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Title

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Journal

ISSN

Authors

Friedemann, S
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et al.

Publication Date

DOI

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Peer reviewed

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Band-structure and anomalous contributions to the Hall effect of YbRh₂Si₂

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Abstract

We report on Hall effect measurements on YbRh₂Si₂ single crystals with different residual resistivity and on LuRh₂Si₂ single crystal. The temperature dependence of the linear-response Hall coefficient of YbRh₂Si₂ is described by the anomalous Hall effect and the normal contribution incorporating multi-band effects. Sample dependencies at low T are found and explained by slight changes in the charge-carrier concentrations.
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YbRh₂Si₂ is a stoichiometric heavy fermion (HF) compound showing non-Fermi-liquid (NFL) properties in a wide temperature range above the antiferromagnetic transition at $T_N = 70$ mK [1]. T_N is found to be continuously suppressed with small magnetic fields to $T = 0$ accessing the quantum critical point (QCP) [2]. The QCP in YbRh₂Si₂ is best described by the local scenario [3]. This is mainly supported by earlier Hall effect studies [4] in which the Hall effect of YbRh₂Si₂ was measured while tuning the material through the QCP. Here, the Hall coefficient R_H as a mirror of the Fermi surface volume was found to show a crossover which sharpens to a discontinuous jump if extrapolating $T \rightarrow 0$. It was concluded that the Fermi surface volume abruptly changes at the QCP. This crossover was followed up to 500 mK introducing a new energy scale which is confirmed by other transport properties as well as thermodynamic quantities [5]. In order to understand differences found in $R_H(T)$ of newer samples

we extended the measurements to samples of varying quality including the sample used in Ref. [4] and to the non-magnetic analog LuRh₂Si₂.

Single crystals of YbRh₂Si₂ and LuRh₂Si₂ were synthesized with an In flux-growth technique as described earlier [1]. All samples were polished to thin plates and prescreened via $\rho(T, B)$ to ensure In free samples. Samples of thickness t between 30 and 80 μm were contacted via spot welded gold wires. The current I was applied in the crystallographic ab-plane and the magnetic field B along the crystallographic c-axis of the samples inducing the Hall voltage V_{xy} perpendicular to I and B (see inset of Fig. 1). The Hall resistivity was derived from the asymmetric component of the field-reversed Hall voltage, $\rho_H(B) = t[V_{xy}(+B) - V_{xy}(-B)]/2I$. The comparison of the symmetric component with the transversal magnetoresistivity measured simultaneously was used as a consistency check. R_H was calculated in the low-field limit from the initial slope of the Hall resistivity, $R_H = (\delta\rho_H(B)/\delta B)_{B=0}$. Measurements down to 2 K were performed in a commercial PPMS, measurements between 17 mK and 6 K in a dilution refrigerator newly set up for these experiments.

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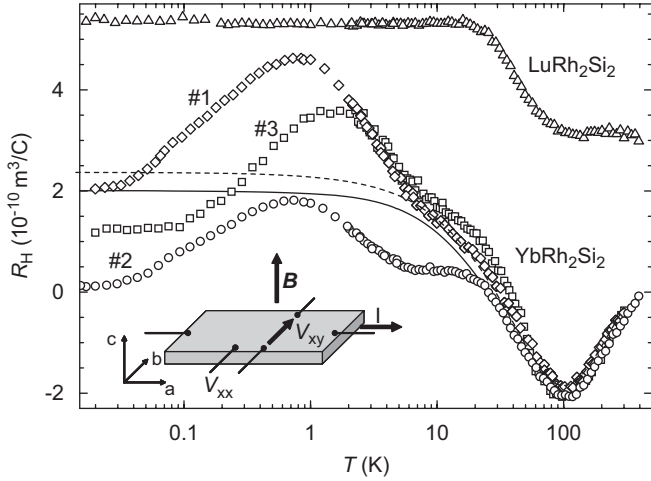*E-mail address:* Sven.Friedemann@cpfs.mpg.de (S. Friedemann).

Fig. 1. Initial-slope Hall coefficient of three selected $YbRh_2Si_2$ samples and of $LuRh_2Si_2$. The solid (dashed) line are fits of Eq. (1) to the data of sample 2 (1) above 25 (7) K, where R_H^n was assumed to be constant. At lower temperatures they are obtained by extrapolation according to Eq. (1) with C and R_H^n obtained from the high temperature fit. The inset sketches the setup.

Fig. 1 shows $R_H(T)$ between 17 mK and 400 K for selected $YbRh_2Si_2$ samples of different residual resistivity ratio, RRR (sample 2: RRR = 120 and 3: RRR = 40) including the very same sample used in Refs. [4,6] (sample 1: RRR = 70) which was remeasured in the new setup. Furthermore, the Hall coefficient of $LuRh_2Si_2$ is displayed.

