Magnetism and superconductivity in non-centrosymmetric topological RPdBi half-Heusler semimetals

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Topological Insulators (TIs), lacking spontaneously symmetry-breaking ordered states, are characterized by the presence of gapless boundary modes with chirality. In the so-called Z2 two and three-dimensional systems, these topologically protected metallic states have the potential for realizing new technologies in spintronics and quantum computation. Besides the intriguing topological boundary states per se, the combination of topologically ordered and symmetry-breaking ordered states such as superconductivity and magnetic order gives rise to new and exotic collective modes in topologically non-trivial materials. In particular, antiferromagnetism breaks time reversal and translational symmetries simultaneously, but can be preserved together, yielding a new, antiferromagnetic TI [1]. Despite extensive studies on bismuth-based TI materials, only a few materials have been identified that may harbor the combination of symmetry-breaking and topological phases.

One such promising candidate class of materials for the realization of combined topological and symmetry-breaking orders is the family of cubic *R*PdBi (*R*=rare earth) half-Heusler compounds [2]. These compounds are located at the border between topologically trivial and non-trivial electronic structure, allowing the band inversion strength to be tuned via atomic number, lattice density, and spin-orbit coupling strength. The *R* ions occupy a face-centered-cubic (fcc) lattice that renders magnetic structures ideal for antiferromagnetic TI's, while the superconductivity that emerges in this non-centrosymmetric crystal structure is exotic, providing unique opportunities to investigate the interplay of these states not only with each other but also with TI properties.

We have performed a systematic study of the superconductivity and magnetism in polycrystalline and single crystals of the half-Heusler series *R*PdBi (*R* = Y, Sm, Gd, Tb Dy, Ho, Er, Tm, and Lu) using magnetization, susceptibility, specific heat, charge transport, and neutron diffraction [3].

The 4f electrons are expected to be localized and this has been confirmed by bulk measurements, which can be simply described by crystal-field-split free R^{3+} ion moments. Fig. 1a shows the neutron magnetic diffraction pattern for DyPdBi on a powdered sample of crushed single crystals, with strong magnetic Bragg peaks corresponding to half-integral reflections of an fcc type-II antiferromagnet. This magnetic structure is characterized by a doubling of the simple fcc Dy unit cell along all three crystallographic directions as illustrated in the inset of Fig. 1b, with ferromagnetic layers stacked antiferromagnetically along the [111] direction, a magnetic symmetry of particular interest for topological antiferromagnetism [1]. The *R* = Tb and Ho materials exhibit the identical spin structure. A mean-field fit of the temperature dependence of the intensity of the (1/2, 1/2, 1/2) Bragg peak (Fig. 1b) establishes the antiferromagnetic transition temperature $T_N = 4.9$ K for a single crystal of TbPdBi, in excellent agreement with the transport and magnetic measurements and previous measurements on powders [4].

The superconductivity in *R*PdBi is revealed by low temperature charge transport and magnetic measurements, as summarized in the phase diagram of Fig. 2 where the superconducting transition temperature T_C and T_N are plotted as a function of the de Gennes factor $dG = (g_J-1)^2 J(J+1)$. Here g_J is the Landé factor and J is the total angular momentum of the R^{3+} ion Hund's rule ground state. T_N clearly scales well with *dG* for *R*PdBi, which indicates a Ruderman-Kittel-Kasuya-Yoshida (RKKY) exchange interaction between the conduction electrons and the local magnetic moments that induces the long-range magnetic order. On the other hand, T_C is suppressed linearly with *dG*, which indicates that the magnetic R^{3+} ions break the superconducting pairs. This coexistence of magnetism and superconductivity in this system serves as a prototype platform to elucidate the coupling of topological order with symmetry-breaking states.

