Experimental report

17/08/2021

Proposal: **5-54-369** **Council:** 10/2020

Title: Neutron polarimetry study of the spin density wave phase in Fe1+xTe:

Research area: Physics

This proposal is a new proposal

Main proposer: **Chris STOCK**

Experimental team:

Local contacts: Anne STUNAULT

Samples: Fe1+xTe

Instrument	Requested days	Allocated days	From	To
D3	4	4	18/03/2021	22/03/2021

Abstract:

Fe1+xTe displays incommensurate magnetic ordering near the magnetic and structural transition temperature. We wish to investigate the polarization matrix in this phase to determine the nature of it and also whether it is a spin density wave or a helical structure. The experiment requires the use of cryopad to measure the full polarization matrix.

Proposal 5-54-369, 4 days on D3
Neutron polarimetry study of the spin density wave phase in $Fe_{1+x}Te$

Introduction

$Fe_{1+x}Te$ is composed of van der Waals layers of edge-sharing $FeTe_4$ tetrahedra. The interstitial iron concentration tunes the magnetic properties of the compound. This D3 experiment is performed on a $Fe_{1.06}Te$ sample, having a first-order transition at 75K, where an antiferromagnetic structure appears along b-axis, $\vec{k} = (0.5, 0, 0.5)$, with a structural transition from tetragonal space-group P4/nmm to monoclinic $P2_1/m$ [1].

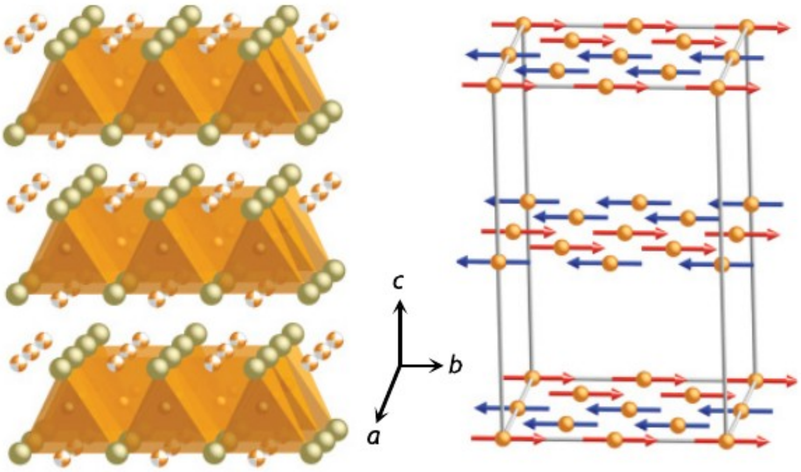

Figure 1: Nuclear and magnetic structure of $Fe_{1+x}Te$. From [2].

The aim of is this experiment on D3 is first; to measure the full polarization matrices for several magnetic reflections and at different temperatures, to see if the magnetic moments are canted from b-axis, as previously measured by spin-polarized scanning tunneling microscopy (STM) on the surface of $Fe_{1+x}Te$ compounds [3]. Then, we are studying temperature-dependence near the transition temperature to see if spin-density waves appear in this sample.

Polarization matrices

The sample is aligned in the (H0L) plane. Full polarization matrices were measured for several magnetic reflections, at different temperatures. The P_{zz} element of nuclear reflection (200) was measured regularly to track the time-decay of the He spin filter efficiency. This allows to correct the measured polarization values.

For a magnetic moment purely aligned along b-axis, the polarization matrix for each (H0L) reflection should be diagonal, with absolute values equal to 1. If the moments are tilted from b-axis towards c-axis (as measured by STM in [3]), the P_{yy} and P_{zz} elements differ in amplitude from 1. The general form of the polarization matrix is given by:

$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -x & 0 \\ 0 & 0 & x \end{pmatrix}$ with x deviating more from 1 with higher canting, and higher Q.

