Experimental report

02/12/2022

Proposal:	**EASY-1034**
Council:	4/2021
Title:	Complex incommensurate magnetic structure of FeMnP0.77Si0.23
Research area:	Materials

This proposal is a new proposal

Main proposer:	**Johan CEDERVALL**
Experimental team:	
Local contacts:	Thomas HANSEN

Samples: FeMnP0.73Si0.27

Instrument	Requested days	Allocated days	From	To
D20	5	5	25/09/2021	26/09/2021

Abstract:

Materials based upon Fe2P provides great opportunities for magnet refrigeration. Materials for magnetic refrigeration should, in the ideal case, be ferromagnetic and show a large entropy change when magnetised. Fe2P-type materials have such properties and the physical properties can be further tuned with substitutions to ensure suitable materials for real world applications. Upon substitution of Fe2P with Mn and Si, FeMnP0.75Si0.25 (synthesised within our group) reveals ordering into in an incommensurate structure. We studied the very similar compound FeMnP0.73Si0.27 using INS and the diffraction profile represents that of FeMnP0.75Si0.25. However, even though linear spin wave theory should be able to reproduce the excitations in the polarised state, using the magnetic wave vector determined previously, this has not been the case. When examining the old diffraction data (exp. in Prague), it was found that the signal to noise ratio and the maximum overall intensity is poor. We therefore ask for two diffraction patterns for the compound FeMnP0.73Si0.27, at RT and 2 K. This would allow us to examine the nuclear and magnetic structure so that the INS data can be fully interpreted.

EXPERIMENT TITLE: ”Complex incommensurate magnetic structure of $FeMnP_{0.73}Si_{0.27}$”
PROPOSAL NUMBER: (EASY-1034)
EXPERIMENTAL TEAM: Johan CEDERVALL
INSTRUMENT: D20

Introduction

Global warming and an increasing industrialisation of the world increases the need for efficient cooling for both refrigeration and heat pumps. An energy efficient alternative to achieve this is magnetic refrigeration, which is based on an effect where a material changes its temperature when being magnetized [1,2]. Compounds based on Fe_2P, such as $(Fe,Mn)_2(P,Si)$, are among the most promising candidates for room temperature magnetic refrigeration via the magnetocaloric effect with great potential to reduce the amount of energy necessary for refrigeration. An optimised magnetocaloric material displays a first order ferromagnetic transition with enhanced entropy change. $Fe_{1-x}Mn_xP_{1-y}Si_y$ yields tuneability of both the ferromagnetic transition and magnetic moment of the compound [3] thus further optimising the magnetocaloric effect. To fully understand the interactions a model system of $FeMnP_{0.73}Si_{0.27}$ have been studied with Inelastic Neutron Scattering (INS), and the results showed temperature dependent scattering features at low Q, which needs could only be resolved with Small Angle Neutron Scattering (SANS) [4].

Experimental details and analysis

Powder samples of $FeMnP_{0.73}Si_{0.27}$ were synthesised using the drop synthesis techniques followed by sintering and annealing at 1373 and 1073 K, respectively [5]. The samples were pre-characterized XRD and magnetic measurements. INS have also been employed at the instrument IN5 at ILL. Neutron diffraction experiments were performed using the instrument D20 at room temperature (RT) and 2 K to elucidate the complex magnetic structure.

Results

Rietveld refinements of the room temperature data, figure 1, shows two Fe_2P-type phases (space group $P\bar{6}2m$), where the main phase have a phase fraction of 97(1) wt.%. In the refinement a clear site preference were found for Fe and Mn, visualised in figure 1. According to previous reports [6], and the unit cell parameters, the main phase will become ferromagnetic (FM) and the minority phase antiferromagnetic (AFM) upon cooling. At 2 K, a phase transition have occurred for both phases and magnetic peaks have appeared. The phase fractions for the FM and AFM phases are refined to 76(1) and 24(1) wt.%, respectively. The FM phase can easily be modelled with a propagation vector **k** = (000), and the magnetic moments aligned along the a-axis. For the AFM phase, a strong magnetic reflection are seen at ~0.45 $Å^{-1}$, which gives an incommensurate magnetic structure with **k** = (0.375(1) 0 0). This results in the helical magnetic structure seen in figure 2. The results from this study will help to interpret the results from our INS study and when combined with these results and theoretical modelling will lead to advancement of our understanding in the $(Fe,Mn)_2(P,Si)$ system.

