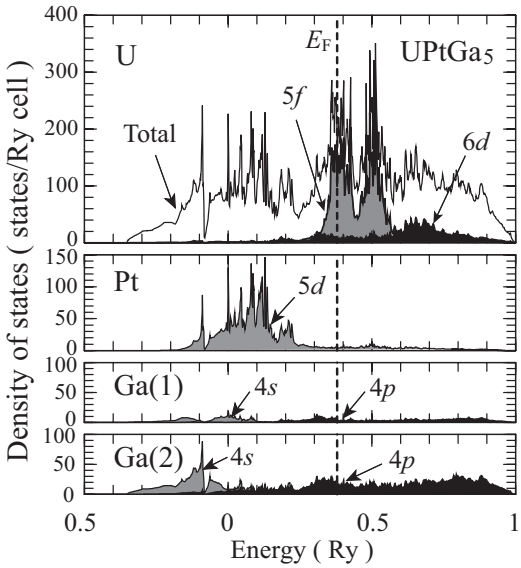

Fig. 1. Total and partial density of states partitioned into the U, Pt, Ga(1) and Ga(2) sites.

value is $\gamma_{\rm exp}$=57 mJ/K^2 mole [3]. The enhancement factor ($\lambda = \gamma_{\rm exp}/\gamma_{\rm b} - 1$) is thus found to be of a small value of 1.53.

The Fermi surfaces are composed of $5f$-rich bands with 30 to 34 band-indices, which are adopted to a number counted up from the bottom of the valence electron. In Fig. 2 the shape of the Fermi surfaces is shown within a tetragonal Brillouin zone in the antiferromagnetic state. All the Fermi surfaces except the band 34-electron surface have cylinder-like shapes with open structure along the [001] direction.

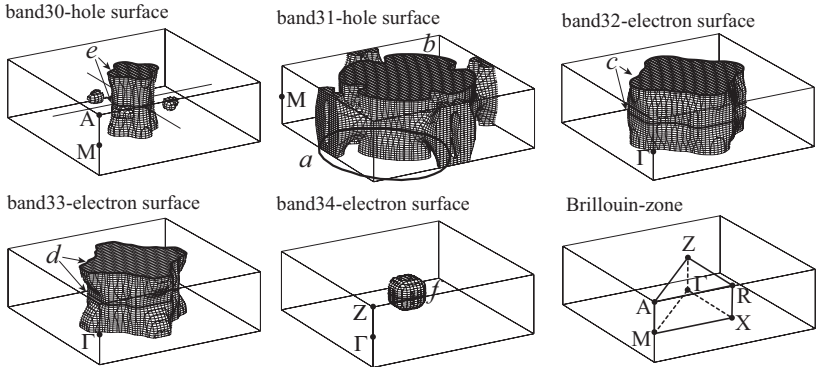

Fig. 2. Fermi surface of antiferromagnet $UPtGa_5$. The band30- and band31-hole surfaces are drawn at the center of the Γ point in the Brillouin zone and the band32- to band34-electron surfaces are centered as the M point.

The extremal cross-sectional area (ECSA) of the Fermi surface is proportional to the dHvA frequency. Fig. 3 shows a quantitative comparison between the theoretical (solid lines) and the observed results (circles) [4] in the angular dependence of the dHvA frequencies. The theoretical branch a, d and e in Fig. 3 obviously correspond to the experimental branch ε, α_1 (α_2) and γ, respectively. The orbits of the theoretical branches with respect to the [001] field direction are presented in Fig. 2. The branch α_3 naturally originates from the branch c or/and a part of the branch b_1 and b_2, each of which is the branch b (Fig. 2) in the case that the center of ECSA is set at the Z and Γ point. The remaining branch f is not observed here. Additionally the cyclotron masses at the [001] field angle for branch a, b, c, d, e and f are given as 3.63, 4.81, 3.43, 3.19 and 3.04, 1.65 and 1.56 in units of electron mass m_0, though it is not discussed here for lack of space.

For the magnetic properties the spin- and orbital-moment at the U site are calculated as $-2.55\mu_{\rm B}$ and $2.84\mu_{\rm B}$, respectively. The local magnetic moment is thus $0.29\mu_{\rm B}$. It is in good agreement with the experimental value of $0.24\mu_{\rm B}$ [1].

It is thus suggested that $UPtGa_5$ should be a $5f$-band antiferromagnet in a viewpoint of the fermiology and magnetic moment.

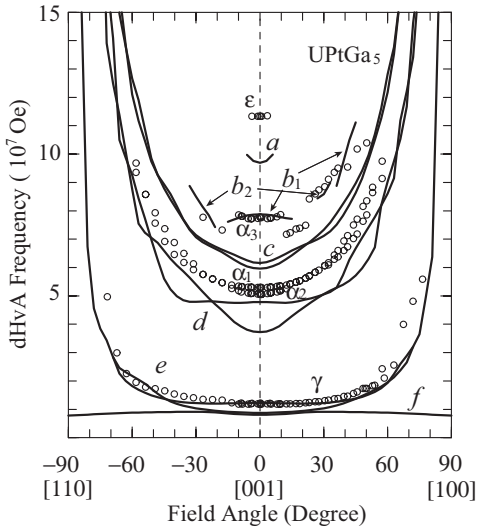

Fig. 3. Comparison between theoretical and experimental results of de Haas–van Alphen frequencies in $UPtGa_5$. The theoretical results are indicated by solid lines and the experimental results are denoted by circles [4].

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