Experimental report

05/10/2015

Proposal: 5-31-2387 **Council:** 10/2014

Title: The magnetic and nuclear structureof Fe5SiB2 and AlFe2B2

Research area: Materials

This proposal is a new proposal

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Samples: AlFe2B2
Fe5SiB2

Instrument	Requested days	Allocated days	From	To
D1B	0	2	15/05/2015	17/05/2015
D20	2	0		

Abstract:

Magnetic materials are crucial components in many components used in renewable energy applications. Especially, new permanent magnets without rare earth elements are needed for energy conversion devices. Here we would like to investigate the temperature dependences of the magnetic- and crystal structure of two new magnetic materials, Fe5SiB2 and AlFe2B2. The compounds are synthesized with isotope pure 11B to minimize the absorption from the sample. The results expected from these measurements are important for the possible application of these materials in renewable energy applications.

EXPERIMENT TITLE: "The magnetic and nuclear structure of Fe_5SiB_2 and $AlFe_2B_2$"
PROPOSAL NUMBER: (5-31-2387)
EXPERIMENTAL TEAM: Martin SAHLBERG, Johan CEDERVALL and Mikael ANDERSSON
INSTRUMENT: D1B

Introduction

Magnetic materials for energy applications, such as permanent magnets and magnetic refrigeration, have become more important for a sustainable future [1, 2]. Permanent magnetic materials are used to harvest energy, in generators for example in wind turbines, and in electric vehicles [1] and magnetocaloric materials will reduce the energy consumption for refrigeration purposes [2]. Because of this, two new materials have been studied, one permanent magnet (Fe_5SiB_2) and one magnetocaloric ($AlFe_2B_2$).

Fe_5SiB_2 is a ferromagnetic tetragonal compound without rare earth elements. The tetragonal structure is good for the possibility of an easy axis of the magnetization in the manufactured magnet and a magnet without rare earth elements is preferred due to their expensiveness. Fe_5SiB_2 crystallizes within the space group I4/mcm with the unit cell parameters a = 5.5498(2) Å and c = 10.3324(5) Å with two magnetic iron cites. The magnetic moments are aligned along the c-axis below the Curie temperature at 784 K [3] and at lower temperatures, around 140 K, Mössbauer spectroscopy reveals that the material undergoes a spin reorientation and the magnetic moments fall down to the ab-plane.

$AlFe_2B_2$ is an ferromagnetic orthorhombic compound that is recently discovered as a magnetocaloric material [4]. The compound crystallizes in the space group Cmmm with the unit cell parameters a = 2.9233(10) Å, b = 11.0337(14) Å, c = 2.8703(3) Å. I has a layered structure where slabs of (Fe_2B_2)-units is alternated with Al layers. The Curie temperature have been reported to around room temperature with magnetic moments around 1 μ_B/Fe-atom.

Experimental details and analysis

Powder samples were synthesized via high temperature synthesis techniques. Arc-melting from the pure elements were followed by annealing at 1273 and 1173 K for Fe_5SiB_2 and $AlFe_2B_2$ respectively. The samples were pre characterized with XRD (Bruker D8) as well as magnetic measurements (MPMS SQUID magnetometer as well as a PPMS VSM system both from Quantum Design). Neutron diffraction was performed at the beamline D1B. For both samples the collection were done for 3 h at specific temperatures (16, 150, 200, 300 and 500 K for Fe_5SiB_2 and 16, 150, 200, 300 and 500 K for $AlFe_2B_2$) and upon ramping between all temperature steps (3 minutes per diffraction pattern). The diffraction patterns were analyzed with the FullProf software [5] utilizing the Rietveld method [6]

Preliminary results

For Fe_5SiB_2 all patterns were collected below T_C so there are magnetic contributions in all diffraction patterns. There are however differences where the proposed spin reorientation occurs. Intensities from magnetic scattering changes are seen in figure 1. Analyzing these intensities differences gives the structures in figure 2 with the spin along the tetragonal c-axis above the spin-flip temperature and in the ab-plane along the a-axis at low temperatures. The magnetic moments have been refined

