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Electronic properties of cerium and uranium compounds with $HoCoGa_5$-type tetragonal structure

Takahiro Maehira[1], **Masahiko Higuchi**[2] **and Akira Hasegawa**[3]

[1] Advanced Science Research Centre, Japan Atomic Energy Research Institute, Tokai, Ibaraki 319-1195, Japan
[2] Department of Physics, Shinshu University, Matsumoto, Nagano 390-8621, Japan
[3] Niigata University, Niigata 950-2181, Japan

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Abstract

Relativistic energy band calculations have been carried out for $CeIrIn_5$, $CeCoIn_5$, $UFeGa_5$, $UCoGa_5$ and $URhGa_5$ under the assumption that f electrons are itinerant. The main Fermi surface sheet of $CeIrIn_5$ is quite similar to that of $CeCoIn_5$, which is a quasi-two-dimensional Fermi surface. The Fermi surface sheets of $UCoGa_5$ are quite similar to those of $URhGa_5$, which are all small in size and closed in topology. $UFeGa_5$ has a quasi-two-dimensional Fermi surface and a lattice-structure-like Fermi surface.

1. Introduction

In recent years, f-electron compounds with the $HoCoGa_5$-type tetragonal crystal structure such as $CeMIn_5$ (M = Ir, and Co) and $UTGa_5$ (T = Fe, Co, and Rh) have been studied intensively, both theoretically and experimentally, because they show various kinds of anomalous properties due to the f electrons, such as Pauli paramagnetism and heavy fermion and unconventional superconductivity. To understand the electronic properties of these materials, the features of the ground state should first be clarified. For this purpose, it is quite important to investigate the Fermi surface both experimentally and theoretically. $CeMIn_5$ and $UTGa_5$ are paramagnetic in the ground state [1–3]. Owing to their simple crystal structure and paramagnetism, $CeMIn_5$ and $UTGa_5$ are appropriate subjects for a fundamental study of the nature of the f electrons.

In order to calculate the energy band structure of the cerium and uranium compounds, relativity should be taken into account because of the large atomic numbers of the constituent atoms. In this paper, the energy band structures for $CeMIn_5$ and $UTGa_5$ are calculated by using the relativistic linear augmented-plane-wave (RLAPW) method [4]. In the RLAPW method, the four-component relativistic plane wave is augmented by a linear combination of the solutions for the spherically symmetrical potential. The exchange and correlation potential is treated in the local density approximation (LDA). The spatial shape of the one-electron potential is determined in the muffin-tin approximation. Self-consistent calculations are carried out for the experimental lattice constants.

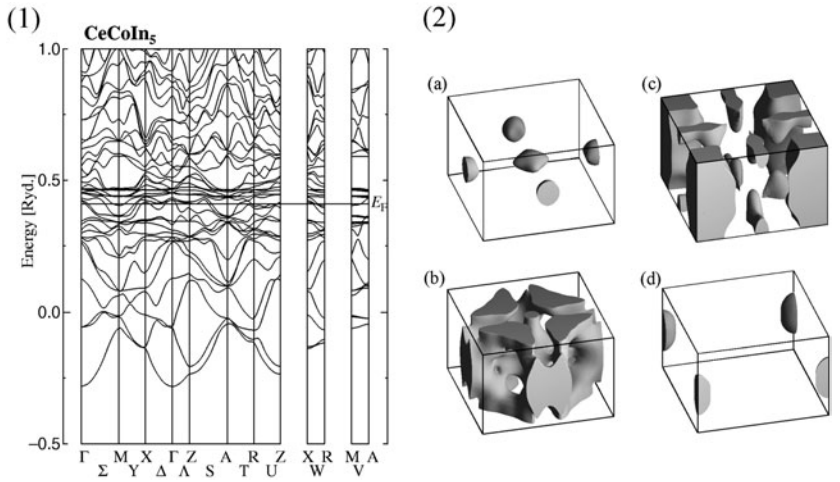

Figure 1. (1) Energy band structure calculated for $CeCoIn_5$. E_F shows the Fermi energy. (2) The Fermi surface for $CeCoIn_5$ centred at the Γ point in the Brillouin zone. (a) The small hole sheet of the Fermi surface in the 13th band. (b) The large hole sheet of the Fermi surface in the 14th band. (c) The large electron sheet of the Fermi surface in the 15th band. (d) The small electron sheet of the Fermi surface in the 16th band.

