Experimental Report

11/01/2014

Proposal:	**5-41-698**	**Council:**	4/2012	
Title:	Magnetic structure of $SmFeO_3$			

This proposal is a new proposal

Researh Area: Physics

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Samples: $SmFeO_3$
$Sr_3YCo_4O_{10.5}$

Instrument	Req. Days	All. Days	From	To
D9	10	10	26/07/2012	30/07/2012
			26/11/2012	02/12/2012

Abstract:

Very recently room-temperature multiferroic properties of SmFeO3 have been reported [6]. Density functional theory calculations explain the ferroelectricity in this exciting material with the calculated canted antiferromagnetic structure (T_N~670 K). This renders single crystal neutron measurements highly desirable now. Despite the strong neutron absorbtion crossection of the Sm ion we found conditions where the total absorbtion is comparably small. This could be realized by an optimized sample geometry and the use of 0.511 A hot neutrons in a measurement at the D9 diffractometer. Our single crystal neutron measurements reveal an exciting first result: the spin configuration calculated in Ref. [6] can not be correct, since we observe quite strong magnetic intensities that should be absent for this calculated magnetic structure. We obtain a different magnetic symmetry and our magnetic structure is able to explain the ferroelectric properties with the inverse Dzyaloshinskii-Moriya interaction as well. After our first measurement we propose to perform a more detailed measurement at room-temperature now and also a 2nd measurement in the high-temperature magnetic phase (T_SR = 480 K).

Experimental report for D9 measurement of multiferroic $SmFeO_3$

$SmFeO_3$ crystallizes in the well-known perovskite structure [1]. Very recently, the discovery of ferroelectric polarization in $SmFeO_3$ has been reported concomitantly with the onset of antiferromagnetic ordering at $T_N \sim 670$ K in this compound [1]. The origin of its multiferroic properties above room-temperature i.e. the origin of the ferroelectric polarization in $SmFeO_3$ is highly debated [2–3]. A further spin-reorientation transition occurs at $T_{SR} \sim 480$ K in this material [1]. In the initial publication an inverse Dzyaloshinskii-Moriya interaction based mechanism has been reported to be the driving force of the ferroelectric properties of $SmFeO_3$ [1]. The underlying magnetic structure was calculated by ab initio calculations [1]. However, it has been demonstrated that this calculated k=0 magnetic structure with magnetic ions located at inversion centers can not be responsible for a spin-orbit-coupling driven ferroelectric polarization by $S_i \times S_j$ in this material since inversion symmetry will not be broken [2]. Finally, a different alternative magnetoelastic mechanism based on J $S_i \circ S_j$ exchange-striction has been proposed to be responsible for the ferroelectric polarization in SmFeO 3 [3]. In order to elucidate the physical properties of this highly controversially discussed $SmFeO_3$ -system we studied this intriguing system experimentally now.

In this D9 measurement we were able to measure the magnetic structure of $SmFeO_3$ ***for the first time*** experimentally by neutron diffraction despite the highly neutron absorbing properties of the Sm ion (~5900 barn for 2200 m/s neutrons). *This was achieved by the high incident neutron energy available at the D9 diffractometer as well as by the optimized sample geometry chosen*. The magnetic structure of $SmFeO_3$ has been measured in the two different magnetic phases i.e. at 300 K below and at 515 K above the spin-reorientation transition T_{SR}.

156 reflections have been measured at 300 K. The R-values of our magnetic and crystal structure refinement amount to $R(F^2)$: 18.7% and $Rw(F^2)$-factor : 21.1%. Other magnetic structures could be excluded. **Fig. 1** shows the Fcalc/Fobs plot indicating the goodness of our fit for our "300 K refinement". The finally obtained spin structure is shown in **Fig. 2**. This results already now prove that the interpretations in Ref. [1] can not be correct.

In a similar manner the 515 K spin structure could be obtained by the measurement of 156 reflections using a furnace (see **Fig. 3 & 4**). Also the "515 K spin structure" contradicts the whole interpretation presented in Ref. [1].

