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Low temperature transport and thermodynamic properties of $YbPd_2Si$

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Abstract

A novel ternary compound has been found at the 1:2:1 position among the Yb–Pd–Si phases, where $YbPd_2Si$ crystallises in the ordered Fe_3C-structure. $YbPd_2Si$ is characterised by Kondo lattice features at higher temperatures and, presumably, antiferromagnetism at 2.1 K. A quasi-quartet crystal field ground state governs the physics at low temperature.

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The present investigation is devoted to Yb intermetallics, which in many respects are considered as hole-analogues to cerium-based compounds. Motivated by our discovery of heavy fermion superconductivity in $CePt_3Si$ we commenced a systematic exploration of RE–TM–Si compounds, where RE are rare earths (mostly Ce, Eu and Yb) and TM are noble metals (mostly Pd and Pt). In order to determine the relevant interaction mechanisms in $YbPd_2Si$, we have carried out susceptibility and isothermal magnetisation measurements, specific heat and electrical resistivity studies in an extended temperature and field range.

Single-phase $YbPd_2Si$ was synthesised by argon arc melting elemental ingots of >99.9 mass% purity. Vapour losses of Yb were carefully compensated by weighing samples before and after arc melting until phase purity was achieved and finally checked by EMPA. The crystal structure was determined from X-ray single crystal data and was found to be isotypic with a fully ordered Fe_3C type (space group Pnma). A sketch of this structure is shown in Fig. 1. The lattice parameters a, b, c in (Å) are 7.1775, 6.9335, 5.4406 for $YbPd_2Si$.

In general, physics of Ce and Yb based intermetallic compounds comes from a balance of the Kondo effect, the RKKY interaction and crystalline electric field (CEF) effects. Distinct hints to the Kondo effect in $YbPd_2Si$ are obvious from the temperature dependent resistivity $\rho(T)$, displayed in Fig. 2(a). The most important characteristics found at zero external field are a negative slope of $\rho(T)$ below about 20 K and a maximum at 8.5 K. While the former refers to the Kondo effect in the CEF ground state, the latter can be considered as a signature of coherence, originated from the periodic arrangement of the Yb ions in $YbPd_2Si$. The rapid decrease of the resistivity below that maximum results from the onset of long range magnetic order as evidenced by the anomaly of $d\rho/dT$ [inset of Fig. 2(a)]. Moreover, the pronounced change of the slope of $\rho(T)$ is a typical feature of a magnetic phase transition, in fine agreement with the heat capacity results (see below). The application of external fields causes an overall decrease of the electrical resistivity as well as a shift of the low temperature resistivity maximum to higher temperatures. These observations are typical features of Kondo lattices where the quenching of the Kondo interaction by external

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magnetic fields depletes the scattering intensity and thus reduces $\rho(T)$. We note that the change of the resistivity at lowest temperatures and at fields of 12 T reaches more than 50%.

The magnetic configuration of the Yb ion can be proven by susceptibility measurements $\chi(T)$, where data of a 1 T run are shown in Fig. 2(b). The almost linear temperature dependence of $\chi^{-1}(T)$ above about 50 K refers, in fact, to the magnetic state Yb-$4f^{13}$. A fit according to the modified Curie–Weiss law yields a temperature independent Pauli-like susceptibility $\chi_0 = 4 \times 10^{-5}$ emu/mol, an effective moment $\mu_{\rm eff} = 4.39\mu_B$ and the paramagnetic Curie temperature $\theta_p = -19.5$ K. The effective magnetic moment is close to the theoretical value associated with the Yb^{3+} state, i.e., $4.54\mu_B$. The slight curvature of the inverse magnetic susceptibility observed below 50 K is attributed to CEF effects. A negative paramagnetic Curie temperature follows also in terms of the Kondo effect.

Below about 2.1 K, magnetic order is obvious from the capacity data, $C_p(T)$ for $YbPd_2Si$ (compare Fig. 3). The inset of Fig. 3 displays the entropy gain up to 10 K, yielding at 10 K about 10 J/mol K, thus referring to a quasi-quartet as CEF ground state, with a splitting of the two low lying doublets by about 1 meV or smaller. Such a CEF driven configuration is rather rare in Yb-based compounds [1,2].

The anomaly right at the transition temperature is somewhat smaller than expected for ordering in a doublet as ground state and is supposed to be a consequence of the

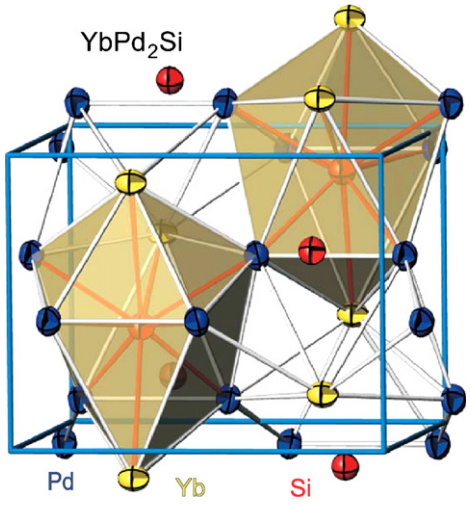

Fig. 1. Crystal structure of $YbPd_2Si$ with ordered Fe_3C-type. Bonds and polyhedra indicate the tetrakaidekahedral coordination $[Pd_6Yb_3]Si$ around the Si atom.