The polarization matrices measured during the experiment are given below:

Reflection (0.5 0 0.5) at T=2.00 K
$$\begin{pmatrix} -0.985(4) & 0.036(7) & 0.099(7) \\ -0.002(7) & -0.983(4) & 0.093(7) \\ 0.111(7) & 0.070(7) & 0.981(4) \end{pmatrix}$$

Reflection (0.5 0 0.5) at T=60.00 K
$$\begin{pmatrix} -0.976(7) & 0.02(1) & 0.10(1) \\ 0.00(1) & -0.983(7) & 0.07(1) \\ 0.10(1) & 0.09(1) & 0.979(7) \end{pmatrix}$$

Reflection (1.5 0 0.5) at T=2.00 K
$$\begin{pmatrix} -0.97(2) & 0.02(3) & 0.10(3) \\ 0.02(3) & -0.93(2) & 0.02(3) \\ 0.13(3) & 0.03(3) & 1.01(2) \end{pmatrix}$$

Reflection (1.5 0 0.5) at T=60.00 K
$$\begin{pmatrix} -0.98(3) & 0.06(4) & 0.08(4) \\ 0.06(4) & -1.00(3) & 0.03(3) \\ 0.16(4) & 0.11(4) & 0.97(3) \end{pmatrix}$$

Reflection (1.5 0 1.5) at T=2.00 K
$$\begin{pmatrix} -0.97(3) & 0.06(4) & 0.14(4) \\ 0.02(4) & -0.96(3) & 0.13(4) \\ 0.12(4) & 0.04(4) & 0.98(3) \end{pmatrix}$$

Reflection (1.5 0 1.5) at T=60.00 K
$$\begin{pmatrix} -1.06(5) & -0.08(5) & 0.04(5) \\ 0.05(5) & -0.92(5) & 0.11(5) \\ 0.08(6) & 0.25(6) & 0.90(5) \end{pmatrix}$$

Reflection (2.5 0 0.5) at T=2.00 K
$$\begin{pmatrix} -0.9(2) & 0.0(2) & 0.3(1) \\ 0.3(2) & -1.0(1) & 0.3(2) \\ 0.3(2) & -0.1(2) & 1.0(2) \end{pmatrix}$$

Reflection (0.5 0 0.5) at T=65.00 K
$$\begin{pmatrix} -0.973(7) & 0.045(9) & 0.097(9) \\ 0.004(9) & -0.976(7) & 0.092(9) \\ 0.122(9) & 0.095(9) & 0.984(7) \end{pmatrix}$$

Reflection (0.5 0 0.5) at T=30.00 K
$$\begin{pmatrix} -0.993(5) & 0.029(8) & 0.080(8) \\ 0.004(8) & -0.980(5) & 0.090(8) \\ 0.117(8) & 0.069(8) & 0.983(5) \end{pmatrix}$$

Reflection (1.5 0 0.5) at T=65.00 K
$$\begin{pmatrix} -0.97(3) & 0.02(3) & 0.11(3) \\ 0.03(3) & -0.96(3) & -0.00(3) \\ 0.11(4) & 0.08(3) & 0.96(3) \end{pmatrix}$$

Reflection (1.5 0 0.5) at T=30.00 K
$$\begin{pmatrix} -1.01(2) & 0.04(3) & 0.13(3) \\ -0.00(3) & -1.00(3) & 0.05(3) \\ 0.14(3) & 0.07(3) & 1.03(3) \end{pmatrix}$$

Reflection (1.5 0 1.5) at T=65.00 K
$$\begin{pmatrix} -0.98(3) & 0.03(4) & 0.12(4) \\ 0.01(4) & -0.98(4) & 0.06(4) \\ 0.11(4) & 0.04(4) & 0.93(4) \end{pmatrix}$$

Reflection (1.5 0 1.5) at T=30.00 K
$$\begin{pmatrix} -0.99(3) & 0.06(4) & 0.00(4) \\ 0.02(4) & -1.06(4) & 0.16(4) \\ 0.03(4) & 0.05(4) & 0.97(3) \end{pmatrix}$$

Reflection (0.5 0 0.5) at T=68.00 K
$$\begin{pmatrix} -0.93(2) & 0.04(2) & 0.11(2) \\ 0.01(2) & -0.93(2) & 0.09(2) \\ 0.10(2) & 0.08(2) & 0.98(2) \end{pmatrix}$$

