# Single Crystal Magnetic Structure Determination of NdBiPt

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Based on a model proposed by [1], NdBiPt was considered as candidate of a new family of antiferromagnetic topological insulator (AFTI). In their proposed model, translational and time-reversal symmetry are broken due to magnetically induced spin-orbit coupling, while their product is conserved. We conducted single crystal neutron scattering experiments on NdBiPt to determine the magnetic order. Our results indicate that given the observed magnetic structure, this compound does not fall under the symmetry class described in [1] .

NdBiPt crystallizes in the cubic Half-Heusler crystal structure with space group F43m [2]. This structure consists of four interpenetrating fcc lattices shifted by [¼, ¼, ¼] where the [½, ½, ½] position is an ordered vacancy. The compound has a lattice constant of 6.76 Å with $Nd^{3+}$ located on the [0, 0, 0], Bi on the [¼, ¼, ¼], and Pt on the [¾, ¾, ¾] position, and permutations of [0, ½, ½]. NdBiPt is a semi metal with a low carrier density of 3 x $10^{15}$ $cm^{-3}$, and a high carrier mobility [3]. In the high temperature regime the magnetic susceptibility of the $Nd^{3+}$ shows a Curie-Weiss behaviour with a Curie-Weiss temperature $\Theta_W$ of -23 K. However, we present results that show that the compound orders at a lower Néel temperature of around $T_N$ = 2.18 K. Single crystals of NdBiPt where grown using Bi flux. Nd, Bi and Pt of high purity where placed in a ceramic crucible in the ratio 1:15:1 and then sealed in a quartz ampule. The melt was kept at 1200 °C for two days and then cooled down to 550 °C over a week. After two days the ampules where then taken out of the furnace and centrifuged to separate the flux from the crystals which where further characterized by x-ray diffraction. Three crystals of the size of about 2 x 1 x 1 $mm^3$ where co-aligned on a 99.9% pure Al plate. The experiment was carried out at the C5 tripe axis spectrometer at the National Research Council (NRC) in Chalk River. To obtain a good separation between the nuclear and magnetic Bragg peaks the crystal was aligned in the (hhl) scattering plane. Data was collected at different temperatures and corrected for background. The peaks where fit with a Gaussian function:

$$G(x) = B + A \cdot \exp\left[\frac{-4 \cdot \log(2) \cdot (x - x_0)^2}{s^2}\right] \quad (1)$$

To determine the direction of the magnetic moment, the intensities at ±(110) and perpendicular at ± (001) have been compared. The Intensities observed at these two sites differ roughly by a factor of 15, suggesting that the moment is aligned with the momentum of the incoming neutron, along [001] (Fig.1 (a)&(b)). There is no magnetic signal at the (001) position underneath the critical temperature, up to some second order scattering from the ± (111) nuclear peak. Due to the cubic structure of the crystal the magnetic moment can point along any of the six edges of the cube. Along four of these edges the form factor cancels leaving only the ±[001] direction. Therefore we can conclude that the magnetic moment of the $Nd^{3+}$ ion points normal to the {100} family of planes forming domains of orientations where the moment lies along the directions [100], [010] or [001]. This results in antiferromagnetic ordered planes along the propagation vector τ = (100) which does not lead to the necessary symmetry breaking to qualify for an AFTI.

The amplitude of the moment was determined by scaling observed magnetic intensities at the reciprocal lattice vector $Q$ using the relation:

$$\left|F_{mag}(Q)\right|^2 = \frac{I_{mag}(Q) \cdot \sin\phi}{C(Q) \cdot \sin^2\alpha} \quad (2)$$

where $I_{mag}$ is the observed intensity,

$\sin^2\alpha = 1 - \left(\hat{Q} \cdot \hat{\mu}\right)^2$, is the scattering angle and

$C(Q)$ can be determined from nuclear peaks, calculating the structure factor from known scattering lengths. The magnetic structure factor can be written as [4] (equation 3):

$$F_{mag}(Q) = \frac{\gamma_n r_0}{2} \cdot \mu \cdot f(Q) \cdot \sum_j \exp\left[2\pi i\left(hx_j + ky_j\right)\right]$$

with $\gamma_n r_0 / 2 = 2.69 \cdot 10^{-15}\, m / \mu_B^2$, indicating the

product of neutron gyromagnetic ratio times the electron radius. To calculate the magnetic form factor $f(Q)$, we used a dipole approximation [4]. Solving for $\mu$ results in a magnetic moment of 3.90 ± 0.1 $\mu_B$, which is close to the result obtained from susceptibility measurements with a $\mu$ = 3.83 $\mu_B$. Figure 1(c) shows the temperature dependence of the integrated intensity of the (110) magnetic peak as we cross the transition temperature. To obtain the correct Néel temperature of $T_N$ = 2.1767 ± 0.0005 K the data was fitted to the scaling law (inset Fig. 1(c)) [5]:

$$I = C \cdot \left(1 - \frac{T}{T_N}\right)^{2\beta} \qquad (4)$$

with a critical exponent of β = 0.3704 ± 0.003, which is close to the value predicted for a three dimensional Ising antiferromagnet (β = 0.333). Figure 1 (d) shows the temperature dependence of the Lorentzian peak width, which is proportional to the average inverse correlation length. One can see long range order becoming infinite as we cross the transition temperature.