REFERENCES:

[1] J.-H. Lee et al., **Phys. Rev. Lett. 107**, 117201 (2011)

[2] R. D. Johnson et al., **Phys. Rev. Lett. 108**, 219701 (2012)

[3] J.-H. Lee et al., **Phys. Rev. Lett. 108**, 219702 (2012)

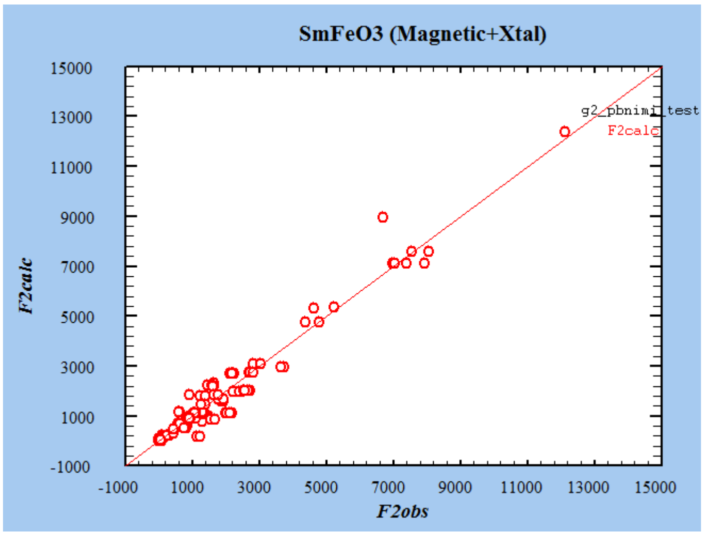

Figure 1: Resulting Fcalc/Fobs plot of the magnetic structure refinement of $SmFeO_3$ at 300 K.

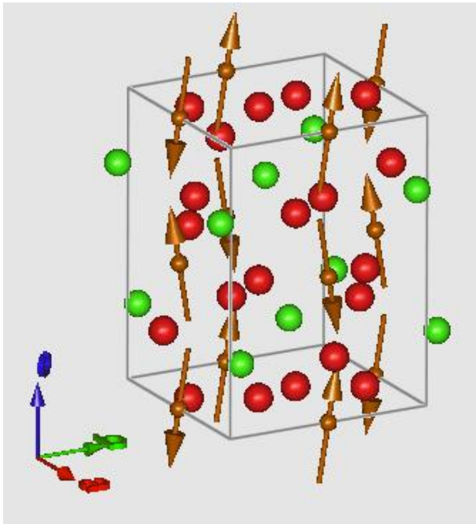

Figure 2: Magnetic structure of $SmFeO_3$ at 300 K. (Fe^{3+}-spins indicated by the arrows; red: O-ions; green: Sm-ions.)

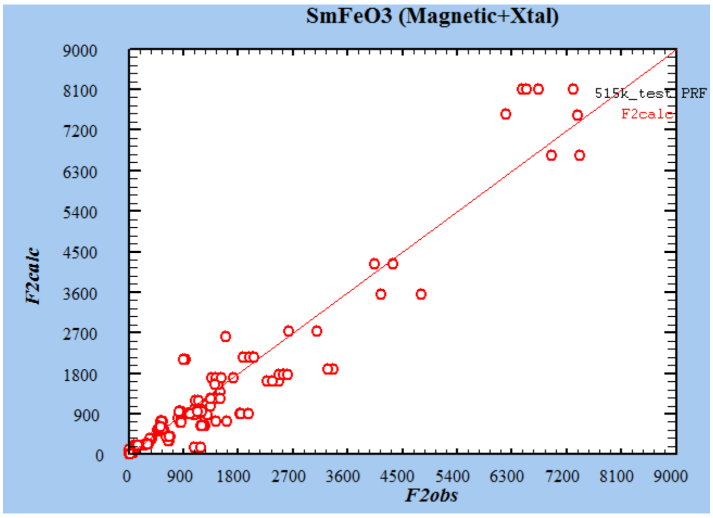

Figure 3: Resulting Fcalc/Fobs plot of the magnetic structure refinement of $SmFeO_3$ at 515 K. Probably due to the use of a furnace the scattering is larger.

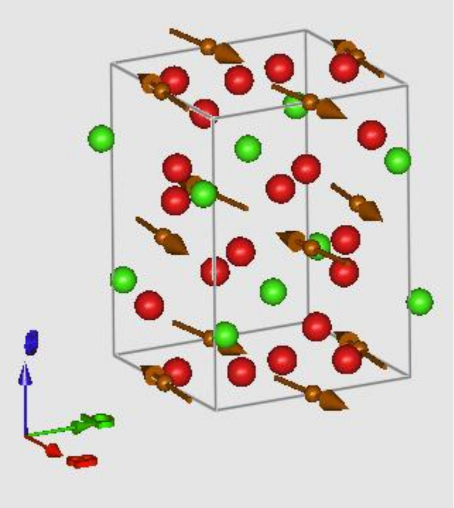

Figure 4: Magnetic structure of $SmFeO_3$ at 515 K. (Fe^{3+}-spins indicated by the arrows; red: O-ions; green: Sm-ions.)