Experimental Report

06/12/2013

Proposal: **5-31-2296** **Council:** 10/2012

Title: High-pressure neutron diffraction study of incommensurate magnetic ordering in Fe1.141Te.

This proposal is a new proposal

Research Area: Materials

Main proposer: **JORGENSEN J.- E.**

Experimental Team: JORGENSEN J.- E.
HANSEN Thomas

Local Contact: HANSEN Thomas

Samples: Iron telluride, Fe1.141Te

Instrument	Req. Days	All. Days	From	To
D20	5	5	23/05/2013	27/05/2013
			12/06/2013	13/06/2013

Abstract:

Magnetisation and resistivity measurements as well as high-pressure neutron diffraction have shown the existence of novel pressure induced phases at low temperature in Fe1.087Te. A transition from commensurate to incommensurate order was observed at about 1.6 GPa and 6 K and and the magnetic order is suppressed at about 2.8 GPa. The iron richer compound Fe1.141Te shows incommensurate magnetic ordering below 63 K at ambient pressure. It is proposed to study the incommensurately magnetically ordered phase of Fe1.141Te at high pressures. The experiment will yield information on the stability as well as on the pressure dependence of the magnetic propagation vector of this phase and the results are of interest in relation to the understanding of pressure-induced superconductivity in the iron pnictides e.g. BaFe2As2.

Experimental Report Proposal 5-31-2296

High-pressure neutron powder diffraction study of incommensurate magnetic ordering in $Fe_{1.141}Te$

Iron pnictide and chalcogenide compounds have recently attracted much attention due to their superconducting and magnetic properties. Superconductivity with critical temperatures up to 55 K has been observed in the $LaFeAs(O_{1-x}F_x)$ compounds while the iron chalcogenide compound $FeSe_{1-x}$ becomes superconducting below with 8 K [1-3]. In contrast to $FeSe_{1-x}$, superconductivity has not been observed in the $Fe_{1+x}Te$ compounds which order magnetically at low temperatures. Studies of chemical doping and pressure effects as well as the interplay between magnetic ordering, structural instability and superconductivity in the iron pnictide and chalcogenide compounds compounds are therefore of great interest. $Fe_{1.141}Te$ was studied at high pressures and low temperatures on the D20 diffractometer using the Paris-Edinburgh pressure cell using a wave length of 2.41 Å. Data were recorded as a function of temperature for pressures in the range from 0.4 to 2.55 GPa and Pb was be used as internal standard for the determination of the pressure. An additional series of ambient pressure measurement was performed using a closed cycle He refrigerator. Data analysis was be performed by the Rietveld method using the models for the chemical and magnetic structures described in ref. [4]. The results of the preliminary data analysis are described below.

Powder patterns of $Fe_{1.141}Te$ were measured in the temperature range from 7 to 95 K at ambient pressure. Fig. 1 shows a thermodiffractogram plot of $Fe_{1.141}Te$. The splitting of the (112) and (200) reflections shows that a transition from tetragonal to monoclinic symmetry is taking place at 58 K. Magnetic scattering at $2\theta \approx 21°$ is observed below this temperature showing that the structural transition is accompanied by the onset of magnetic ordering.

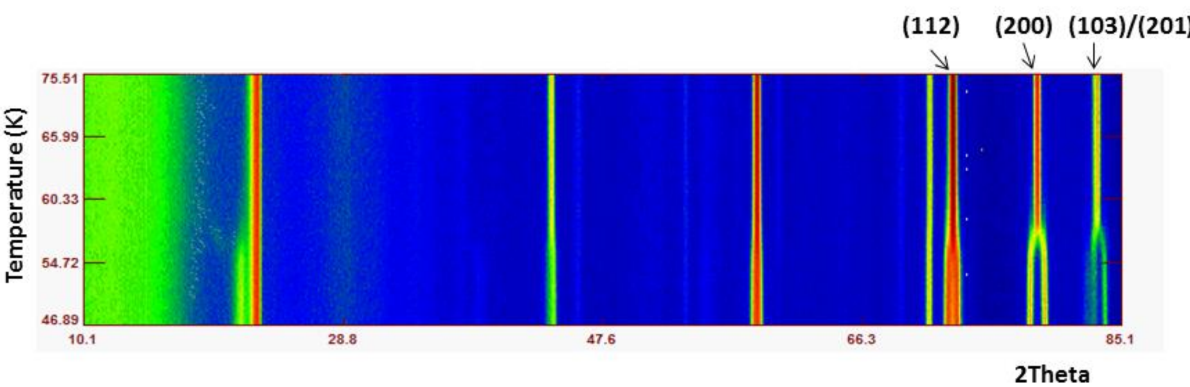

Fig. 1. Thermodiffractogram of $Fe_{1.141}Te$. Indexing corresponds to the tetragonal *P4/nmm* unit cell. A tetragonal to monoclinic structural phase transition is observed at 58 K, and magnetic scattering is seen to appear at $2\theta = 21°$ below this temperature indicating the onset of antiferromagnetic ordering.

