

# Magnetic and Transport Properties of Possibly Topologically Nontrivial Half-Heusler Bismuthides RMBi (R = Y, Gd, Dy, Ho, Lu; M = Pd, Pt)

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High quality single crystals of some representatives of half-Heusler family were grown from Bi-flux. For single crystals characterization, X-ray diffraction and scanning electron microscopy techniques were used. The low-temperature physical properties of the synthesized crystals were determined by means of magnetization, magnetic susceptibility, electrical resistivity and heat capacity measurements. For each compound but LuPtBi, the electrical resistivity varies in a semimetallic manner at high temperatures, and exhibits a metallic character at low temperatures. LuPtBi is metallic in the whole temperature range studied. The bismuthides HoPdBi, LuPdBi, LuPtBi and YPtBi were found superconducting below the critical temperature  $T_c = 0.7, 1.8, 0.9,$  and  $0.96$  K, respectively. For the compounds GdPdBi, DyPdBi and HoPdBi, an antiferromagnetic ordering was found to set in below  $T_N = 12.8, 3.7,$  and  $1.9$  K, respectively. HoPdBi is thus an intriguing material in which both cooperative phenomena coexist.

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## 1. Introduction

Half-Heusler phases form a large family of materials, which crystallize with the noncentrosymmetric MgAgAs-type structure and exhibit a variety of physical properties. Thermoelectrics, superconductors, shape memory alloys, spintronic materials, topological insulators are just few examples of the observed characteristics, some of them useful for practical applications [1].

Rare-earth (R) containing bismuthides RMBi with M being palladium or platinum form a very exciting group of half-Heusler phases, as a few of them have been predicted theoretically to be topological insulators [2, 3]. Besides non-trivial topology, these compounds attract attention due to interesting combination of their physical behaviors. For example, coexistence of superconductivity and non-trivial topology could be a turning point in quantum computing [4, 5]. Remarkably, the superconductivity in these materials possibly has an unconventional character with mixed spin-singlet/spin-triplet pairing symmetry [6]. Most recently, a novel concept of antiferromagnetic topological insulator (AFTI) has been introduced for the RMBi phases, that combines non-trivial topology with long-range magnetic ordering [7].

In this article, we briefly review our experimental results obtained to date in the course of our comprehensive investigations of the RMBi compounds.

## 2. Experimental details

High-quality single crystals of the RMBi ternaries were grown in Bi flux. Purity of the elemental constituents

was R: 99.9 wt%, Pd: 99.99 wt%, Pt: 99.9 wt%, Bi: 99.999 wt%. Excess of flux was removed by centrifugation and then etching with nitric acid. X-ray diffraction performed on an Oxford Diffraction Xcalibur four-circle diffractometer confirmed the cubic MgAgAs-type crystal structure. The refined lattice parameter was  $a = 6.613, 6.634, 6.666, 6.565, 6.630,$  and  $6.570$  Å for HoPdBi, DyPdBi, GdPdBi, LuPdBi, YPtBi, and LuPtBi, respectively, in good agreement with literature data [8].

Chemical composition of the obtained single crystals was examined on a FEI scanning electron microscope (SEM) equipped with an EDAX Genesis XM4 spectrometer. The crystals were found homogeneous and free of foreign phases, with the stoichiometry very close to the equiatomic one.

Electrical transport and heat capacity measurements were performed in the temperature range from 0.4 K to 300 K and in magnetic fields up to 9 T using a Quantum Design PPMS platform. DC and AC magnetic susceptibility measurements were carried out in the temperature interval 0.5–20 K employing a Quantum Design MPMS-XL SQUID magnetometer equipped with an iHelium3 refrigerator.

## 3. Results and discussion

For all the single crystals studied but that of LuPtBi, the temperature dependences of the electrical resistivity  $\rho(T)$  (see Fig. 1a) indicate a semiconducting-like behavior at high temperatures. However, when temperature drops below a certain value  $T^*$ , different for distinct materials, a metallic behavior is observed ( $d\rho/dT > 0$ ). Only LuPtBi shows a metallic-like conductivity in the whole temperature range inspected. The overall behaviors of  $\rho(T)$  are similar to those reported for poly- [9] and single-crystalline [6, 10–13] samples.

