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ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Role of the coupling between transition-metals and rare-earths in the metamagnetic behaviour of Ba_2LnFeO_5 perovskite derivatives	**Experiment number:** HC-2350
Beamline: ID12	**Date of experiment:** from: 08/04/16 to: 11/04/16	**Date of report:** 03/07/2016
Shifts: 12	**Local contact(s):** F. Guillou	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

In oxides containing both transition-metal (*3d*) and rare-earth (*4f*) cations, the *3d-3d* interaction is largely predominant in the overwhelming majority of cases. As a general rule, the *3d-4f* and *4f-4f* interactions only play a role at temperatures much lower than the magnetic spin ordering, which is itself dictated solely by the *3d-3d* coupling. Recently, we synthesized a new family of perovskite derivatives in which the *3d-3d* and *3d-4f* interactions turn out to be of comparable strengths [1]. These compounds of formulation Ba_2LnFeO_5 (Ln = Sm, Eu, Gd, Dy, Ho, Er, Yb, as well as Y) exhibit a peculiar lattice structure in which isolated FeO_4 tetrahedra are linked by LnO_6 octahedra. As a result, the usually strong superexchange (SE) Fe-O-Fe coupling is absent and one is left in a situation where only a weaker super-superexchange (SSE) Fe-O-O-Fe mechanism competes with SE Fe-O-Ln. Magnetic and calorimetric measurements showed that each of these Ba_2LnFeO_5 compounds exhibits a unique, antiferromagnetic transition involving both the *3d* and *4f* ions. When applying magnetic field at $T \ll T_N$, the magnetization curves display puzzling behaviors depending on the *4f* cation. It remains that the interpretation of the metamagnetic-like effects is hard to establish on the basis of bulk magnetometry only. XANES/XMCD experiments have been carried out at the Fe K-edge and Ln $L_{2,3}$-edges in order to disentangle the transition-metal and rare-earth contributions in the global magnetic response of a few representative Ba_2LnFeO_5 compositions.

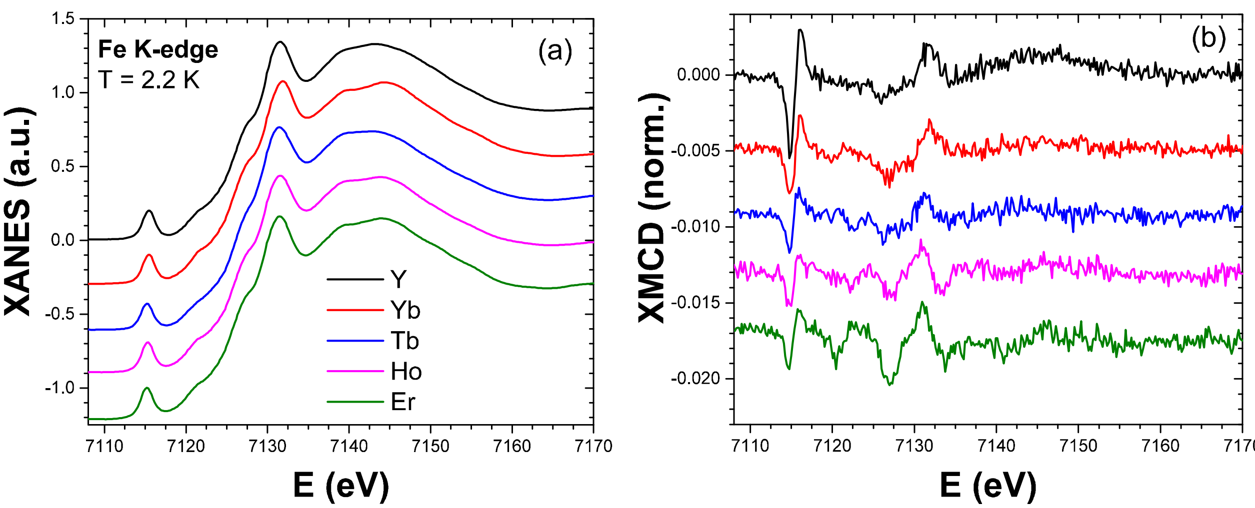

Fig.1. (a) Isotropic x-ray absorption spectra (XANES) at the Fe K-edge of selected Ba_2LnFeO_5. (b) Corresponding X-ray magnetic circular dichrosim (XMCD) spectra.

The Fe K-edge XANES and XMCD spectra measured at T = 2.2 K are presented in Fig.1. One can observe a great similarity of both the XANES and XMCD spectral shapes for all Ba_2LnFeO_5 materials. The five selected compositions present an intense pre-peak on the XANES spectra particularly pronounced due to the tetrahedral environment of Fe. It is associated with the largest XMCD feature in Fig .1(b). It should be highlighted that the XMCD spectral shape of the Ba_2LnFeO_5 Ln= Yb, Tb, Ho, Er is similar to that of Ba_2YFeO_5. This is a crucial point for further analysis, as it demonstrates that the Fe K-edge XMCD is not dominated by hybridization with rare-earth states, so that the Fe K-edge XMCD truly represents the Fe (*4p*,*3d*) moments.