The characteristics of $LuRh_2Si_2$ are typical of a non-magnetic intermetallic system. The resistivity ρ is linear in T above ≈ 100 K with $\rho(300 \text{ K}) = 20 \,\mu\Omega$ cm. The magnetoresistance is quadratic for small fields. All these properties are consistent with a simple metallic system.

In $LuRh_2Si_2$ $R_H(T)$ is positive at all T and constant below 20 K and above 100 K. Between these temperatures the Hall coefficient changes its value by a factor of 1.6. Band-structure calculations for $LuRh_2Si_2$ [7] reveal two hole-like bands at the Fermi energy. Therefore, we approximate the observed T dependence by a simple two-band model in the low-field limit [8] where $R_H(T)$ is the mobility weighted sum of two bands of positive charge carriers. The data are well described assuming one band dominating at high temperatures due to its high mobility arising from lower phonon scattering rates and the other band dominating the low temperature Hall coefficient by its enhanced mobility due to a lower scattering rate at residual scatterers. The crossover temperature between these limits is determined by the Debye temperature known from specific heat measurements. Surprisingly, very similar behavior of $R_H(T)$ has been observed in the non-magnetic La analogs of the Ce-115's [9].

A negative sample-independent $R_H(T)$ is found for all $YbRh_2Si_2$ samples at high temperatures, followed by a minimum at $T \approx 100$ K and a sign change at $T \approx 20$ K. However, below 25 K sample dependencies are obvious.

$R_H(T)$ exhibits a maximum at ≈ 1 K for all samples but with different absolute values and at slightly different temperatures. At lowest temperatures $R_H(T)$ saturates at different values R_H^0. Furthermore, for sample 2 of highest quality, a plateau between 7 and 13 K is found at a value quite close to R_H^0. For the other samples a shoulder is observed in this temperature range roughly pointing towards R_H^0 for each sample.

The Hall effect of HF compounds is usually the sum of a normal contribution, $R_H^n(T)$, reflecting the band-structure and an anomalous contribution due to skew scattering of the conduction electrons on the orbital f moment, $R_H^a(T) = C\rho(T)\chi(T)$, with χ the susceptibility and C a constant [10]:

$$R_H(T) = R_H^n(T) + R_H^a(T) = R_H^n(T) + C\rho(T)\chi(T). \quad (1)$$

Previously, the Hall effect of sample 1 was described by Eq. (1) with the normal contribution being constant and equal to the low-T saturation value, $R_H^n(T) = R_H^0$ [6].

However, for samples 2 and 3 this does not hold true. Fits of Eq. (1) with constant R_H^n to the high temperature data yield similar normal contributions which thus differ from R_H^0 (cf. solid line in Fig. 1). If we incorporate the multi-band effects observed in $LuRh_2Si_2$ we can understand $R_H(T)$ of these samples down to lowest T. The step observed for $LuRh_2Si_2$ is also present in $YbRh_2Si_2$. Particularly, sample 2 shows the same slope of $R_H(T)$ for $7 \text{ K} \leqslant T \leqslant 100$ K, even the step height is identical (although shifted by $-5 \times 10^{-10} \text{ m}^3 \text{ C}^{-1}$). Thus, $R_H(T)$ may be described by Eq. (1) if we take into account the T-dependent normal Hall coefficient seen in $LuRh_2Si_2$ and the constant C being lowered below the coherence temperature as often found in HF [10]. Furthermore, we are now able to account for the sample dependencies within the two-band model used for $LuRh_2Si_2$. Here, the low-T value R_H^0 strongly depends on the charge-carrier concentration n_l of the low-T dominating band. Thus, the different R_H^0 are reasonably explained by small deviations of n_l suggesting the normal contribution to be dominant below 100 K.

The dominance of $R_H^n(T)$ at low T is further supported by the absence of any scaling between ρ_0 and R_H^0 expected for the anomalous Hall effect in the $T = 0$ limit where $R_H^a(T = 0) = C\rho_0\chi(T = 0)$ with $\chi(T = 0)$ usually less sample dependent than ρ_0. The slight variation of n_l would also request for a scaling of ρ_0 and R_H^0 but this might be hidden by a change of the impurity concentration for different samples.

According to this analysis $R_H(T)$ is expected to be almost temperature independent below 10 K. By contrast the data show a pronounced maximum around 1 K superposed to the underlying constant contribution. We associate this maximum with the NFL properties of $YbRh_2Si_2$.

To conclude, the Hall effect of $YbRh_2Si_2$ is described by contributions of the anomalous and the normal Hall effect reflecting the band structure. The band-structure

effect is deduced by analyzing the Hall effect of $LuRh_2Si_2$ in terms of a two-band model. Below $100\,K$, the normal Hall effect dominates and is superposed by a broad maximum at $T \approx 1\,K$ assigned to the NFL properties. Sample dependencies are explained in the two-band model by small deviations of the charge-carrier concentration.

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