Proceedings of the European Conference Physics of Magnetism 2011 (PM'11), Poznań, June 27–July 1, 2011

Kondo Screening Effect and Ferromagnetic Order in UCu_2Si_2

R. Troć[a,*], M. Samsel-Czekała[a] and B. Coqblin[b]

[a]Institute of Low Temperature and Structure Research, Polish Academy of Sciences
P.O. Box 1410, 50-950 Wrocław 2, Poland

[b]Laboratoire de Physique des Solides, CNRS-Université Paris-Sud, 91405 Orsay, France

Electrical resistivity and low temperature magnetoresistivity measurements made on a single crystal of UCu_2Si_2 are reported. By using as a phonon reference the temperature dependence of the electrical resistivity of $ThCu_2Si_2$ we could establish that UCu_2Si_2 has both a ferromagnetic and a Kondo behaviour. Such a phenomenon can be described by the underscreened Kondo lattice model. The magnetoresistivity revealed the presence of magnetic fluctuations within the ferromagnetic order as it was reported previously for UGe_2. Also one of the calculated Fermi surface sheets exhibits nesting properties, being in perfect agreement with the previous neutron diffraction data, supporting the possibility of a presence of the spin density wave phase. In this ternary silicide, where the strong ferromagnetic behaviour exists, this phase is signalised by magnetic fluctuations.

PACS: 73.43.Qt, 75.30.Mb, 75.30.Fv, 71.18.+y

1. Introduction

Previous bulk ac and dc magnetic susceptibility, as well as neutron-diffraction data reported in the literature, reviewed by Kuznietz et al. [1], revealed ferromagnetic (FM) ordering of UCu_2Si_2 aligned along the tetragonal axis below the Curie temperature T_C being equal to 103(3) K with values of the uranium ordered moment at 4.2 K either 1.61(5) or 2.0(1) μ_B/U at. Moreover, curves of the ac and dc magnetic susceptibility versus T discussed in Ref. [1] indicated also a tiny anomaly just above T_C connected with another magnetic phase transition. The performed recent magnetic studies on single-crystalline samples of this ternary compound have either revealed [2, 3] or not [4] the existence of the above anomaly at 106 K. Nevertheless, both these measurements of the magnetization show a similarly large anisotropy in the FM state with a magnetic easy-axis of [001] and a hard-axis of [100] below T_C = 100(1) K [2] or 104(1) K [3]. The ordered moments found from the magnetization at 2 and 1.9 K are respectively 1.55 [4] and 1.8 μ_B/U at. [2, 3]. Furthermore, there exists a difference in the results of these two measurements concerning the appearance of the above tiny anomaly. Matsuda et al. [2, 3] measured the field dependence of the magnetization in the temperature range 100–106 K and found a clear metamagnetic transition already in applied fields of an order of 0.1 T, indicating an evidence of antiferromagnetic (AFM) ordering above T_C. Then, a full confirmation of this fact came from very detailed neutron diffraction measurements of Honda et al. [5], so that UCu_2Si_2 transforms above T_C into a long-period, amplitude-modulated antiferromagnet having a spin-density-wave (SDW)-like order vanishing at T_N = 106 K. No such magnetic phase has been detected in the single-crystalline magnetization studies of Ref. [4], next confirmed also by specific heat measurements [6]. One cannot exclude, however, the fact that in the latter case both the transitions, i.e. FM and AFM ones, occur at the same temperature while the concept of two $5f$ electron subsystems for the uranium atom in this ternary compound will be taken into account.

We present here the electrical transport properties, probed on a single-crystalline sample under a magnetic field up to 8 T and the topology of our calculated Fermi surface (FS). The compound UCu_2Si_2 is ferromagnetic with a large Curie temperature and has also a Kondo behaviour as we will see in the next section. Thus, it belongs clearly to the underscreened Kondo lattice (UKL) systems, which has been studied recently theoretically [7, 8] and also observed in some uranium or neptunium compounds.

