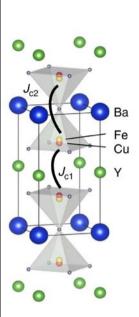
Experimental report

Proposal: 5-23-695				Council: 10/2	016		
Title:	Tuning	Tuning multiferroicity in RBaCuFeO5 perovskites with chemical pressure					
Research	area: Physic	2S					
	-						
This propos	al 18 a contin	uation of 5-31-2380					
Main proposer:		Maria Luisa MEDARDE BARRAGAN					
Experimental team:		Maria Teresa FERNANDEZ DIAZ					
Local contacts:		Maria Teresa FERNA					
C ,							
Samples:	PrBaCuFeO						
	NdBaCuFeC LaBaCuFeC						
	154SmBaCuFeC						
	154SmBaCu 153EuBaCu						
	160GdBaCu						
	TbBaCuFeC						
	DyBaCuFeC						
	HoBaCuFe						
	TmBaFeCu						
	ErBaCuFeO						
	YbBaCuFe						
	LuBaCuFeC						
Instrumer	nt		Requested days	Allocated days	From	То	
				•			
D2B			3	2	09/12/2016	11/12/2016	

We propose to investigate the impact of "chemical pressure" in the crystal structure of the high-temperature magnetoelectric multiferroic YBaCuFeO5 through the replacement of Y3+ by trivalent 4f lanthanide ions. The obtained information should provide insight about the link between the evolution of the multiferroic order temperature and the modification of the lattice due to the lanthanide contraction. This information may help to design other materials with improved multiferroic properties.

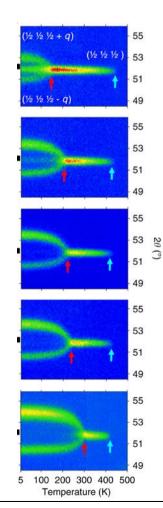
Scientific Report

The goal of this experiment was to investigate additional ways of tuning the spiral ordering



temperature of the layered perovskite YBaCuFeO₅ [1], whose crystal structure is schematically shown in Fig. 1. The renewed interest on material, extensively investigated during the 80's [2,3] due to its parentage with the high-temperature superconductor YBa₂Cu₃O_{6+x}, is the recent observation of magnetism-driven ferroelectricity at an unexpectedly high temperatures. As reported in refs. [4,5], spontaneous electrical polarization develops in YBaCuFeO₅ below T_{N2} ~ 240K, coinciding with a spin-reorientation of the Fe³⁺ and Cu²⁺ magnetic moments [4,5]. This reorientation involves a change in the periodicity of the magnetic order, which is commensurate with the crystal unit cell above T_{N1} (k_c = ½ ½ ½) and becomes incommensurate below this temperature.

Fig. 1. Crystal structure of YBaCuFeO₅ (from ref. 7)

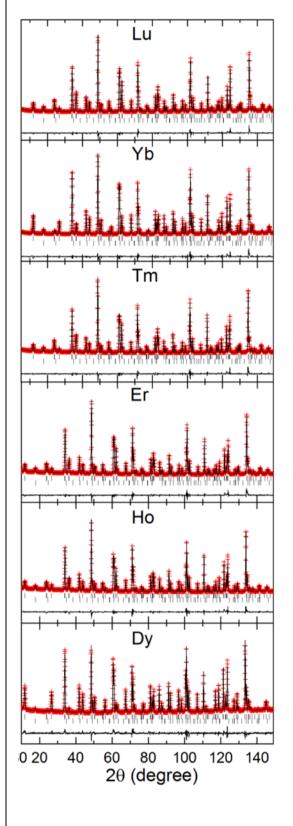


As part of Mickael Morin's PhD work, we recently succeeded to prepare YBaCuFeO₅ ceramic samples of unprecedented quality in our group at the PSI [6]. We also reported the first model for the low temperature incommensurate phase, which is of spiral type. Moreover, we managed to increase the spiral order temperature up to 310K using a novel route based in the targeted manipulation of the Cu/Fe chemical disorder in the structure [7]. As shown in Fig. 1, the spiral order temperature, signaled by the red arrow, is quite low for the sample with the smallest amount of disorder (154K, upper panel), but it increases up to 310K for the most disordered sample (310K, lowest panel). At the same time, the paramagnetic-to-collinear transition temperature (indicated by a blue arrow) displays the opposite behavior. From Fig. 2, it is clear that both temperatures should merge for larger degrees of disorder.

Fig. 2. Low angle part of the neutron powder diffraction patterns of 5 YBaCuFeO₅ samples with different degrees of disorder (from ref. 7)

Fig. 3. Neutron powder diffraction patterns of the RBaCuFeO₅ layered perovskites at RT measured at D1B using 1.59A.

In the present experiment we have tried to reach this limit by combining a maximal chemical



disorder with a targeted manipulation of some magnetic exchange couplings. For this purpose we prepared the RBaCuFeO₅ series (R = Lu, Yb, Tm, Er, Ho, and Dy) aimed to change Jc1 (see Fig. 1). Unfortunately. highest the spiral transition temperature, which corresponds to R = Dy, was 312K, only slightly higher than in the case of quenched YBaCuFeO₅ (see Fig. 2). Nevertheless, the data recorded on D2B (Fig. 3) allowed to understand the reasons of this behavior. These results, combined with those extracted from data obtained at the Swiss neutron source SINQ for other layered perovskites, were recently accepted for publication in Science Advances

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