Reflection (2.5 0 0.5) at T=30.00 K
$$\begin{pmatrix} -1.1(2) & -0.1(2) & 0.0(2) \\ 0.2(2) & -1.2(2) & -0.0(2) \\ 0.3(2) & 0.1(2) & 0.8(2) \end{pmatrix}$$

Reflection (1.5 0 0.5) at T=68.00 K
$$\begin{pmatrix} -1.00(5) & 0.01(6) & 0.15(5) \\ 0.05(5) & -0.80(6) & -0.06(6) \\ 0.09(6) & 0.05(5) & 0.93(6) \end{pmatrix}$$

The diagonal elements are fairly equal in amplitude to 1, showing an axial magnetic structure along b-axis. The non-diagonal elements differ from 0, even within the uncertainties. This can be accounted to incomplete polarization of the incident beam and small misalignments which lead to additional experimental errors. This can be further corrected as described in [4]. The measurement of purely nuclear Bragg peak (200) which should lead to an identity polarization matrix proves the underestimation of the uncertainties in the data analysis.

Reflection (2 0 0) at T=68.00 K
$$\begin{pmatrix} 0.994(6) & -0.006(6) & -0.030(7) \\ -0.044(7) & 0.999(6) & -0.005(7) \\ -0.007(7) & 0.032(7) & 0.999(5) \end{pmatrix}$$

Q-scans

Some H-scans were performed at different temperatures (see Figure 2), to track the temperature-dependence of the propagation vector along a^*-axis. The eventual apparition of spin-density wave near the transition temperature should imply a variation of the propagation vector from (0.5, 0, 0.5). The intensities are fitted to a Gaussian, the mean value giving the actual H component of the propagation vector.

The slight difference from antiferromagnetic $\vec{k} = (0.5, 0, 0.5)$ can be explained by the fact the sample was aligned in the paramagnetic phase, and lattice parameters change after the structural transition [5]. Within the instrumental resolution of D3, the propagation vector seems constant as a function of temperature, but more accurate tracking could be performed on D10 for example.

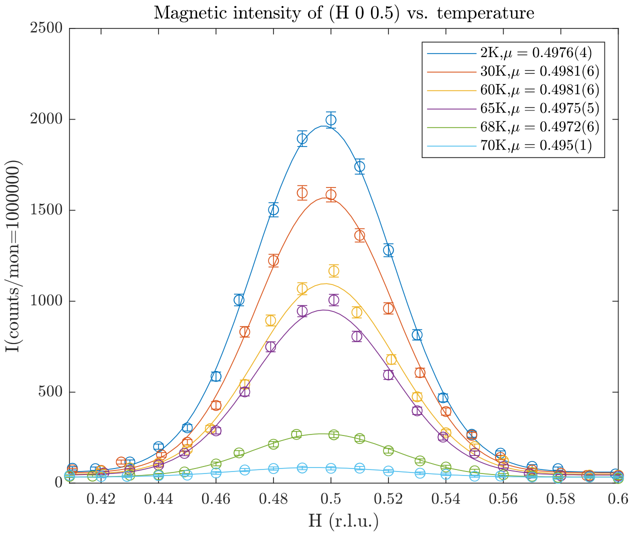

Figure 2: H-scans as a function of temperature

Temperature-dependence of P_{xx} and P_{zz}

Matrix elements P_{xx} and P_{zz} were further tracked as a function of the temperature. As described above $P_{zz} = +1$ in the case of magnetic moments aligned along b-axis. This value can be reduced if the moments are canted. However, in absence of chiral magnetic scattering P_{xx} is theoretically equal to 1. From the data, the amplitude of both elements deviates from 1 above 70K. Yet it seems that $-P_{xx} = P_{zz}$, which could indicate an underestimation of the spin filter efficiency (the data shown here is still corrected, by tracking the polarization of a nuclear peak), or this can be due to the low magnetic intensity near the transition temperature.