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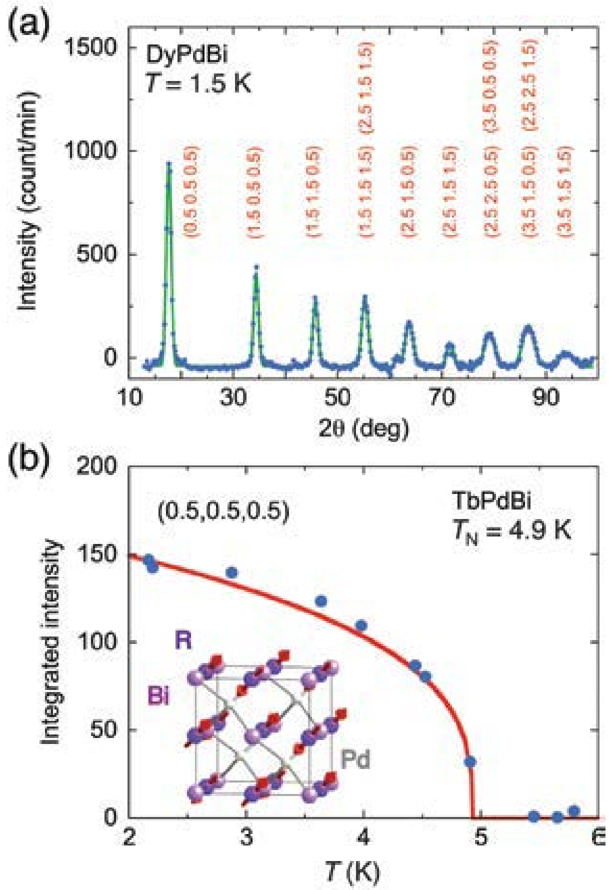

FIGURE 1: Antiferromagnetic order characterized by elastic neutron diffraction. (a) Low temperature magnetic diffraction pattern of DyPdBi obtained by subtracting the background data (18 K) from low temperature data (1.5 K). Labels indicate the series of half-integer antiferromagnetic peaks. (b) Intensity of the (1/2, 1/2, 1/2) magnetic Bragg peak for single-crystal TbPdBi. Solid curve is a mean-field fit to the data, and the inset shows a schematic of the antiferromagnetic spin structure.

In summary, we have investigated the coexistence of magnetism and superconductivity in the single-crystal *R*PdBi series. The magnetic rare earth members investigated so far exhibit an antiferromagnetic state characterized by ferromagnetic planes of spins stacked antiferromagnetically along the [111] direction, induced by the RKKY interaction between conduction electrons and localized moments. All *R*PdBi members except GdPdBi are superconductors. The anticorrelation between the magnetism and superconductivity is revealed by the scaling with the de Gennes factor, indicating *R*PdBi not only to be a new family of interesting magnetic superconductors, but together with their topological properties promise to be prototype systems to elucidate the emergence of novel quantum states of matter.

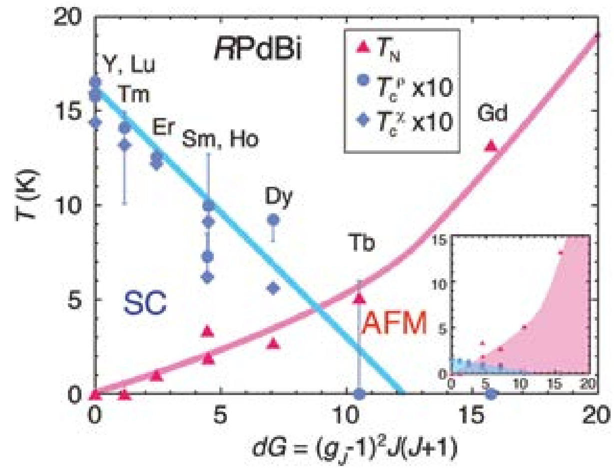

FIGURE 2: Phase diagram of the *R*PdBi series, demonstrating the evolution of the superconducting and antiferromagnetic states as a function of de Gennes factor $dG = (g_J\text{-}1)^2 J(J+1)$. The superconducting transition T_c (blue) is obtained from the midpoint of the resistive transition (circles; upper and lower error bars indicate onset and zero resistance) and the onset of diamagnetism in ac susceptibility (diamonds), and Néel temperatures T_N (red triangles) are obtained from dc magnetic susceptibility. The plotted T_c is scaled by a factor of 10, and solid lines are guides to the eye. Note that T_c (T_N) for SmPdBi is lower (higher) than that for HoPdBi. Inset: unscaled T_c and T_N versus *dG*.

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