The *p*,*T*-phase diagram of $Fe_{1.141}Te$ based upon the results of high-pressure neutron powder diffraction is shown in Fig. 2. The diagram contains three phases: The paramagnetic phase with space group *P4/nmm*, which is stable above ≈58K at ambient pressure. This phase is stabilized down to the lowest measured temperatures (6K) at pressures higher than ≈2.3 GPa. The monoclinic low temperature phase with space group $P2_1/m$ and commensurate bicollinear antiferromagnetic order and propagation vector **k** = (½ 0 ½) was found to be stable up to a pressure of approximately ≈ 0.8 GPa at 6K. The third observed phase has orthorhombic symmetry (space group *Pmmn*) and incommensurate antiferromagnetic order. The magnetic structure of this phase is closely related to the magnetic structure of the monoclinic phase but has a sinusoidal modulation with propagation vector **k** = (δ 0 ½) with δ = 0.391(2) at 1.1 GPa and δ = 0.332(2) at 2.1 GPa. The orthorhombic phase is stable in the pressure range from ≈0.8 to ≈2.3 GPa at the lowest measured temperatures. The measured *p,T*-phase diagram suggests the existence of magnetic quantum phase transitions in $Fe_{1.087}Te$, which are of great interest in relation to the understanding of the physical properties including superconductivity of the iron pnictides and chalcogenides [5].

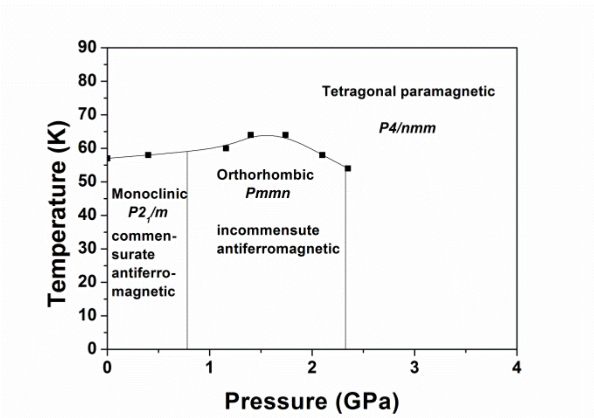

Fig. 1. Schematic *p,T* phase diagram of $Fe_{1.141}Te$. No magnetic ordering was observed in the tetragonal phase. The propagation vector for the commensurate antiferromagnetic ordering in the monoclinic phase is **k** = (½ 0 ½) while it is **k** = (δ 0 ½) with 0.332(2) ≤ δ ≤ 0.391(2) for the incommensurate magnetic ordering within the orthorhombic phase, see text.

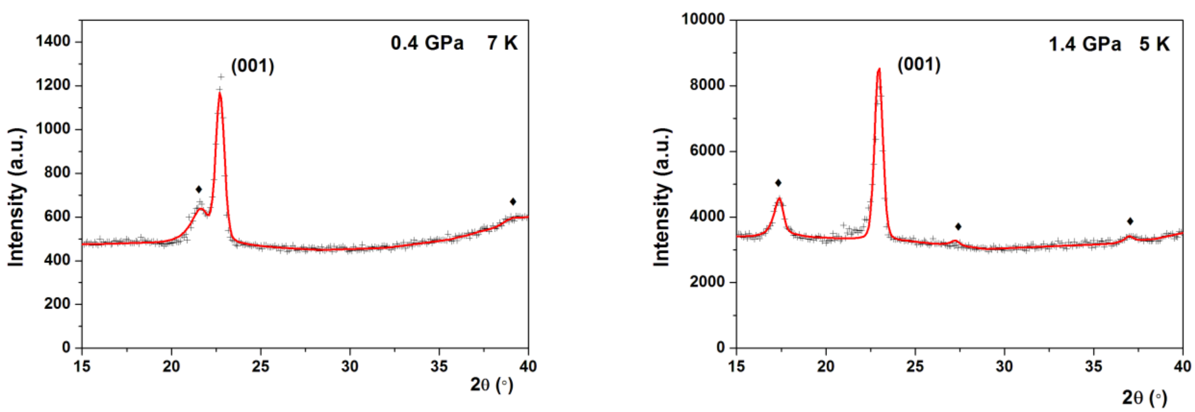

Fig. 2. Powder diffraction profiles of $Fe_{1.141}Te$ at 0.4 GPa and7 K and 1.4 GPa and 5K. Magnetic Bragg peaks are marked with (♦). The magnetic ordering is commensurate antiferromagnetic with propagation vector **k** = (½ 0 ½) at 0.4 GPa while it is incommensurate antiferromagnetic with **k** = (0.346(1) 0 ½) at 1.4 GPa.

References: [1] F.C. Hsu et al., Proc. Nat. Acad. Sci. **105** 14262 (2008). [2] Y. Kamihara et al., J. Am. Chem. Soc. **130** 3296 (2008), [3] H. Takahashi et al., Nature **453** 376 (2008), [4] J.-E. Jørgensen *et al.*, *EPJB (2013) 86 18.* [5] E. Abrahams et al., J. Phys.: Condens. Matter **23** 223201.