ESRF	**Experiment title:** Rationalization of the molecular packing influence on the properties of a Single Ion Magnet by an in situ SXRD and XRR study.	**Experiment number**: HC-631
Beamline: ID03	**Date of experiment**: from: 26/06/2013 to: 02/07/2013	**Date of report**: 31/08/2013
Shifts: 18	**Local contact(s)**: Jakub Drnec	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Roberta Sessoli (Dipartimento di Chimica, Universita' degli studi di Firenze)

Matteo Mannini (Dipartimento di Chimica, Universita' degli studi di Firenze)

Luigi Malavolti (Dipartimento di Chimica, Universita' degli studi di Firenze) *

Valeria Lanzillotto (Dipartimento di Chimica, Universita' degli studi di Firenze) *

Giovanni Lepore (Dipartimento di Scienze della Terra, Universita' degli studi di Firenze) *

Francesco Carla' (ESRF, Grenoble) *

Report:

As described in the proposal the purpose of the experiment was to investigate the relation between structural properties, film thickness and magnetic behaviour of $TbPc_2$ films deposited on Au(111).

The orientation of molecules in such kind of systems shows a dependence on coverage. For monolayers and thin film molecules are absorbed flat on the surface whereas stand up as the film grows thicker molecules[1]. For the $TbPc_2$/Au(111) system some structural information have been deduced by magnetic properties (extracted by an XMCD experiment)[1] but so far only little is known about the bulk structure of this thin films excluding the STM characterization of monolayer deposits[2].

Our experiment at ID03 started with a characterization of samples grown on Au/mica prepared *ex situ* before the experiment. Extended reflectivity data clearly shows a preferential orientation in the crystalline structure of the film along the direction perpendicular to the surface. Unfortunately due to the poor quality of the substrate was impossible to identify an epitaxial relation between the Au and the film lattice. Nevertheless the *ex situ* sample analysis allowed us to get extremely valuable information about reciprocal space position of the $TbPc_2$ structure on Au.

As planned, the experiment proceeded then with the *in situ* growth of $TbPc_2$ thick films on Au(111) bulk single crystal. Structural evolution of the film was investigated during the growth monitoring reciprocal space position where Bragg peaks from film structure were

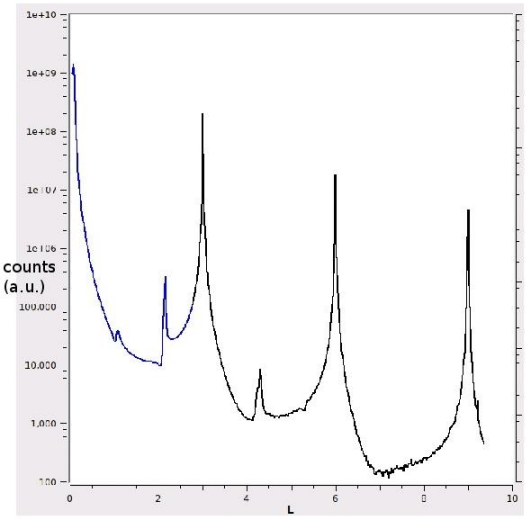

Fig. 1 Extend reflectivity of Au(111)/TbPc2 (extimated thickness: 60MLs)

supposed to appear (as observed on the test ex-situ samples). Due to radiation damage we decided to repeat the control measure used for the growth control process only every 30 minutes during the growth. As the thickness of about 60MLs was reached a short characterization of few rods was performed before cooling down the sample to 20K in order to perform further investigation in condition where beam damage could be limited.

No significant changes in the film structure was induced by the temperature change.

A complete characterization of the film structure was performed measuring an hk mesh at a complete rod set.

Data clearly show that the film is crystalline up to the thickness reached during the experiment and no molecules crystallized in powder-like structure are present on the surface. The structure of the film appears to be ordered respect to the Au main axis as an epitaxial relation is present with the Au(111) substrate. Nevertheless given the complexity of the substrate (substrate surface is Herringbone reconstructed) this matter will be object of a further investigation. A detailed analysis of the data is presently in progress.

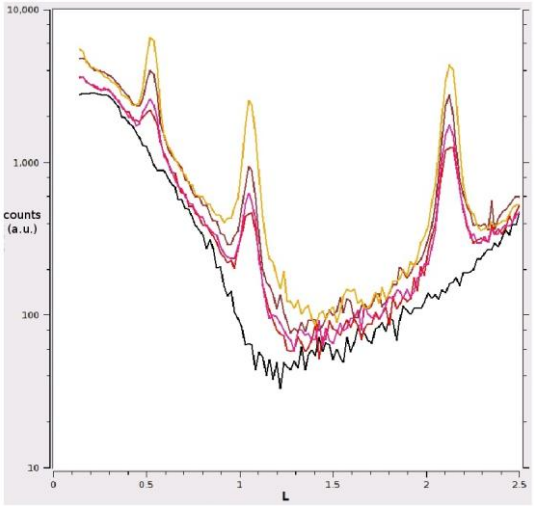

Fig. 2 TbPc2 growth monitored measuring surface rod at h=-.102, k=.213

References

[1] L. Margheriti, D. Chiappe, M. Mannini, F. Pineider, P. Sainctavit, L. Joly, A. Fraile-Rodriiguez, M.-A. Arrio, C.C. dit Moulin, W. Wernsdorfer, A. Cornia, D. Gatteschi, Others, P.P.-E. Car, F.B. de Mongeot, J.C. Cezar, F.M. Piras, A. Magnani, E. Otero, A. Caneschi, R. Sessoli, Adv. Mater. 22 (2010) 5488.

[2] K. Katoh, Y. Yoshida, M. Yamashita, H. Miyasaka, B.K. Breedlove, T. Kajiwara, S. Takaishi, N. Ishikawa, H. Isshiki, Y.F. Zhang, T. Komeda, M. Yamagishi, J. Takeya, J. Am. Chem. Soc. 131 (2009) 9967.