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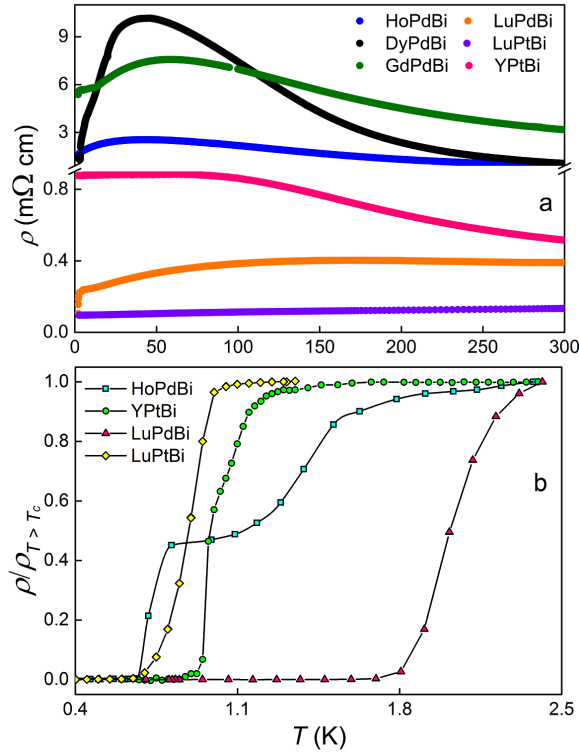


Fig. 1. (a) Temperature dependences of the electrical resistivity of single-crystalline RPdBi ( $R = \text{Ho, Dy, Gd, Lu}$ ) and RPtBi ( $R = \text{Y, Lu}$ ) measured above 2 K. (b) Normalized electrical resistivity data ( $\rho_T > T_c$ ) versus temperature measured for superconducting half-Heusler phases down to 0.4 K.

As displayed in Fig. 1b, YPtBi, LuPtBi, HoPdBi, and LuPdBi exhibit superconductivity below 0.96, 0.9, 0.7, and 1.8 K, respectively (see also our papers [14–16]). These values of the critical temperature agree fairly well with those reported before [6, 11–13]. The superconducting transitions have been confirmed for each compound by means of AC magnetic susceptibility measurements. As an example, Fig. 2 presents the temperature variations of the real,  $\chi'_{AC}$ , and imaginary,  $\chi''_{AC}$ , components of the AC susceptibility of single-crystalline HoPdBi. The onset of superconductivity at  $T_c = 0.9$  K can be easily identified on  $\chi'_{AC}(T)$  and  $\chi''_{AC}(T)$ , and the behavior of both components above  $T_c$  is fully in line with the antiferromagnetic ordering at  $T_N = 1.9$  K [15] (see also Fig. 3a).

The inset to Fig. 2 shows the AC driving field dependencies of  $\chi'_{AC}$  and  $\chi''_{AC}$  of HoPdBi taken at  $T = 0.49$  K. Both curves have shapes typical for type-II superconductors. The lower critical field,  $B_{c1}$ , derived from these data is as small as about 10  $\mu\text{T}$ . Similar magnitude of  $B_{c1}$  was reported for other half-Heusler superconductors [14, 17].

The DC magnetic susceptibility measurements carried out on single crystals of DyPdBi and GdPdBi revealed their antiferromagnetic ordering below  $T_N = 3.7$  and 12.8 K, respectively (see Fig. 3). These Néel

