Magnetic Order and SdH Effect in Half-Heusler Phase ErPdBi

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Single crystals of ErPdBi were grown from Bi-flux. The crystal structure of MgAgAs-type was confirmed using X-ray diffraction. Magnetization, magnetic susceptibility, electrical resistance and heat capacity measurements revealed an antiferromagnetic phase transition at \( T_N = 1.2 \) K. At high temperatures, the electrical resistance has a semiconducting-like character \((dR/dT < 0)\). The resistance starts decreasing with decreasing \( T \) below 15 K and shows a very sharp drop below \( T_N \) but remains finite down to 0.4 K. Hence, no obvious evidence of superconductivity was found in the electrical transport data. On the other hand, the real part of AC magnetic susceptibility is negative below \( T_C = 1.6 \) K and its imaginary component has a clear maximum at this temperature that might be associated with the onset of superconducting state. The electrical resistance revealed Shubnikov-de Haas oscillations in magnetic fields 8–33 T. Their amplitude decreases with increasing \( T \) and disappears above 10 K. Cyclotron mass determined from this dependence is 0.21 \( m_0 \).

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1. Introduction

An equiatomic compound ErPdBi crystallizes in a noncentrosymmetric structure of the half-Heusler MgAgAs-type (space group \( F\overline{4}3m \)) \cite{1}. Similar rare-earth (\( RE \)) based \( RExPdBi \) phases \cite{2–4} exhibit localized antiferromagnetic behavior below the ordering temperature \( T_N \sim 2\)–13 K. It has recently been proposed that some of these compounds can be considered as topological insulators (TI) \cite{5, 6}, i.e. analogs of the intensively studied Hg(Cd)Te and Bi\(_2\)Se\(_3\) systems. TI is a novel state of quantum matter having a full insulating gap in the bulk and topologically protected gapless surface or edge states on the boundary \cite{7}. The family of half-Heusler compounds includes not only metallic and semiconducting materials, but also superconducting compounds which exhibit band inversion. Such unique combination of superconductivity and band inversion, seen e.g. in LuPtBi \cite{8}, YPtBi \cite{9, 10} and LuPtBi \cite{11} makes these ternaries promising candidates for topological superconductors. Furthermore, a coexistence of superconductivity \((T_c = 1.22 \) K) and antiferromagnetic order \((T_N = 1.06 \) K) has recently been reported for a potentially topological compound ErPdBi \cite{12}. However, as stated by authors of Ref. \cite{12}, their single crystals may have been contaminated by an impurity phase PdBi\(_2\) superconducting below 1.7 K, and thus strongly influenced the observed physical properties of the samples studied.

2. Experimental details

High quality single crystals of ErPdBi were grown in Bi flux. The X-ray diffraction analysis revealed single phase with the MgAgAs-type cubic crystal structure and the lattice parameter of 6.589 Å, consistent with the previous reports \cite{1–4, 12}. Electrical transport and heat capacity measurements were performed in the temperature range from 0.4 K to 300 K using a Quantum Design Physical Property Measurement System (PPMS). Electrical resistance measurements in high magnetic fields up to 34 T were performed in a 10 ms pulse magnet. DC and AC magnetic susceptibility measurements were carried out in the temperature interval 0.5–1.8 K using a Quantum Design MPMS-XL magnetometer equipped with an helium3 refrigerator.

3. Results and discussion

The low-temperature dependence of the magnetic susceptibility of ErPdBi is shown in Fig. 1. Magnetic susceptibility was measured in zero-field-cooled (ZFC) and field-cooled (FC) regimes. Maxima in both \( \chi(T) \) curves indicate antiferromagnetic state below \( T_N = 1.2 \) K. The field variation of the magnetization (inset of Fig. 1) shows no hysteresis nor remanence, and linear \( \sigma(B) \) is typical for an antiferromagnet (abrupt change of slope at 2 T reflects a metamagnetic transition). The \( \chi_{ZFC}(T) \) and \( \chi_{FC}(T) \) curves split below the temperature of 1.65 K, which coincides with features in the temperature dependences of the AC magnetic susceptibility.

As can be inferred from Fig. 2, the real component \( \chi' \) of the AC susceptibility is negative below \( 1.6 \) K and saturates at a small positive value above \( 1.7 \) K. The imaginary component \( \chi'' \) has a maximum at 1.6 K, which does not move with changing the frequency of driving field. Following Ref. \cite{12}, these features can be associated with the onset of superconducting state in PdBi\(_2\) that is likely present in the single crystals studied here as a minor phase.