**References**


[1] R.S. Mong et al. Phys. Rev. B 81, 245209 (2010).
[2] P.C. Canfield et al. J. Appl. Phys 70, 5800 (1991).
[3] D. T. Morelli et al. Phys. Rev. B 53, 12896 (1996).
[4] Z. Yamaniet al. Can. J. Phys. 88, 771-197 (2010).
[5] L. P. Kadano et al. Rev. Mod. Phys. 39, 2 (1967).


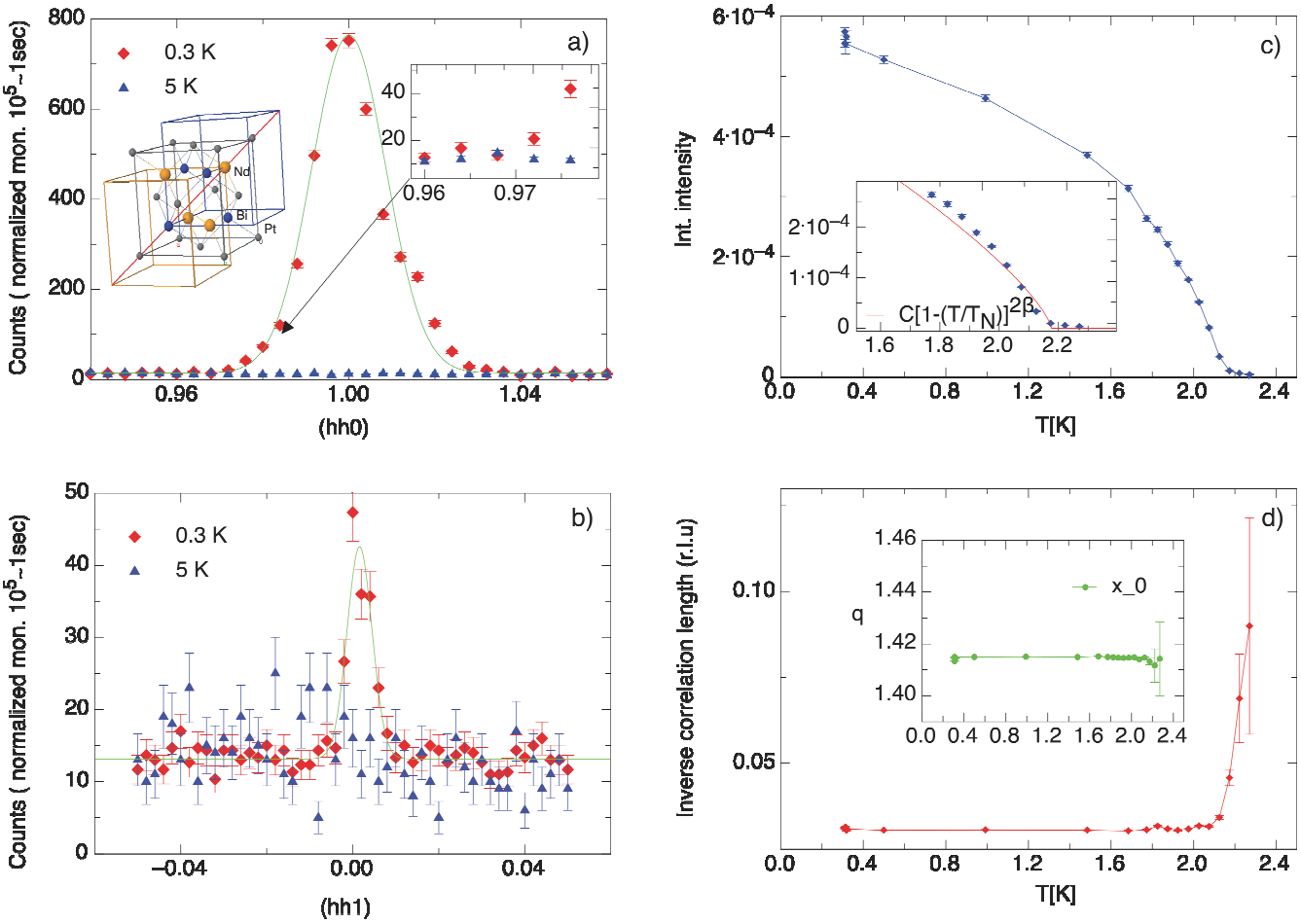


**Fig. 1** (a) (110) magnetic peak above (blue triangles) and underneath (red diamonds) the transition temperature. (b) Scattering of the (001) peak showing second order scattering from the (111) nuclear peak underneath $T_N$. (c) Integrated intensities of the (110) magnetic peak as a function of temperature. Inset: Scaling law fit with β = 0.37. (d) Inverse scattering length and peak position as function of temperature.