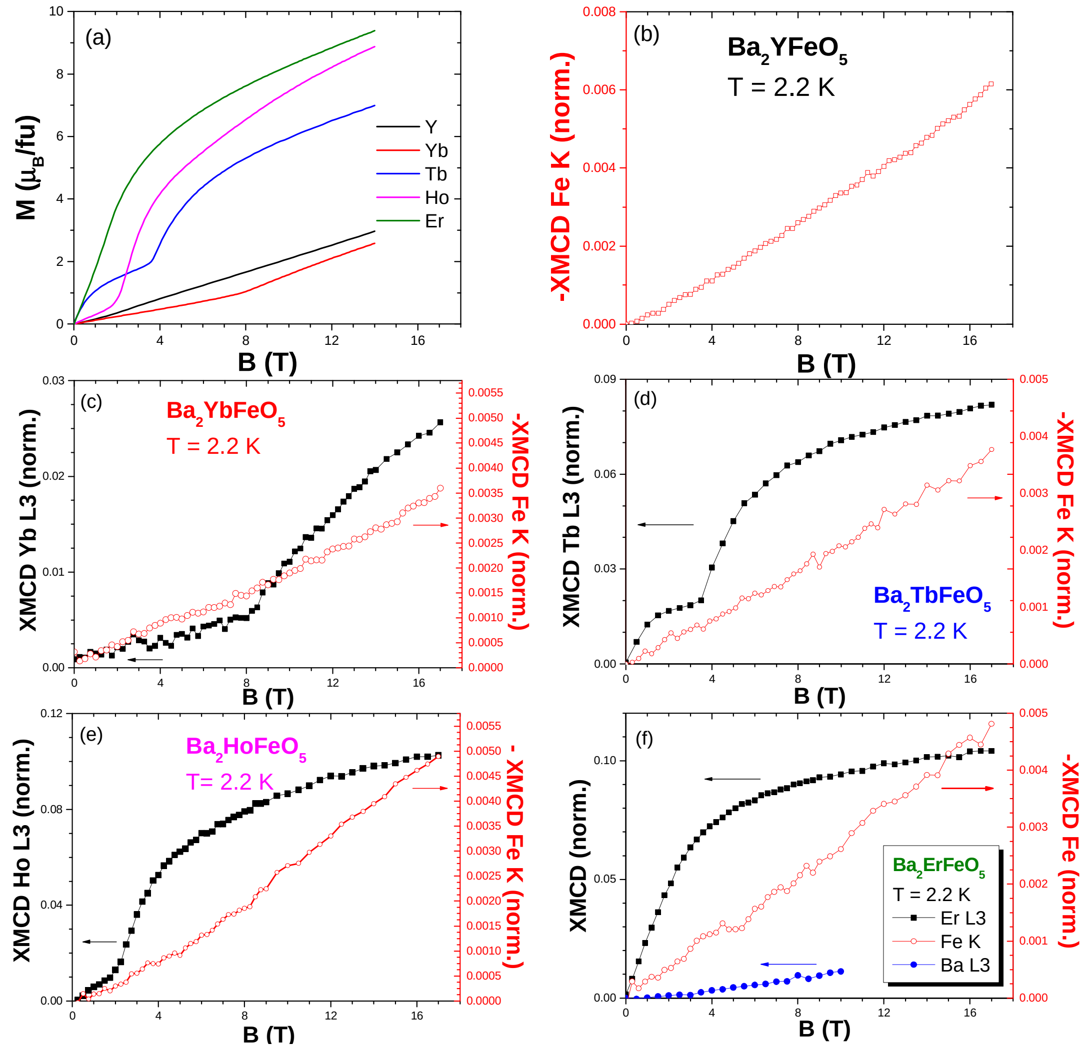

Fig.2. (a) Bulk magnetization measurments. (c)-(f) XMCD as a function of the magnetic field.

XANES and XMCD spectra were measured at the $L_{2,3}$ edges of Yb, Tb, Ho and Er in Ba_2LnFeO_5 materials (an attempt has been done on Y, but unsuccessful due to diffraction peaks). From these XMCD spectra, an energy point has been selected, and its field dependence recorded from -17 to +17 T. Fig. 2 (b) to (f) shows the field dependence of the rare-earth XMCD in regards to that of Fe in the same conditions. One can clearly see that the rare-earth contribution mimics the bulk magnetization measurements shown in Fig. 2 (a), in particular it accounts for most the metamagnetic jump, while the change in curvature on Fe turns out to be rather small.

In addition, Ba XMCD spectra were measured at L_2 and L_3 for Ba_2ErFeO_5. Besides being one of the first measurements of XMCD on barium, these data also show that the induced moments on Ba are dominated by hybridization with Fe states.

To sum up, element specific magnetic information were successfully obtained by XMCD as a function of the magnetic field. At first sight, these data are well suitable to bring new insights into the metamagnetic behavior observed in bulk magnetometry experiments. Further analyses are in progess.

REF: A. K Kundu, V. Hardy, V. Caignaert, and B. Raveau, J. Phys.: Condens. Mat. 27, 486001 (2015).