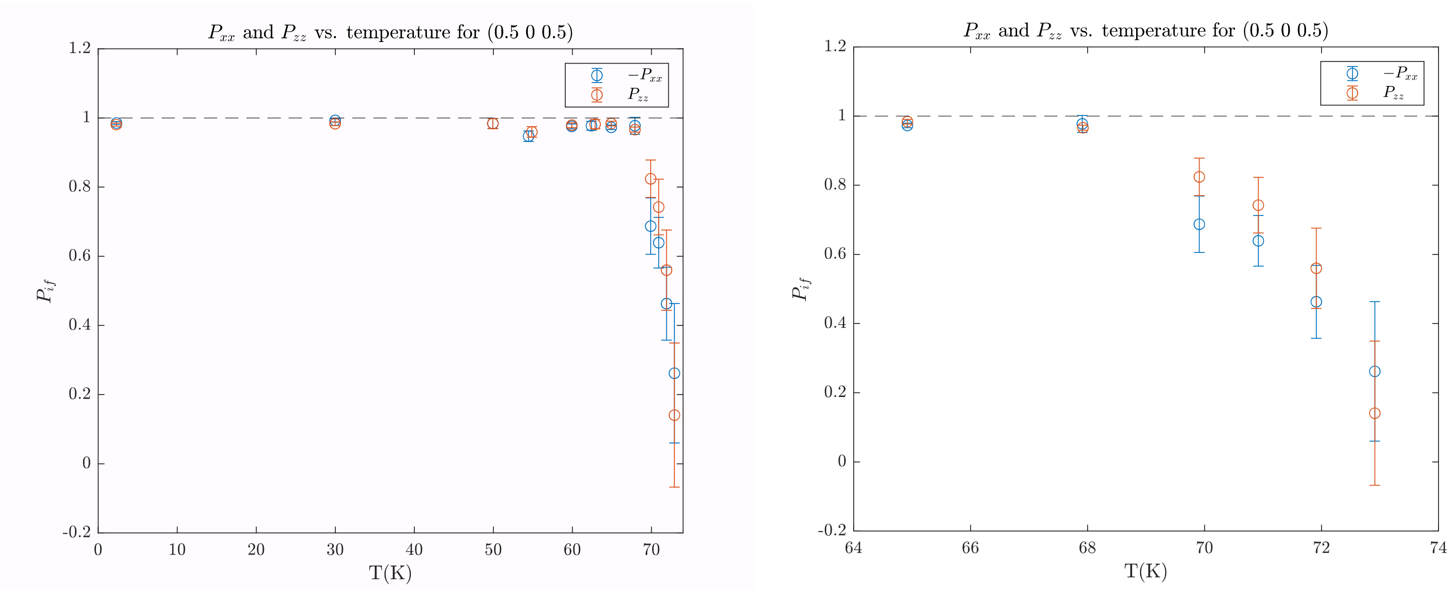

Figure 3: Temperature-dependence of polarization matrices elements.

[1] C. Stock, E. E. Rodriguez, P. Zavalij, M. A. Green, and J. A. Rodriguez-Rivera, Phys. Rev. B **84**, 045124 (2011).

[2] E. E. Rodriguez, C. Stock, P. Zajdel, K. L. Krycka, C. F. Majkrzak, P. Zavalij, and M. A. Green, Phys. Rev. B **84**, 064403 (2011).

[3] C. Trainer, M. Songvilay, N. Qureshi, A. Stunault, C. M. Yim, E. E. Rodriguez, C. Heil, V. Tsurkan, M. A. Green, A. Loidl, P. Wahl, and C. Stock, Phys. Rev. B **103**, 024406 (2021).

[4] N. Giles-Donovan, N. Qureshi, R. D. Johnson, L. Y. Zhang, S.-W. Cheong, S. Cochran, and C. Stock, Phys. Rev. B **102**, 024414 (2020).

[5] S. Li, C. de la Cruz, Q. Huang, Y. Chen, J. W. Lynn, J. Hu, Y.-L. Huang, F.-C. Hsu, K.-W. Yeh, M.-K. Wu, and P. Dai, Phys. Rev. B **79**, 054503 (2009).