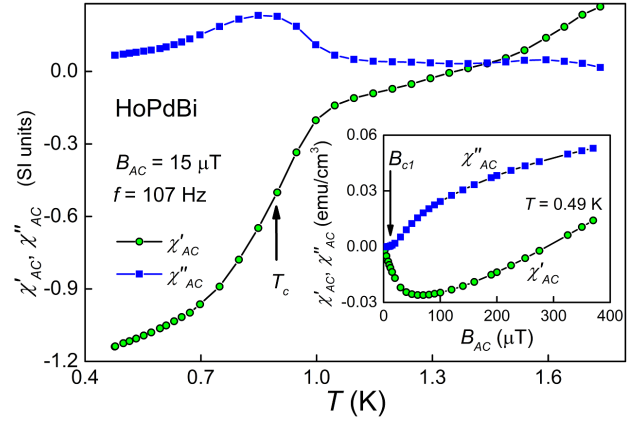


Fig. 2. Temperature dependences of the AC magnetic susceptibility of HoPdBi single crystals, measured in a field 15  $\mu\text{T}$  alternating with a frequency 107 Hz. The arrow indicates the critical temperature. Inset: real and imaginary components of the AC magnetic susceptibility versus driving field measured at 0.49 K. The arrow marks the lower critical field.

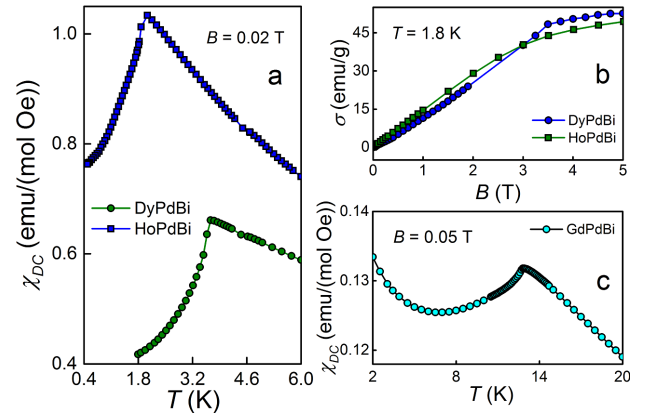


Fig. 3. (a) Low-temperature dependences of the DC magnetic susceptibility of single-crystalline DyPdBi and HoPdBi measured in an applied magnetic field of 0.02 T. (b) Field variation of the magnetization of DyPdBi and HoPdBi single crystals taken at 1.8 K. (c) DC magnetic susceptibility of single-crystalline GdPdBi versus temperature measured in a magnetic field of 0.05 T.

temperatures are close to those reported in the literature [9, 10, 13]. An antiferromagnetic ground state was found also for ErPdBi below 1.2 K [18] ( $T_N = 1.06$  K was reported in Ref. [19]).

At  $T = 1.8$  K, i.e. below  $T_N$ , the magnetization of single-crystalline HoPdBi and DyPdBi varies nearly linearly with increase of the magnetic field up to  $B = 2$  T and 3 T, respectively. In stronger fields, distinct bending in the  $\sigma(B)$  curves is observed (see Fig. 3b), which can be attributed to a kind of metamagnetism. No hysteresis effects nor remanence were found in the  $\sigma(B)$  data in the entire magnetic field range investigated.

The antiferromagnetic phase transitions in GdPdBi and DyPdBi manifest themselves as sharp  $\lambda$ -shaped anomalies in the temperature dependences of the spe-

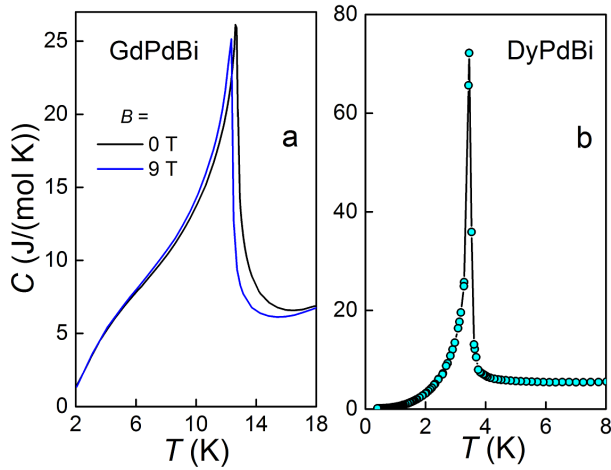


Fig. 4. Low-temperature variations of the specific heat of single-crystalline GdPdBi (a) and DyPdBi (b).

sific heat (see Fig. 4). Applied magnetic field has very weak impact on  $C(T)$  of GdPdBi; a tiny shift of  $T_N$  by only 0.3 K was found in a field of 9 T. As regards the superconducting half-Heusler phases, no anomaly in  $C(T)$  has been found near  $T_c$  for any of the investigated materials [14–16].