The low-temperature specific heat of ErPdBi (Fig. 3) exhibits a clear lambda-shaped anomaly at \( T_N = 1.2 \) K that manifests the antiferromagnetic phase transition. In applied magnetic field the peak in \( C(T) \) broadens

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Fig. 1. DC magnetic susceptibility versus temperature measured in ZFC and FC regimes in a field of 30 Oe. Inset: Magnetic field variation of the magnetization taken at 0.5 K with increasing (empty symbols) and decreasing (solid symbols) magnetic field.

Fig. 2. Temperature dependence of the real and imaginary (inset) AC magnetic susceptibility measured in zero DC field with a 0.027 Oe driving field of different frequency.

and shifts to lower temperatures, as expected for antiferromagnets.

Figure 4 displays the temperature dependence of the electrical resistance of ErPdBi. Above about 20 K, $R(T)$ exhibits a behavior typical of semimetals or narrow band-gap semiconductors, in line with the previous reports [2–4, 12]. Below the maximum near 15 K, the resistance becomes metallic-like. The magnetic ordering at $T_N = 1.2$ K results in a very abrupt decrease of the resistance in the ordered state.

In external magnetic field (see inset of Fig. 4), both the ordering temperature and the resistance drop below $T_N$ decrease, as expected for an antiferromagnet. These results are in perfect agreement with the DC magnetic susceptibility and specific heat data. The anomalies observed at 1.7 K in the AC magnetic susceptibility are not reflected in $R(T)$. Down to 0.4 K, the resistance of our single crystals of ErPdBi remains finite, thus not providing any distinct evidence for superconducting state.

In strong magnetic fields, the resistance of single-crystalline ErPdBi clearly shows Shubnikov – de Haas (SdH) oscillations (Fig. 5), reflecting high mobility of carriers. The SdH oscillations amplitude decreases with increasing temperature and no oscillations are observed for $T > 10$ K. A single oscillation frequency $f_{\text{SdH}} = 21$ T can be extracted from the fast Fourier transform spectra (inset of Fig. 5). The SdH oscillations frequency is directly

Fig. 3. The specific heat measured below 1.3 K in several magnetic fields.

Fig. 4. Electrical resistance as a function of temperature. Inset: Low-temperature resistance in zero and applied magnetic fields.

Fig. 5. Field dependence of the resistance at 2 K. Inset: fast Fourier transform (FFT) spectra of SdH oscillations.
pertained to the cross section $S_F$ of the Fermi surface in momentum space via the Onsager relation: $f_{SdH} = (h/2\pi c)S_F$ where $S_F = \pi k_F^2 / 4\pi$, $k_F$ is the Fermi vector, and $c$ stands for the electron charge. Assuming a 2D character of conductivity one can express the 2D surface carrier density as $n_{2D} = k_F^2 / 4\pi$. By substituting $f_{SdH}$, the Fermi vector $k_F$ is found to be $0.0252 \text{ Å}^{-1}$, that corresponds to the 2D carrier density of $5.01 \times 10^{-11} \text{ cm}^{-2}$. Furthermore, the temperature dependence of the SdH oscillations amplitude can be fitted to the Lifshitz-Kosevich dependence $\Delta R(T)/\Delta R(0) = \lambda(T)/\sinh(\lambda(T))$, where $\lambda(T) = 2\pi^2 k_F T m_{cyc}/(\hbar e B)$, and $m_{cyc}$ is the cyclotron mass [13]. For ErPdBi this analysis yielded $m_{cyc} = 0.21 m_e$, where $m_e$ is the free electron mass (see Fig. 6); $\Delta R$ was obtained by background subtraction from the resistance measured in the field range 8-32 T. The Fermi level is defined by $E_F = m_{cyc} V_F^2$, where the Fermi velocity $V_F$ is related to $k_F$ by $m_{cyc} V_F = k_F$. This yielded $E_F = 23.2 \text{ meV}$ above the Dirac point and $V_F = 1.39 \times 10^8 \text{ m s}^{-1}$.

4. Conclusions

We prepared high-quality single crystals of the half-Heusler compound ErPdBi and determined its low-temperature physical properties. At odds with the recent literature report [12], we have not find any clear-cut evidence for the superconducting state below $T_c = 1.22 \text{ K}$. Instead, our electrical transport, magnetization and heat capacity studies clearly revealed the antiferromagnetic order at $T_N = 1.2 \text{ K}$. Remarkably, this Néel temperature coincides with the reported $T_c$ value and is higher than $T_N = 1.06 \text{ K}$ determined in Ref. [12]. Our measurements indicated semimetallic character of the electrical transport in ErPdBi. Observation of the SdH oscillations confirmed the high quality of the single crystals studied. The electronic transport parameters obtained from the SdH oscillations analysis are similar to those reported in the literature for archetypal topological insulators.

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