2. Result of the calculation

In figure 1(1), the energy band structure calculated for $CeCoIn_5$ is shown. The Fermi energy E_F is located at 0.409 Ryd. Narrow bands, which lie just above E_F and are split into two subbands by the spin–orbit interaction, are identified as the Ce 4f bands. A hybridization between the Ce 4f state and the In 5p state occurs in the vicinity of E_F. The 13th, 14th, 15th and 16th bands form the Fermi surface, which is shown in figure 1(2). These Fermi surface sheets are essentially the same as the previous results [5], with some differences in detail. The total number of holes is equal to that of electrons, which means that $CeCoIn_5$ is a compensated metal. The theoretical electronic specific-heat coefficient γ_{band} is 26.8 mJ K^{-2} mol^{-1}. The experimental electronic specific-heat coefficient γ_{exp} is 300 mJ K^{-2} mol^{-1}. Therefore, the enhancement factor for the electronic specific-heat coefficient, defined by $\lambda = \gamma_{exp}/\gamma_{band} - 1$, is 10.2. This disagreement between γ_{band} and γ_{exp} should be ascribed to the effects of the electron correlation which the LDA fails to take into account.

Similarly, we calculated the energy band structure of $CeIrIn_5$ with the RLAPW method in the LDA. The 13th, 14th, 15th and 16th bands construct the Fermi surface sheets, which are very similar to those of $CeCoIn_5$.

Figure 2(1) shows the energy band structure calculated for $UCoGa_5$. The Fermi energy E_F is located at 0.460 Ryd. Narrow bands, which lie just above E_F and are split into two subbands by the spin–orbit interaction, are identified as the U 5f bands. A hybridization between the U 5f state and Ga 4p state occurs in the vicinity of E_F. The 15th and 16th bands form the Fermi surface, which is shown in figure 2(2). These sheets of the Fermi surface are all small in size and closed in topology. The hole sheets of the Fermi surface, as shown in figure 2(2a), consist of the sheet centred at the Γ point, two equivalent sheets centred at the X points and the sheet which lies across the Σ axis. Figure 2(2b) shows a set of the 16 electron sheets of the Fermi surface in the 16th band. Each electron sheet lies across the T axis and looks like a cushion. The total number of holes is equal to that of electrons, which means that

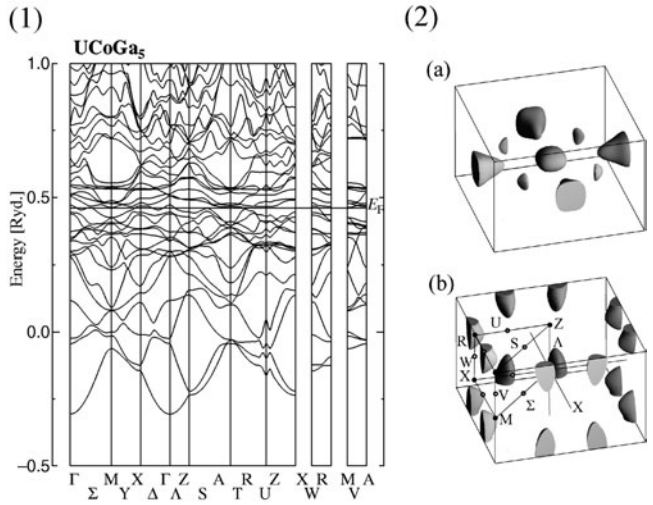

Figure 2. (1) Energy band structure calculated for $UCoGa_5$. E_F shows the Fermi energy. (2) The Fermi surface for $UCoGa_5$ centred at the Γ point in the Brillouin zone. (a) The small hole sheet of the Fermi surface in the 15th band. (b) The small electron sheet of the Fermi surface in the 16th band.

