Experimental Report

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Proposal: **5-31-2252** **Council:** 4/2012

Title: Study of giant magnetization reversal in Bi2FeMnO6, a room temperature magnetodielectric double perovskite

This proposal is a new proposal

Researh Area: Materials

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Samples: Bi2FeMnO6

Instrument	Req. Days	All. Days	From	To
D2B	1	1	15/11/2012	16/11/2012
D1B	1	1	13/11/2012	14/11/2012

Abstract:

We have recently synthesized Bi2FeMnO6, a novel multiferroic compound belonging to the class of bismuth-based double perovskites, in high temperature/high pressure conditions. Single-crystal diffraction allowed the determination of the crystal structure on the basis of an orthorhombic Pnam cell with lattice parameters a=5.573 Å, b= 11.206 Å and c=15.743 Å. The magnetic characterizations indicate an unconventional magnetic behavior as a function of temperature: due to the concomitant presence of competitive interactions, the material undergoes a complex ferrimagnetic transition around 500 K followed, at lower temperatures, by a field-dependent giant reversal of the magnetization. Furthermore, the study of the electric permittivity reveals the presence of magnetodieletric effects, suggesting the intriguing possibility of magnetoelectricity in Bi2FeMnO6. We consider neutron diffraction the best technique to accurately investigate the nuclear structure of the system –in particular for what concerns the Fe/Mn distribution- and, on the other side, to understand the complex magnetic behavior of the compound as a function of temperature.

Study of giant magnetization reversal in Bi_2FeMnO_6, a room temperature magnetodielectric double perovskite

Powder neutron diffraction data collected at the ILL institute allowed a thorough study of both the nuclear magnetic structures of $BiFe_{0.5}Mn_{0.5}O_3$ and their evolution in temperature. The compound shows a complex magnetic behavior characterized by spontaneous magnetization reversal leading to a field-dependent compensation and then to a giant negative response. High resolution neutron diffraction data were collected at the D2B beamline with incident beam wavelengths 1.59 Å at three characteristic temperatures: 10, 310 and 500 K. The data were refined using a distorted perovskite orthorhombic *Pnam* cell with lattice parameters *a*=5.573 Å, *b*= 11.206 Å and *c*=15.743 Å. Thanks to the different scattering factors of iron and manganese in neutron diffraction it was possible to exclude the presence of B-site cation ordering, while no symmetry changes were evidenced in the whole investigated temperature range. The 10 K data show the presence of purely magnetic peaks with propagation vector k = (0 0 0) giving rise to antiferromagnetic G-type magnetic ordering of the B-site transition metals.

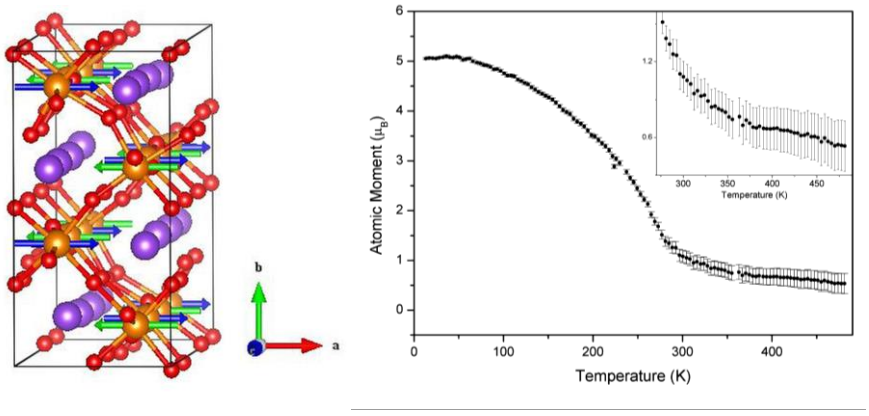

Figure 1. *(left) $BiFe_{0.5}Mn_{0.5}O_3$ magnetic structure. (Right) Refined atomic moment in the 5-500 K range. The inset shows an enlargement of the high temperature region.*

The spin arrangement is shown in Fig. 1, left and involves collinear atomic moments along the *a* direction, with zero component along *b* and *c*, and the presence of isotropic first neighborhood antiferromagnetic interactions.

The high-flux data collected at D1B with λ= 2.52 Å between 10 and 500 K allowed the accurate study of the magnetic structure thermal evolution. On the right panel of Figure 1, the refined atomic moment as a function of temperature is reported, showing a Brillouin-like behavior up to about 290 K, indicating the loss of long range magnetic correlation at this temperature. On the other hand, a weak and broad signal, observed in the 2θ regions where the magnetic reflections are detected, persists up to about 400 K, indicating the presence of small clusters of magnetically ordered TM ions, related to the observed lack of cationic order involving the transition metal atoms. The information provided by neutron diffraction was fundamental in the interpretation of the peculiar magnetization reversal observed in $BiFe_{0.5}Mn_{0.5}O_3$: basing on the completely different ordering temperatures of the solid solution end-members, the mechanism implies, by decreasing the temperature, a composition-dependent progressive ordering of clusters that starts with the iron-rich ones an than extends on the whole solid. The presence of a ferromagnetic component is ascribed to spin-canting, whereas the MRV to the fact that the Fe-Mn interactions, statistically dominant but taking place at lower temperatures, produces a ferromagnetic component which order antiparallel to the preexistent one.