2. Electrical transport results

We have made electrical resistivity measurements on the single-crystalline sample of average quality by using the Cu-flux method, described in the previous paper [4], where the magnetic data are involved. We used the classical method to separate the phonon contribution from the measured resistivity by taking the phonon contribution equal to the electrical resistivity of the non-magnetic, isostructural $ThCu_2Si_2$, prepared by the arc-melting and

* corresponding author; e-mail: R.Troc@int.pan.wroc.pl

annealing procedures. In Fig. 1, we show the three $(\rho - \rho_0^*)(T)$ curves for: (1) UCu_2Si_2, (2) $ThCu_2Si_2$, and (3) their difference $\Delta\rho_{mag}$. The difference presents clearly a $\log T$ behaviour at higher temperatures, characteristic of the single-Kondo effect and the corresponding parameters are given in Fig. 1.

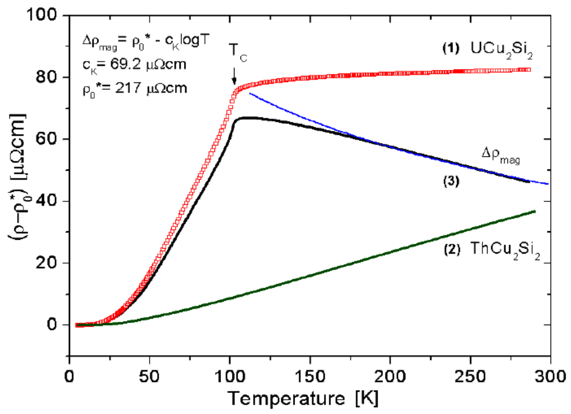

Fig. 1. Temperature dependences of the resistivity difference $(\rho - \rho_0^*)$ for the single crystal of UCu_2Si_2 oriented along the [100] axis (1) and for the polycrystalline sample $ThCu_2Si_2$ (2). The solid line (3) is given as the resulting magnetic resistivity part found by subtracting (2), taken as the phonon part, from the $(\rho - \rho_0^*)(T)$ curve (1).

The compound UCu_2Si_2 presents both a ferromagnetic order with a relatively large Curie temperature of order 100 K and the UKL behaviour characteristic of the Kondo-lattice effect in actinide systems [7, 8]. This new scenario presented here for UCu_2Si_2 enlarges the list of the growing family of the UKL ferromagnetic compounds, with already known some uranium compounds such as UTe [9] or recently neptunium compounds like $NpNiSi_2$ [10] or Np_2PdGa_3 [11]. This peculiar UKL behaviour arises from the localized spins of the actinide atoms which are larger than the $s = 1/2$ conduction electron spins and consequently cannot be completely screened at very low temperatures.

Furthermore, in Figs. 2a and b we have plotted the magnetoresistivity (MR), $\Delta\rho/\rho_0$, as a function of applied magnetic field B and temperature T, respectively, for cases where the current $\boldsymbol{j}$ is flowing along the a axis and the magnetic field is aligned perpendicular to $\boldsymbol{j}$. As seen in Fig. 2, the measured transverse MR of UCu_2Si_2 in the temperature range of the ferromagnetic order has an expected negative sign. However, the temperature dependence of MR is quite unusual. The $\Delta\rho/\rho_0(T)$ function found at $B = 8$ T first goes through a diffuse negative minimum at $T_{\rm min} = 75$ K and then shows a sharp negative minimum at $T_{\rm C} = 103$ K, indicating a critical scattering of electrons. A very rapid change of this dependence as T is increased above $T_{\rm C}$, gives no sign of an existence of another critical scattering for our sample. This fact is supported also by our specific heat

