Experimental report

22/08/2019

Proposal: **5-41-975**

Council: 4/2018

Title: Magnetic structure of the candidate Weyl semi-metal Mn3Ge

Research area: Physics

This proposal is a new proposal

Main proposer: **Andrew Timothy BOOTHROYD**

Experimental team: Jian Rui SOH
Henrik JACOBSEN

Local contacts: Navid QURESHI

Samples: Mn3Ge

Instrument	Requested days	Allocated days	From	To
D3 CPA	3	4	27/09/2018	01/10/2018
ORIENTEXPRESS	0	1		

Abstract:

We propose to investigate the antiferromagnetic structure of Mn3Ge, a candidate magnetic Weyl semi-metal, by spherical neutron polarimetry. The magnetic structure is non-collinear, and we aim to determine which of several theoretically proposed structures is the right one. We also aim to search for the existence of a weak canted ferromagnetic component whose direction determines whether or not the Weyl point exists.

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In this work, the antiferromagnetic (AFM) structure of Mn_3Ge was investigated by spherical neutron polarimetry (SNP) to determine which of the theoretically proposed magnetic structure, as shown in Fig. 1, best describes the magnetic order of the Mn sublattice.

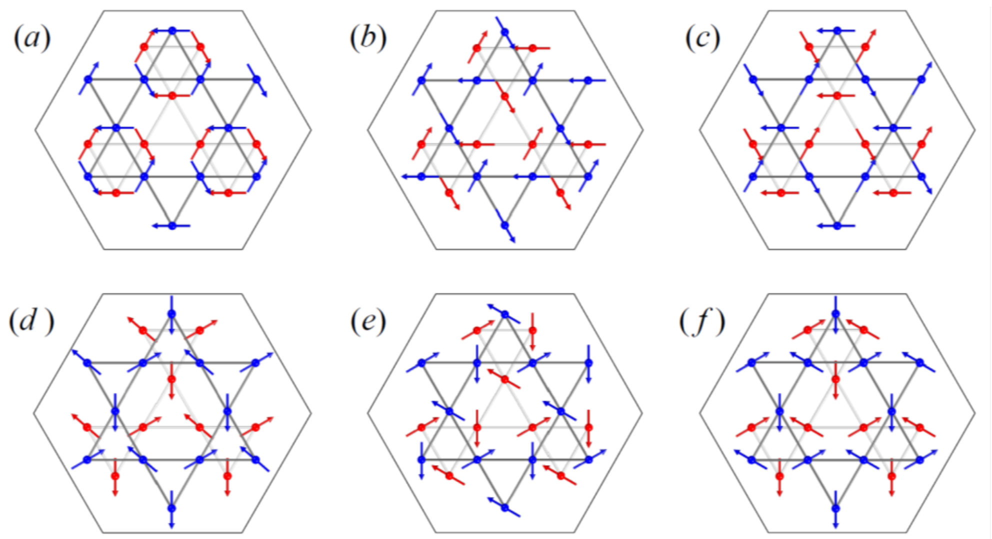

Figure 1. (a)-(f) various spin configurations of manganese moments adapted from [1]. The red and blue spheres correspond to Mn ions residing at Wyckoff position 6*h* with z = 1/4 and 3/4 respectively. Here, the Ge atoms are omitted for clarity.

Elastic neutron scattering of Mn_3Ge was performed on the D3 diffractometer in the horizontal scattering geometry with Henrik Jacobsen and Navid Qureshi, who is the beamline scientist. The crystal was initially mounted with the *b*-axis vertical to access the (h,0,l) reflections and was subsequently rotated by 90°, with the *c*-axis vertical, to study the (h,k,0) family of peaks [See Fig. 2].