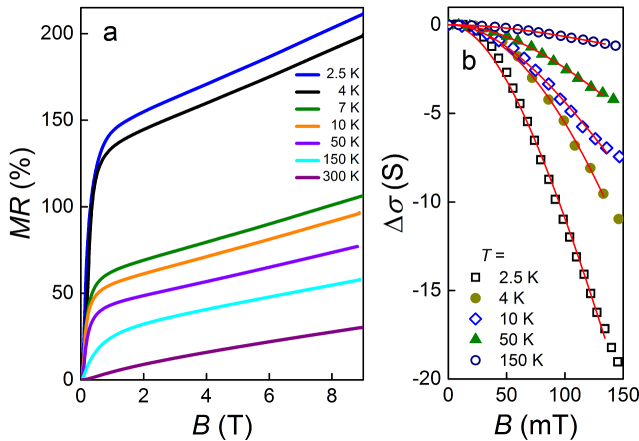


Fig. 5. (a) Transverse magnetoresistance versus magnetic field measured for single-crystalline LuPdBi at several temperatures between 2.5 and 300 K. (b) Low-field dependences of the conductivity isotherms of LuPdBi. The solid lines emphasize a weak antilocalization behavior. Figure adapted from Ref. [15].

The key objective in our on-going detailed studies on half-Heusler bismuthides is experimental verification of the hypothesis on their non-trivial topological nature. In line with the behavior expected for topological insulators, the electrical conduction in a few RMBi compounds was found governed by two parallel channels: semiconducting- and metallic-like, with the former one being negligible at low temperatures (for details see Refs. [14–16]). In weak magnetic fields, the transverse magnetoresistance (MR) of LuPdBi (Fig. 5), HoPdBi and

YPtBi [14–16] exhibits a sharp increase, identified as a weak antilocalization (WAL) effect, which is a characteristic feature of the Dirac materials [20]. In stronger magnetic fields, positive MR of LuPdBi and YPtBi is linear in a wide range of temperature from 2 to 300 K (see Fig. 5a). For the compounds containing magnetic rare-earth, MR is also non-saturating, yet negative at low temperatures, and positive at high temperatures [15].

Most remarkably, in strong magnetic fields, the low-temperature resistivity of single-crystalline LuPdBi, YPtBi and HoPdBi was found to exhibit periodic Shubnikov–de Haas (SdH) oscillations [14–16]. Numerical analyses of the SdH effect yielded several important characteristics of the Fermi surfaces and charge carriers in these materials. Key parameters are listed in Table I and compared to that of Refs. [6, 13]. For all the compounds investigated, the effective masses are very small, and the Berry phases are finite. Moreover, the derived values of the Berry phase are very close to those theoretically predicted for the Dirac fermions.

TABLE I

Parameters obtained from the SdH data of RMBi.

Material	Frequency [T]	Berry phase	Effective mass, $m_e$	Ref.
YPtBi	24.7	$0.7\pi$	0.15	[16]
	46	–	0.15	[6]
HoPdBi	78.5	$1.3\pi$	0.44	[15]
	143.9	$0.76\pi$	0.28	[15]
LuPdBi	11.9	$0.72\pi$	$< 0.5$	[13]

#### 4. Conclusions

At low temperatures, single-crystalline YPtBi, LuPtBi and LuPdBi exhibit superconductivity, while DyPdBi, GdPdBi and HoPdBi order antiferromagnetically. Most interestingly, the latter phase shows a coexistence of the two cooperative phenomena. All the compounds studied except LuPtBi are semimetals with two parallel conduction channels of semiconducting and metallic character. LuPtBi behaves like a poor metal in the whole range of temperatures covered.

For HoPdBi, LuPdBi and YPtBi, strong clues at their non-trivial topology were obtained from the electronic transport data. These include weak antilocalization effect, non-saturating magnetoresistance, as well as very small effective masses of charge carriers and non-zero Berry phases determined from the SdH oscillations.

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