Experimental report

18/02/2017

Proposal: **5-31-2405** **Council:** 4/2015

Title: The magnetic structure of 154SmCo5

Research area: Chemistry

This proposal is a new proposal

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Samples: 154SmCo5

Instrument	Requested days	Allocated days	From	To
D1B	2	2	09/12/2015	11/12/2015

Abstract:

The magnetic structure of the classical permanent magnet material SmCo5 will be studied within the whole range of ferro- and ferrimagnetically ordered states (2 K up to approximately 1050 K) by neutron powder diffraction. This will complement older studies at short wavelengths or during in situ studies of the hydrogenation behaviour of SmCo5. In contrast to that earlier work, this experiment will use a setup optimized for magnetic scattering and allow an accurate mapping of magnetic moments as a function of temperature. This will allow us to follow the changeover from the ferro- to a ferrimagnetic state at 354 K in more detail and to check for a previously suggested change back to ferromagnetism around 537 K. The strong neutron absorption will be overcome by using a sample with isotopically pure 154 Sm.

The magnetic structure of $^{154}SmCo_5$ (experiment 5-31-2405)

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Objectives

$SmCo_5$ is one of the strongest permanent magnet materials with one of the highest coercitivities known do date [1]. Studies of the magnetic structure of samarium compounds are very scarce due to the enormous neutron absorption cross section of ^{nat}Sm for thermal neutrons [2]. This might be overcome by using short wavelengths, as was done in [3], where a ferromagnetic behaviour was found for the temperature range 4.2 K ≤ T ≤ 300 K. Samarium's magnetic moments are rather small and a change to ferromagnetic ordering was predicted to occur at 350 K, where the spin contribution to the magnetic moment was expected to become larger than the orbital one [3]. Another opportunity to solve the absorption problem is the use of isotopic pure ^{154}Sm with a considerably lower absorption cross section [2]. This allows a wider choice of wavelengths, which are better suited for magnetic scattering.

A previous study suggested the magnetic form factor of samarium to change its sign for T = 354 (2) K (ferro- to ferromagnetic) and back to ferromagnetic at 537(2) K [4]. However, for an unambiguous statement standard uncertainties were too large and the incorporation of deuterium in the samples could not be ruled out completely. Therefore, we have taken temperature dependent neutron powder diffraction data on a $^{154}SmCo_5$ sample on D1B.

Experimental Details

In order to overcome the high neutron absorption by samarium, isotopically enriched $^{154}SmCo_5$ was prepared from $^{154}Sm_2O_3$ (as received from Trace Sciences International) by a modified ORD (oxides-reduction-diffusion) method [4]. Neutron diffraction patterns were collected as a function of temperature (cryostate for 6 K ≤ T ≤ 320 K, furnace for 300 K ≤ T ≤ 1100 K) on the neutron powder diffractometer D1B. All data sets were evaluated using the Rietveld technique, thus leading to complete structural models and a detailed picture of the magnetic structure.

Results and Discussion

Refinement of nuclear and magnetic structure of $SmCo_5$ confirmed the hexagonal $CaCu_5$ type crystal structure and the alignment of all magnetic moments along crystallographic c (Fig. 1). Temperature dependent diffraction data show a smooth variation of structural and magnetic parameters. Magnetic moments of both crystallographically distinct cobalt atoms are not significantly different over the whole temperature range (Fig. 2). They are almost constant at 2.2 μ_B for 6 K ≤ T ≤ 250 K and decrease with increasing temperature to about 0.5 μ_B just below the Curie temperature. Samarium's magnetic moment starts at 0.9 μ_B at 6 K and first decreases with increasing temperature to a minimum around 700 K, but stays positive. Approaching the Curie temperature it increases again and becomes even larger than cobalt's magnetic moment (Fig. 2). There is no change in the sign if the magnetic moment of any of the atoms in the whole investigated temperature range between 6 K and the Curie temperature. $SmCo_5$ is thus a ferromagnet and does not switch to a ferrimagnetic state as suggested before [3, 4].

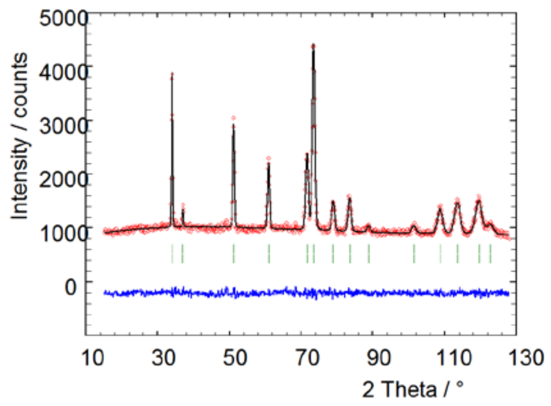

Fig. 1: Rietveld refinement of the nuclear and magnetic structure of $^{154}SmCo_5$ based on neutron powder diffraction data (D1B, λ = 2.52 Å, T = 6 K)

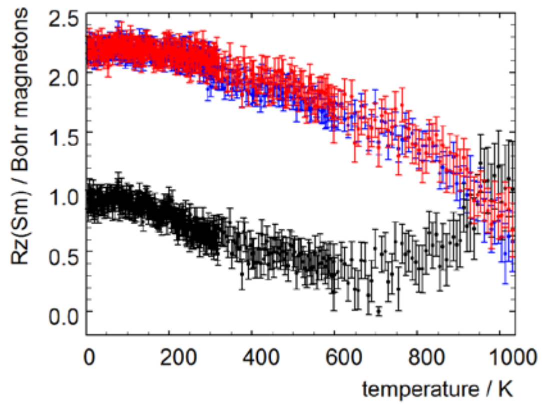

Fig. 2: Magnetic moment μ in Bohr magnetons μ_B along crystallographic c axis of Sm (black), Co1 (red), Co2 (blue) as a function of T as determined by sequential refinement on 459 neutron powder diffraction data sets

Literature

[1] S. Legvold, Rare Earth Metals and Alloys, in: Handbook on Ferromagnetic Materials (E. P. Wohlfarth, Ed.), North Holland, **1980**, Vol. *9*, 183

[2] V. F. Sears, *Neutron News* **1992**, *3*, 26-37

[3] D. Givord , J. Laforest, J. Schweizer, F. Tasset, *J.Appl.Phys.***1979**, *50*, 2008–2010

[4] K. L. A. Belener, H. Kohlmann, *J. Magn. Magn. Mater.* **2014**, *370*, 134-139