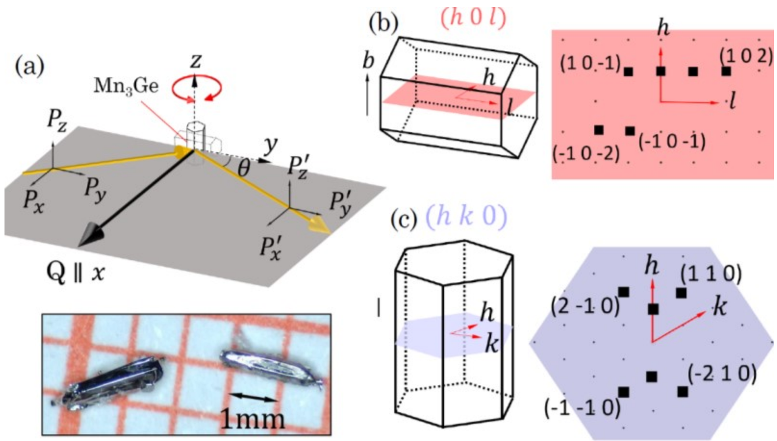

Figure 2. (a) The experimental set-up of the SNP of Mn_3Ge in the horizontal diffraction geometry. The insert shows single crystals obtained by the flux growth. (b), (c) Depicts the crystal orientations with *b*- and *c*-axis vertical, respectively, to access the (h,0,l) and (h,k,0) family of peaks. The reflections that were studied in this work are labelled with black squares.

The full polarisation matrices for the various reflections are shown in Fig. 3. The panels (a) and (c) correspond to measurements performed in the (h,0,l) and (h,k,0) planes respectively. For each reflection, I present the 9 elements of the measured matrix P_{ij} from left to right, P_{xx}, P_{xy}, P_{xz}, P_{yx}, P_{yy}, P_{yz}, P_{zx}, P_{zy} and P_{zz}. I find that the neutrons suffers from negligible depolarisation. This is best exemplified in the matrix elements P_{zz} for the (1,0,0)* reflection in Fig.3(a) and P_{yy} for peaks (1,0,0), (-2,1,0), (1,1,0)*, (-1,-1,0) in Fig.3(c) which are all almost unity.

Using the Mag2Pol program [4], we set up the 6 different magnetic structure models depicted in Fig. 1. Magnetic domains were also incorporated in each spin configuration model (giving rise to three domains) where all of the in-plane Mn moments in each domain are rotated by $\pm 120^{o}$ about the *c*-axis relative to those in the other two domains. For each model (a)-(f), I calculated the associated 9 matrix elements for all of the measured reflections and refined the domain population in a least-squares fit to the measured polarisation matrices of all the reflections. Models (a) – (d) can all be excluded, leaving us with (e) and (f) to consider.

I present the calculated polarisation matrices for both spin configurations in Fig. 3. For the (h,0,l) reflections, there is strong agreement between the measured and calculated P_{ij} [Fig.3(a),(b)]. However, as the calculated matrix elements from both models are very similar, it is difficult to ascertain, solely based on the measurements in the (h,0,l) plane, which model uniquely describes the magnetic structure of Mn_3Ge.

This ambiguity can be resolved by considering the (h,k,0) reflections. For instance in model (e), there are disparities between the measured and calculated P_{xy} and P_{zy} matrix elements for the (-2,1,0)*, (1,1,0) and (2,-1,0) reflections [Fig. 3(c)]. Conversely, this discrepancy is not seen in model (f), which fit the measured matrices very well [Fig.3d)]. This strongly suggests that the Mn^{2+} moments in Mn_3Ge orders with a magnetic structure shown in Fig. 1(f).

References

[1] P. J. Brown *et al.,* J. Phys. Condens. Matter **2** 9409-9422(1990)
[2] S. Tomiyoshi, et al., J. Mag. Mag. Mat. **31**-**34**, 629-630 (1983)
[3] T. Nagamiya et al. Sol. State. Comm. **42**, 385 (1982)
[4] N. Qureshi, J. Appl. Crystallogr. **52**,(2019)