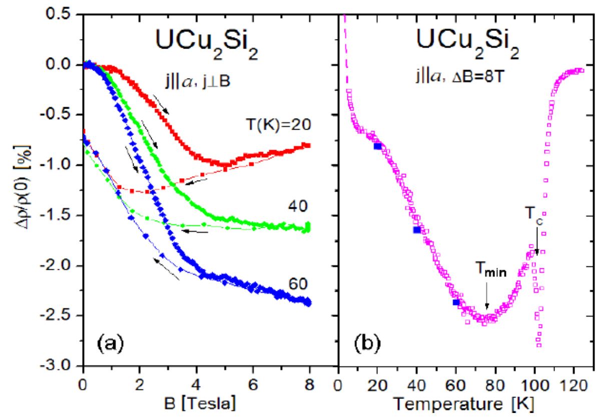

Fig. 2. The low-temperature magnetoresistivity for the UCu_2Si_2 single crystal, oriented along the [100] direction, plotted (a) versus applied magnetic fields up to 8 T taken for three temperatures (indicated in the figure) and (b) versus temperature at 8 T. The blue (dark) squares are the 8 T–MR values found from the field dependences of MR at the three temperatures of part (a).

measurements [6]. Having in mind the above diffuse anomaly in the transverse MR, one can see a similarity with an anomaly previously observed in transverse MR of UGe_2 [12], pointing to the presence of strong magnetic fluctuations deeply below $T_{\rm C}$. As in UGe_2, we have also observed at $T_{\rm min}$ anomalies in the temperature derivative of the resistivity $d\rho(T)/dT$, as well as in the specific heat results [6]. Thus, the above similarity and the discussion about the Fermi surface (see below) may provide another example of the superconductivity coexisting with the FM order under applying pressure, owing to a depression of the magnetic fluctuations being of probable SDW origin (see for discussion Ref. [12]).

3. The Fermi surface

The Fermi surface (FS) of UCu_2Si_2 in the FM state ordered along the c axis was calculated based on the fully-relativistic band structure results, presented in [13], obtained by the full-potential local-orbital (FPLO) code [14] in the local spin-density approximation with orbital-polarization correction (LSDA+OP) [15]. The corresponding densities of states were displayed in Fig. 2a in Ref. [13] and the total magnetic moment of 1.9 $\mu_{\rm B}$/U at. was given in Table 2 of the same reference.

The computed FS of UCu_2Si_2 exists in three non-degenerate bands (no. 91-93). The FS sheet originating from the 92th band is visualized in Fig. 3 and it contains a small flat electron pillow, centred at the Z point of the tetragonal Brillouin zone (BZ) of the $ThCr_2Si_2$-structure type (Fig. 3a). A similar FS element has recently been detected in the de Haas–van Alphen experiment and ascribed to the δ orbit, being drawn on the FS sheet, calculated by the relativistic spin-polarized linearized augmented plane wave (RSPLAPW) band-structure method, and presented in Fig. 3c of Ref. [16].

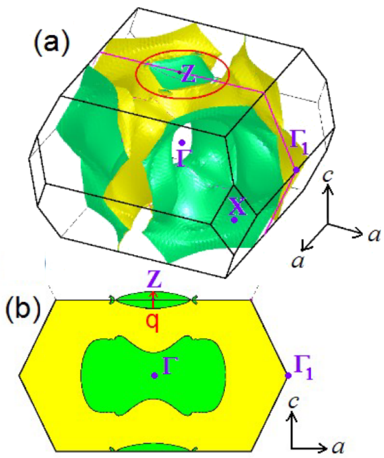

Fig. 3. The FS sheet in the 92th band of UCu_2Si_2 in the FM ordered state (along the c axis), computed using the LSDA+OP approach, drawn in the tetragonal BZ of the $ThCr_2Si_2$-type (a), and its section in ac-plane (b), where the red arrow denotes the nesting vector $\boldsymbol{q}$ = [0, 0, 0.116] for the spanning surfaces of the electron pillow, being centred at the Z point. Green (dark) and yellow (light) colours correspond to electrons and holes, respectively.

The ac plane section of our FS sheet, displayed in Fig. 3b, shows that the electron pillow has almost perfect nesting properties along the c axis with the nesting vector $\boldsymbol{q}$ = [0, 0, 0.116] (marked by the red arrow). It turns out that this vector and the magnetic propagation vector of the incommensurate SDW phase [5] have identical magnitude and direction. It supports a possibility of arising (e.g. under pressure) superconductivity mediated by the magnetic fluctuations, like it was proposed in the case of UGe_2 [12].

