Magnetic structure of the possible antiferromagnetic topological insulator GdBiPt

N. R. Lee-Hone,[1] D. H. Ryan,[1] R. A. Müller,[2] and A. D. Bianchi[2]
[1)] *Physics Department and Centre for the Physics of Materials, McGill University, 3600 University Street, Montreal, Quebec, H3A 2T8, Canada*
[2)] *Département de Physique, Univerisité de Montréal, Montréal H3C 3J7, Canada*

In 2010, Mong *et al.*[1] described the new antiferromagnetic topological insulator (AFTI) class of materials in which time-reversal and translational symmetry are broken, but their product is conserved. The orientation of the magnetic moment may lead to symmetry breaking, which induces spin-orbit coupling resulting in a non-trivial topological phase. This spin-orbit term is maximal if the moments are aligned ferromagnetically in (1 1 1) planes which are stacked antiferromagnetically along the body diagonal. Half-Heusler compounds have been suggested as possible candidates for this class of materials. In particular, Mong *et al.*[1] proposed that GdBiPt has the required properties.

GdBiPt crystallizes in the face centered cubic MgAsAg-type structure with space group $F\bar{4}3m$ (No. 216). The Gd, Bi, and Pt atoms occupy the *4a* (0, 0, 0), *4d* (3/4, 3/4, 3/4), and *4b* (1/2, 1/2, 1/2) sites.

Previous x-ray resonant magnetic scattering experiments,[2] were unable to determine the complete magnetic structure of GdBiPt, but did rule out the moments being along the [1 1 1] direction. To verify whether GdBiPt satisfies the required magnetic structure for an AFTI, a direct measurement of the moment direction via powder neutron diffraction was undertaken.

The neutron diffraction pattern taken at 20 K (top panel of figure 1), well above the Néel temperature, shows only nuclear reflections. The pattern can be refined with the expected MgAsAg-type structure. On cooling to 3.6 K the gadolinium moments order and several magnetic, reflections appear (middle panel of figure 1). All of the magnetic peaks can be indexed as $(\frac{2n-1}{2}\ \frac{2n-1}{2}\ \frac{2n-1}{2})$ reflections with n =1, 2, ..., indicating that the magnetic unit cell is doubled along the [1 1 1] direction of the crystallographic cell. Plotting the intensity of the first magnetic peak against temperature in figure 2 gives a Néel temperature of 9.41(14) K, in agreement with $T_N = 9.55(4)$ K determined from ^{155}Gd Mössbauer measurements on the same sample. The transition temperature is slightly higher than the previously reported values of 8.6 K[2] and 9 K[3].

The BasIreps program (part of the Fullprof Suite[4]) was used to find the basis functions of the irreducible representations of the $F\bar{4}3m$ space group with $\mathbf{k}=[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$. Two sets of basis functions were found, and the real and imaginary components are shown in table I. The first set of basis functions places the gadolinium moments along the body diagonal of the cubic structure. The $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$ peak is forbidden in this configuration, but it is clear from the 3.6 K pattern in figure 1 that this is

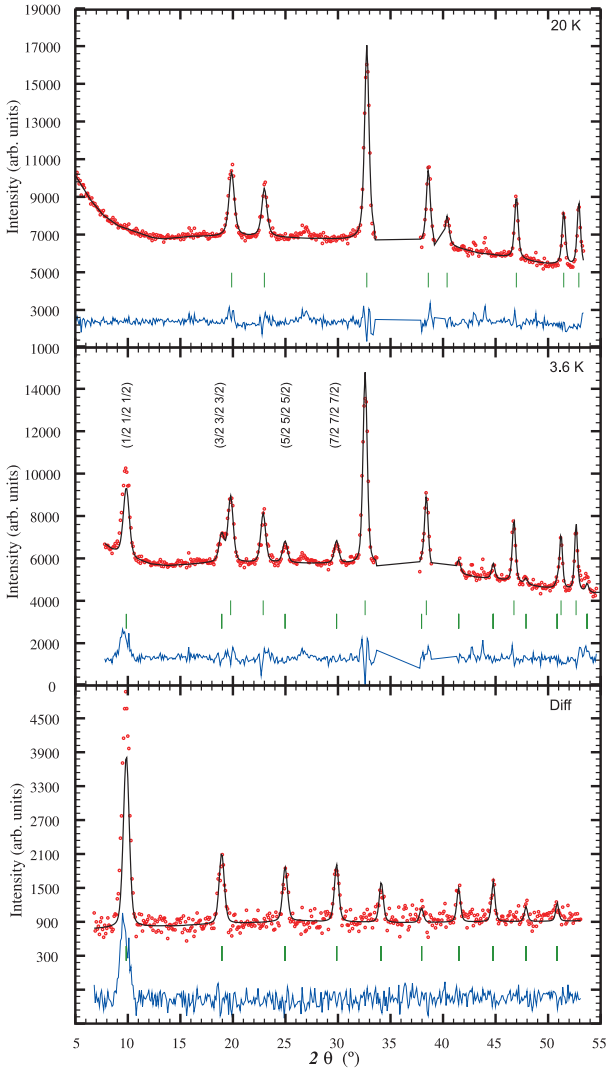

FIG. 1. Neutron powder diffraction patterns for GdBiPt taken above (20 K, top panel) and below (3.6 K, middle panel) the Néel temperature. The bottom panel shows the fit to the difference between the 3.6 K and 20 K patterns, which only has magnetic peaks. The solid line through the data is a the refinement while the solid line below each pattern shows the residuals. In the 20 K pattern (top), the bragg markers are for the nuclear contribution. In the 3.6 K pattern (middle), the first row of bragg markers is the nuclear contribution, and the bottom row is the magnetic contribution. Finally for the difference pattern (bottom), the bragg markers are for the magnetic phase only.