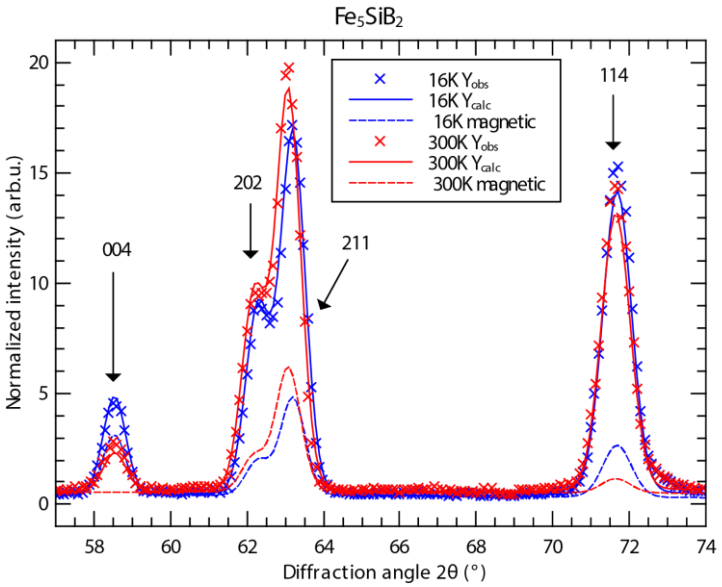

Figure 1. Neutron powder diffraction patterns revealing the magnetic transition for $Fe_5Si^{11}B_2$. λ = 2.52 Å.

to 2.1 and 1.7 μ_B/Fe-atom for the two iron cites at high temperature and 2.3 and 2.1 1.7 μ_B/Fe-atom for the low temperature case.

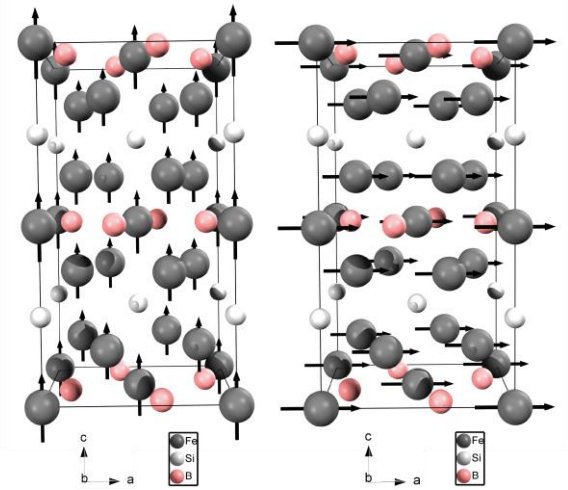

Figure 2. Magnetic structures for Fe5SiB2 at 300 K (left) and 16 K (right). The length of the arrows corresponds with

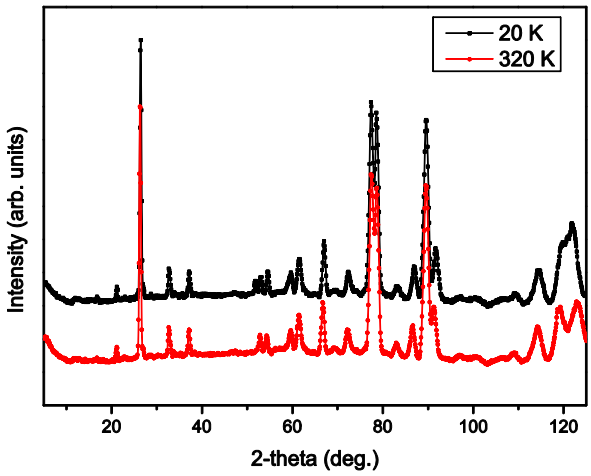

Figure 3. Neutron diffraction patterns above (320 K) and below (20 K) the Curie temperature. λ = 2.52 Å.

The collections for the $AlFe_2B_2$ sample were performed both below and above T_C and reveled a ferromagnetic structure with the magnetic moments along the a-axis with a magnetic moment of 1.4 μ_B/Fe-atom. The magnetic structure can be seen in figure 4.

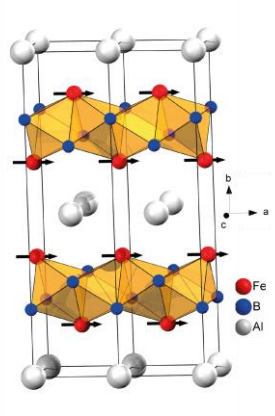

Figure 4. Magnetic structure for AlFe2B2. Magnetic moments are aligned along the a-axis.

Acknowledgements

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References

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