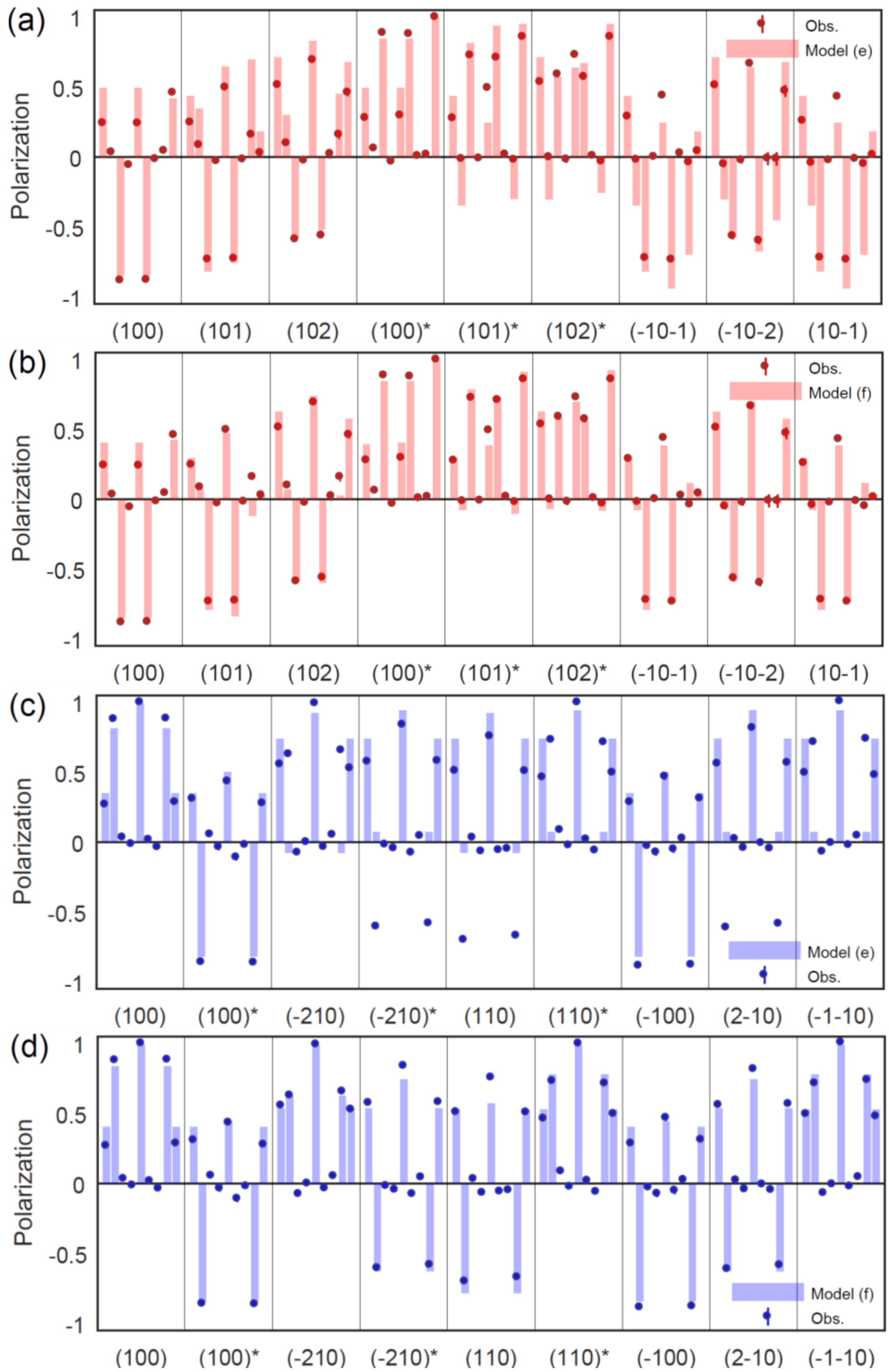

Figure 3. Comparisons between observed and calculated polarisation matrix elements P_{ij} for the Bragg peaks. Panels (a) and (c) correspond to model (e) for the (h,0,l) and (h,k,0) planes respectively. The corresponding panels for model (f) is in (b) and (d). For each reflection, the symbol and bar represent P_{xx}, P_{xy}, P_{xz}, P_{yx}, P_{yy}, P_{yx}, P_{zx}, P_{zy} and P_{zz} from left to right. (* These reflections were repeated with the incident and scattered polarisation reversed.)