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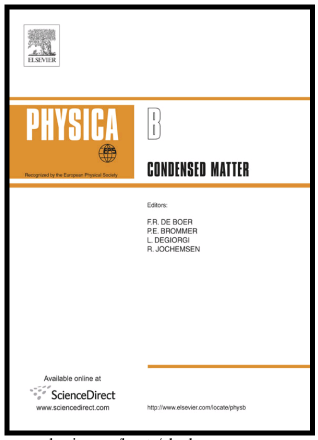

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Magnetic structures of R_EPdBi half-Heusler bismuthides (R_E= Gd, Tb, Dy, Ho, Er).

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Abstract

We present results of neutron diffraction on single crystals of several equiatomic ternary compounds of rare-earth elements with palladium and bismuth, crystallizing with cubic MgAgAs-type structure (half-Heusler phases). Band structure calculations showed that many members of that family possess electronic band inversion, which may lead to occurrence of topological insulator or topological semimetal. But even for the compounds without intrinsic band inversion another way of topologically non-trivial state realization, through a specific antiferromagnetic order, has been theoretically proposed.

Our results show that the antiferromagnetic structures of all studied bismuthides are characterized by the propagation vector, allowing for antiferromagnetic topological insulator state. Therefore, the antiferromagnetic representatives of half-Heusler family are excellent candidates for extended investigations of coexistence of superconductivity, magnetic order and non-trivial topology of electronic states.

Keywords: half-Heusler phases, topological insulators, magnetic structure, rare-earth compounds, neutron diffraction

1. Introduction

Equiatomic ternary compounds of rare-earth elements with palladium and bismuth, crystallizing with the cubic structure of MgAgAs-type, belong to the family of half-Heusler phases intensively studied since band structure calculations have shown that many of them possess band inversion prerequisite for topological non-triviality of electronic states, which may lead to formation of topological semimetal [1]. Among those bearing rare-earth with patially filled f-shell, the band inversion has been shown for ErPdBi and HoPdBi [2, 3], whereas for GdPdBi, DyPdBi and TbPdBi lack of such inversion has been suggested, based on their lattice parameters exceeding a "critical value" of 6.62 Å [4]. Half-Heusler compounds R_EPdBi (with R_E= Gd, Tb, Dy, Ho, Er) have been studied by means of magnetization, electrical transport and heat capacity measurements in wide ranges of temperature and magnetic field. All members of that group are semimetals and order antiferromagnetically at Néel temperatures of 12.8, 5.1, 3.5, 1.9 and 1.1 K, respectively [2, 3, 4, 5, 6, 7]. At temperatures below ≈ 100 K magnetoresistivity of all these compounds is negative. Moreover, in phases with R_E= Dy, Ho and Er the antiferromagnetic order coexists with superconductivity most likely of unconventional nature (due to their common non-centrosymmetric crystal structure and very low carrier densities) [2, 3, 4, 5]. In ErPdBi and HoPdBi clear Shubnikov-de Haas oscillations were observed at low temperatures [3, 5, 6]. Small effective masses and non-trivial Berry phases were extracted from these oscillations, which gave a strong argument in favor of topologically non-trivial properties of those compounds, in agreement with estimations given in Ref. [4], based on lattice constant values.

We present results of single-crystal neutron diffraction indicating that the antiferromagnetic structures of all studied bismuthides are characterized by the $(^1/_2, {}^1/_2, {}^1/_2)$ propagation vector, conforming to the theory of antiferromagnetic topological insulator (AFTI) [8], which proposes that topologically non-trivial electronic states may appear in materials with specific magnetic structures, due to preservation of a combination of two individually broken symmetries: time-reversal symmetry and crystal translational symmetry. Thus, these half-Heusler bismuthides give a pefect playground for extended investigations of coexistence of superconductivity, antiferromagnetism and non-trivial topology of electronic states.

2. Methods

High-quality single crystals of the R_EPdBi ternaries were grown in Bi flux. Purity of the elemental constituents was R_E: 99.9 wt%, Pd: 99.99 wt%, Bi: 99.999 wt%. Excess of flux was removed by centrifugation and etching with diluted nitric acid. X-ray diffraction performed on an Oxford Diffraction Xcalibur four-circle diffractometer or an

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