4. Conclusions

The electronic properties of UCu_2Si_2 have been studied here by the analysis of the electrical transport properties and the calculated Fermi surface topology results. This study establishes very clearly that the compound UCu_2Si_2 is well described by the UKL model in the case of a FM order with a large Curie temperature, which leads to a strong Kondo-ferromagnetic competition.

However, an interesting question remains: although our single crystal has revealed only one phase transition temperature at T_C = 103(1) K, we have some expectation (as found previously for UGe_2) as to the existence of the SDW fluctuations coexisting within all the range of the ferromagnetic ordering. However, as evidenced by neutrons, this SDW phase emerges only in the case of the temperature range $T_C < T < T_N$. The latter conjecture is detected from the present magnetoresistivity results as well as the specific heat data, which will be presented elsewhere. In support to this conjecture, we found also the nesting properties of the Fermi surface in agreement with the neutron diffraction data, from which the existence of the SDW phase was derived.

Acknowledgments

We thank to Z. Bukowski for single crystal growth and to D. Badurski for performing the electrical transport measurements as well as to A. Szajek for making available the FPLO results presented in Ref. [13].

References

[1] M. Kuznietz, H. Pinto, M. Melamud, *Phys. Rev. B* **51**, 16410 (1995).

[2] T.D. Matsuda, Y. Haga, S. Ikeda, A. Galatanu, E. Yamamoto, H. Shishido, M. Yamada, J.-I. Yamaura, M. Hedo, Y. Uwatoko, T. Matsumoto, T. Tada, S. Noguchi, T. Sugimoto, K. Kuwahara, K. Iwasa, M. Kohgi, R. Settai, Y. Õnuki, *J. Phys. Soc. Jpn.* **74**, 1552 (2005).

[3] T.D. Matsuda, Y. Haga, S. Ikeda, A. Galatanu, Y. Õnuki, *Physica B* **359-361**, 1069 (2005).

[4] R. Troć, Z. Bukowski, *Phys. Status Solidi B* **243**, 290 (2006).

[5] F. Honda, N. Metoki, T.D. Matsuda, Y. Haga, Y. Õnuki, *J. Phys., Condens. Matter* **18**, 479 (2006).

[6] R. Troć, A. Pikul, E. Colineau, to be published.

[7] N.B. Perkins, M.D. Núnez-Regueiro, B. Coqblin, J.R. Iglesias, *Phys. Rev. B* **76**, 125101 (2007).

[8] C. Thomas, A.S. da Rosa Simões, J.R. Iglesias, C. Lacroix, N.B. Perkins, B. Coqblin, *Phys. Rev. B* **83**, 014415 (2011).

[9] J. Schoenes, *J. Less-Common Met.* **121**, 87 (1986).

[10] E. Colineau, F. Wastin, J.P. Sanchez, J. Rebizant, *J. Phys., Condens. Matter* **20**, 075207 (2008).

[11] V.H. Tran, J.-C. Griveau, R. Eloirdi, W. Miiller, E. Colineau, *Phys. Rev. B* **82**, 094407 (2010).

[12] R. Troć, *Acta Phys. Pol. B* **34**, 407 (2003) and references therein.

[13] J.A. Morkowski, G. Chełkowska, M. Werwiński, A. Szajek, R. Troć, C. Neise, *J. Alloys Comp.* **509**, 6994 (2011).

[14] FPLO-5, improved version of the original FPLO code by Koepernik, H. Eschrig, *Phys. Rev. B* **59**, 1743 (1999); `http://www.fplo.de` .

[15] O. Eriksson, B. Johansson, M.S.S. Brooks, *J. Phys., Condens. Matter* **1**, 4005 (1989); the above OP implementation in FPLO.5.10-20 by C. Neise, M.Sc. Thesis, TU Dresden 2007; `http://www.ifw-dresden.de/institutes/itf/diploma-and-phd-theses-at-the--itf` .

[16] T.D. Matsuda, S. Ikeda, E. Yamamoto, Y. Haga, H. Shishido, H. Yamagami, R. Settai, Y. Õnuki, *J. Phys. Soc. Jpn.* **79**, 114712 (2010).