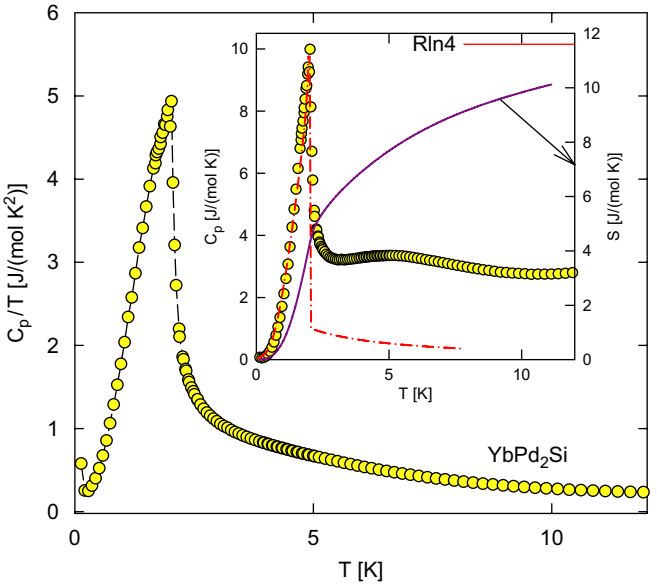

Fig. 3. (a) Temperature dependent specific heat C_p of $YbPd_2Si$ plotted as C_p/T vs. T. The upturn at lowest temperatures results from core contributions. The inset shows a $C_p(T)$ plot and the dashed-dotted line is a fit as described in the text. The solid line refers to the right axis and represents the entropy.

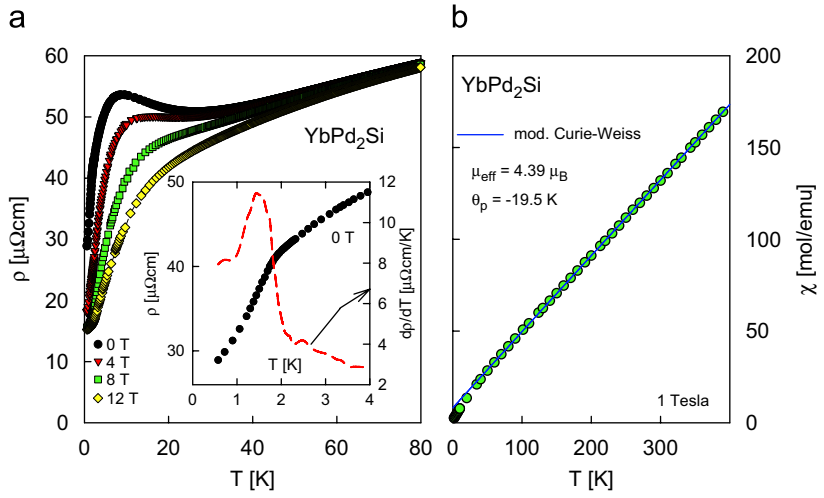

Fig. 2. (a) Temperature dependent electrical resistivity ρ of $YbPd_2Si$ for various external magnetic fields. The inset shows low temperature details of the 0 T measurement. (b) Temperature dependent magnetic susceptibility χ of $YbPd_2Si$ plotted as $1/\chi$ vs. T. The solid line is a least squares fit according to the modified CW-law.

Kondo effect, while the doublet ground state results from the CEF splitting. Considering the Kondo effect as the primary cause of the reduced specific heat anomaly, the resonant level model of Schotte and Schotte [3] can be used, and long range magnetic order is incorporated in terms of the molecular field theory [4]. Adjusting these models to $C_p(T)$ allows estimation of the Kondo interaction strength T_K. Best agreement between the experiment and the predictions of the model is revealed when taking the s–f interaction constant $J = 5.4\,K$ and $T_K = 1.18\,K$ (dashed-dotted line, inset of Fig. 3). Note that for $T_K = 0$, $T_{mag} = J/2$. The model used applies for a doublet as ground state and therefore fails to account for the low lying first excited CEF doublet, present in $YbPd_2Si$.

The Sommerfeld value γ follows from the above model as $480\,mJ/mol\,K^2$. The simultaneous presence of RKKY interaction and the Kondo effect reverses the well known relation $T_K \propto 1/\gamma$. Keeping the RKKY interaction constant while increasing T_K causes γ to rise within a limited range of the ratio J/T_K. If T_K is kept constant, an increasing coupling constant lowers the resulting γ.

In summary, novel $YbPd_2Si$ is a Kondo system exhibiting magnetic order below about 2 K. A slight volume expansion of the lattice is expected to drive the systems towards a magnetic instability at $T = 0\,K$.

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