$UCoGa_5$ is a compensated metal. The theoretical electronic specific-heat coefficient γ_{band} is 4.2 mJ K^{-2} mol^{-1}. This is about half of the experimental value of 7 mJ K^{-2} mol^{-1}. This disagreement between γ_{band} and γ_{exp} should be ascribed to the effects of the electron correlation which the LDA fails to take into account. Similarly, we calculated the energy band structure of $URhGa_5$ with the RLAPW method in the LDA. The 15th and 16th bands construct the Fermi surface, which is very similar to those of $UCoGa_5$.

Figure 3 shows the angular dependence of the theoretical de Haas–van Alphen (dHvA) frequency in $UCoGa_5$. Theoretical dHvA branches, which originate from the hole sheet, are explained as follows: an orbit running on the hole sheet centred at the Γ point (a) and an orbit running on the hole sheet centred at the X point (b). Quantitative comparison reveals, however, that the theoretical frequencies are considerably larger in magnitude than the experimental frequencies [6].

Finally, we discuss the energy band structure of $UFeGa_5$. The 14th and 15th bands construct the Fermi surface sheets. $UFeGa_5$ has an odd number of electrons per primitive cell, and therefore becomes an uncompensated metal in which the numbers of electrons and holes on the Fermi surface are not equal to each other. The electron sheets of the Fermi surface in the 15th band are: cylindrical, Fermi surface and a lattice-structure-like Fermi surface. The origins of the dHvA frequency branches can also be clarified satisfactorily by our theoretical Fermi surface model [7].

3. Conclusions

The theoretical results for the electronic specific-heat coefficient are much smaller than the experimental ones, which suggests the significance of many-body effects in these materials. The disagreements between our calculations and experiments should be ascribed to electron correlations and/or electron–phonon interaction which the LDA fails to take into account. Improvement of the one-electron potential beyond the LDA is a problem for future work.

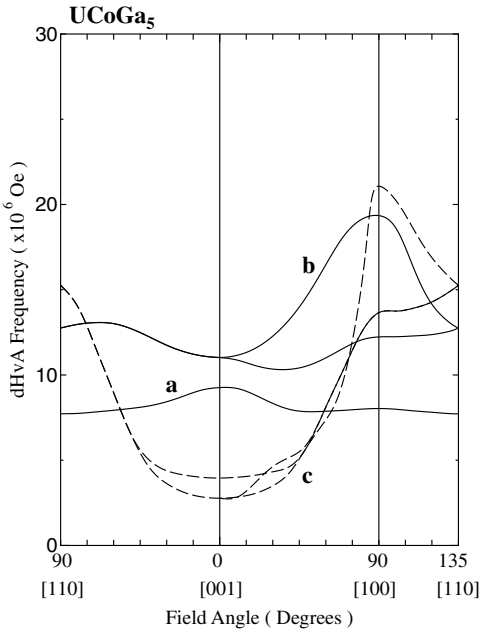

Figure 3. Angular dependence of the theoretical dHvA frequency in $UCoGa_5$. The solid curves and dashed curves show the frequencies calculated from the hole pockets and the electron pockets respectively.

Acknowledgments

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References

[1] Grin Yu N *et al* 1986 *J. Less-Common Met.* **121** 497
[2] Noguchi S *et al* 1992 *J. Magn. Magn. Mater.* **104–107** 57
[3] Sechovsky V *et al* 1992 *J. Magn. Magn. Mater.* **104–107** 11
[4] Higuchi M *et al* 1995 *J. Phys. Soc. Japan* **64** 830
[5] Shishido H *et al* 2002 *J. Phys. Soc. Japan* **71** 162
[6] Ikeda S *et al* 2003 *J. Nucl. Sci. Tech.* at press
[7] Tokiwa Y *et al* 2001 *J. Phys. Soc. Japan* **70** 2982