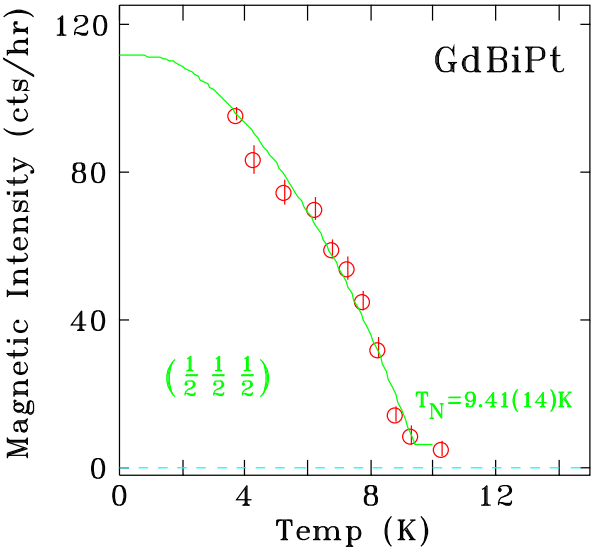

FIG. 2. The intensity of the first magnetic peak $(\frac{1}{2}\ \frac{1}{2}\ \frac{1}{2})$ plotted as a function of temperature. The solid line is a fit to a squared J=$\frac{7}{2}$ Brillouin function to find the Néel temperature.

the strongest of the observed magnetic peaks. We can therefore immediately rule out this structure, in agreement with the aforementioned x-ray resonant magnetic scattering experiments.[2]

	Set 1	Set 2	
BASR	(1 1 1)	(1 -0.5 -0.5)	(-0.5 1 -0.5)
BASI	(0 0 0)	(0 -0.866 0.866)	(-0.866 0 0.866)

TABLE I. Real (BASR) and imaginary (BASI) components of the basis vectors for the two possible magnetic structures generated by BasIreps.

The second set of basis functions contains two equivalent basis vectors. Since the structure is cubic, it is impossible to distinguish them, so the first was chosen for the refinement. The refinements are shown in the middle and bottom panels of figure 1.

The magnetic moments are perpendicular to the propagation vector and form ferromagnetic sheets which are coupled antiferromagnetically along the [1 1 1] body diagonal, as shown in figure 3. The Gd moment was found to be $\mu_{Gd} = 6.1(2)\ \mu_B$ at 3.6 K, which extrapolates to 6.7(2) μ_B at T=0 K, close to the expected value of 7 μ_B. We thus conclude that GdBiPt adopts the required magnetic structure for an AFTI.

[1]R. S. K. Mong, A. M. Essin, and J. E. Moore, Phys. Rev. B **81**, 245209 (2010).
[2]A. Kreyssig, M. G. Kim, J. W. Kim, D. K. Pratt, S. M. Sauerbrei, S. D. March, G. R. Tesdall, S. L. Bud'ko, P. C. Canfield, R. J. McQueeney, and A. I. Goldman, Phys. Rev. B **84**, 220408 (2011).
[3]P. C. Canfield, J. D. Thompson, W. P. Beyermann, A. Lacerda, M. F. Hundley, E. Peterson, Z. Fisk, and H. R. Ott, Journal of Applied Physics **70**, 5800 (1991).
[4]J. Rodriguez-Carvajal, Physica B **192**, 55 (1993).

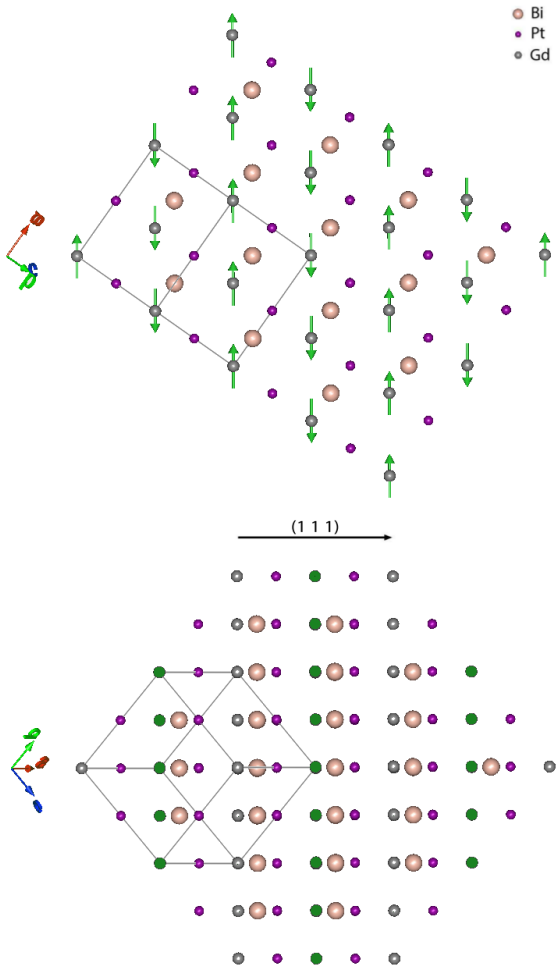

FIG. 3. Two views of the magnetic structure of GdBiPt with the [1 1 1] body diagonal pointing to the right. The lower panel shows the structure rotated by 90° around the [1 1 1] axis relative to the upper panel. The moments are perpendicular to the body diagonal, and form alternating ferromagnetic sheets. The crystal unit cell is outlined, showing the doubling of the unit cell along all three crystallographic axes.