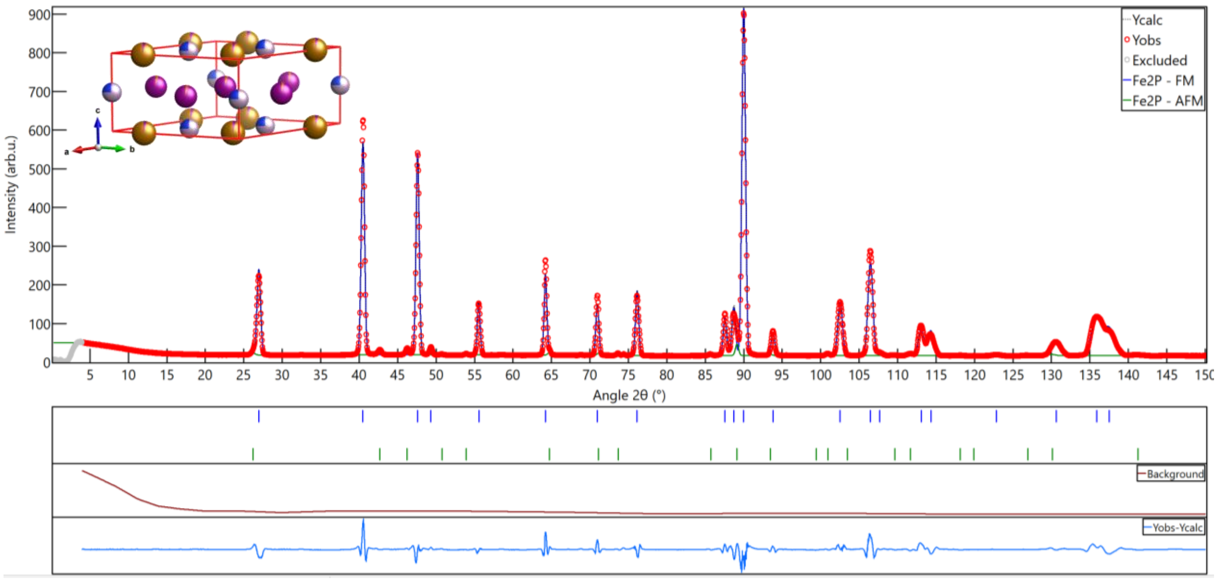

Figure 1. Room temperature neutron diffraction pattern of $FeMnP_{0.73}Si_{0.27}$ refined using two Fe_2P-type models, including the refined model for the main phase.

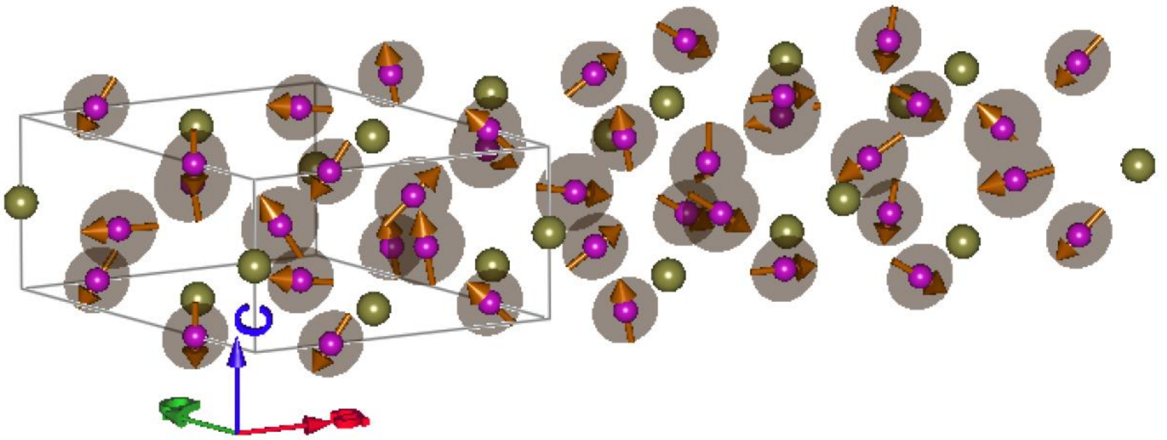

Figure 2. Incommensurate helical magnetic ordering for the AFM structure for $FeMnP_{0.73}Si_{0.27}$ at 2 K. Three nuclear unit cells along *a* are shown for clarity.

Acknowledgements

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References

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