Experimental report

02/05/2022

Proposal: 5-53-305 **Council:** 10/2020

Title: Structural investigation of a possible magnetically-induced Weyl Semi-Metal YbMnSb2

Research area: Physics

This proposal is a continuation of 5-41-1049

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Samples: YbMnSb2

Instrument	Requested days	Allocated days	From	To
D3 Low field <1T	4	4	25/02/2021	01/03/2021

Abstract:

The antiferromagnet YbMnSb2 has recently been identified as a candidate Weyl semi-metal created by a very specific type of magnetic order. We have studied single crystals of YbMnSb2 on D10 and have observed anomalies above 300 K which point to the presence of Weyl fermions. We propose to use polarized neutrons to confirm whether or not YbMnSb2 hosts these exotic quasi-particles or not.

Topological semimetals are materials whose electronic bands have a linear dispersion in the vicinity of the Fermi energy. Examples include crystals where the valence and conduction bands meet at discrete points (as in a Dirac or Weyl semimetal) or along a one-dimensional curve in **k**-space (in the case of nodal line semi-metals). These systems can host fermions that mimic the behaviour of massless fermions and are robust against perturbations due to the protection afforded by the topology of the electronic band structure.

The exploration of magnetic materials with topologically non-trivial electronic band structure has become a key topic of quantum materials physics. The goal of our research is to find novel materials where the electronic states can be controlled by their magnetic order. Recently, $YbMnSb_2$ has been proposed as such a candidate, where the topology of the electronic bands near E_F depend on the spin-configuration of the Mn sub-lattice. The tetragonal crystal structure of $YbMnSb_2$ is described by space group P4/nmm and the unit cell, includes a square sub-lattice of Sb atoms which host the topological fermions. The magnetism is contained in $MnSb_4$ layers.

Depending on whether $YbMnSb_2$ displays G-type, C-type, or canted C-type AFM order, the electronic bands are predicted to give rise to a gapped Dirac crossing, a nodal-line dispersion, or Weyl nodes, respectively. Yet, only Weyl nodes benefit from the topological protection. Hence, it is essential to determine the magnetic order of the Mn sublattice in order to ascertain the nature of the topological fermions in $YbMnSb_2$.

Very recently, we investigated the magnetic order in $YbMnSb_2$ by single crystal neutron diffraction on D10. We confirmed the existence of a dominant AFM component to the magnetic order with propagation vector q = (1,0,0) for temperatures below T_N = 345K, but we also observed anomalies in some weak (00L) Bragg peaks above ~250 K. The (001) and (002) intensities increase by about 5% from 300 to 400K, whereas there is no corresponding increase in the (200) peak.

These anomalies could be structural in origin, but they could also be due to a weak ferromagnetic (FM) moment which could condense into the canted C-AFM structure for $T < T_N$. In fact, a similar anomaly was observed in neutron diffraction from $SrMnSb_2$, and was interpreted as long-range FM order below T_C = 565K.

To distinguish these possibilities, we performed neutron diffraction with a half-polarized setup on D3 in order to separate any magnetic contribution to the reflections which show the anomalous behaviour. We focused on a small set of Bragg peaks in the (H0L) scattering plane which have weak nuclear contributions and which are predicted to have a magnetic contribution in the canted structure. An FM component may depolarize the beam, which would be a clear indication of FM order, but by cooling the sample in a magnetic field we enforced a single FM domain and detect the FM component quantitatively via the nuclear–magnetic interference term in the cross-section.

The results were decisive and we could exclude FM order on the Mn sublattice.