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:** **Mn lattice positions in topological crystalline insulators investigated by x-ray standing wave method**	**Experiment number**: HC-1424
Beamline:	**Date of experiment**: from: 30. 4. 2014 to: 6. 5. 2014	**Date of report**: 28.7.2014
Shifts:	**Local contact(s)**: Oleg Konovalov	*Received at ESRF:*

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Report:

Topological crystalline insulators (TCIs) are new class of topological insulators where topological surface states are protected by crystal symmetries and not by time reversal symmetry as in the so far intensively studied Z_2 topological insulators such as Bi_2Se_3, Bi_2Te_3 or Bi_xSb_{1-x}. In a recent paper, Fu has predicted that SnTe and the ternary alloys of SnTe or SnSe with PbTe and even MnTe have the proper crystal group symmetry to qualify them for a novel manifestation of nontrivial topology [1].

By Mn doping with concentrations up to 15% ferromagnetic order up to above 20 K has been observed in $Pb_{1-x-y}Sn_xMn_yTe$[2,3] due to free carrier mediated RKKY interactions. In the ongoing discussion on the origin of surface band gaps in magnetically doped topological insulators of the Z_2 class, the role of surface, bulk impurities and vacancies has been pointed out in Ref. [4] and has recently been invoked in the interpretation of temperature independent band gaps in $(Bi_{1-x}Mn_x)_2Se$ [5] where an appreciably amount of Mn was found to be incorporated non-substitutionally.

The aim of the beamtime was to contribute to the solution of the crucial problem of the lattice positions of Mn ions in SnTe and SnSe, using x-ray standing-wave technique. We have investigated a series of $Sn_{1-x}Mn_xTe$ layers with various Mn content x, deposited by molecular beam epitaxy onto (111)BaF_2 substrates. The experiments have been performed in a standard diffraction setup, using the photon energy of 10 keV, a linear detector for diffracted radiation and a solid-state fluorescence detector.

For each sample in the series, we have measured standard coplanar reciprocal-space maps (symmetric in diffractions 111, 222, 333 as well as asymmetric 331), standard specular reflectivity scans, and the dependence of the fluorescence spectra on the grazing-incidence angle α_i. For selected samples, we have performed x-ray standing-wave (XSW) scans in asymmetric diffraction $22\bar{2}$. In Figs. 1-3 we displayed examples of measured data for sample with the Mn content of 4%.

From the reciprocal-space maps we determine the lattice parameters of the layer as well as the degree of plastic relaxation of the layer with respect to the substrate. From the α_i-dependence of the fluorescence intensities of various elements we determine the vertical profile of chemical composition of the layers and confirm their chemical homogeneity.

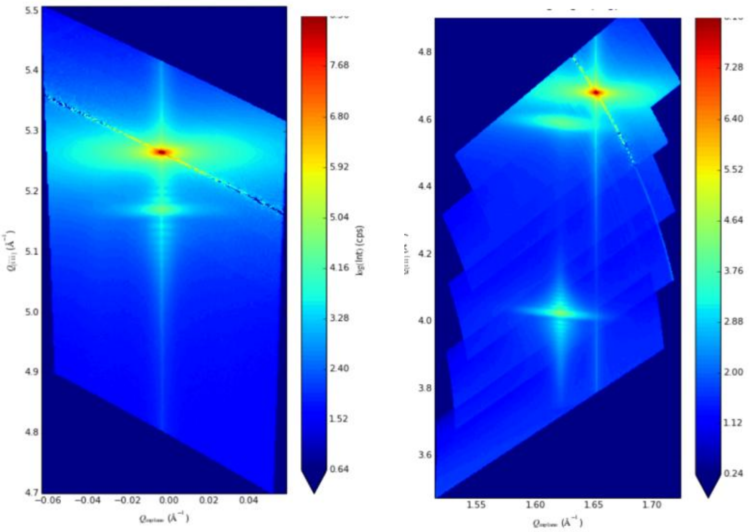

Fig. 1: Coplanar reciprocal space maps of the sample x_{Mn} = 4% taken in symmetric 333 (left) and asymmetric 331 diffractions (right).

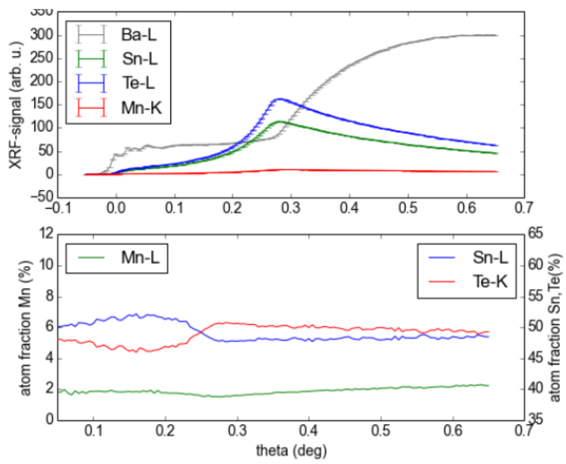

Fig. 2: Dependence of the fluorescence intensities on the glancing incidence angle, sample x_{Mn} = 4%

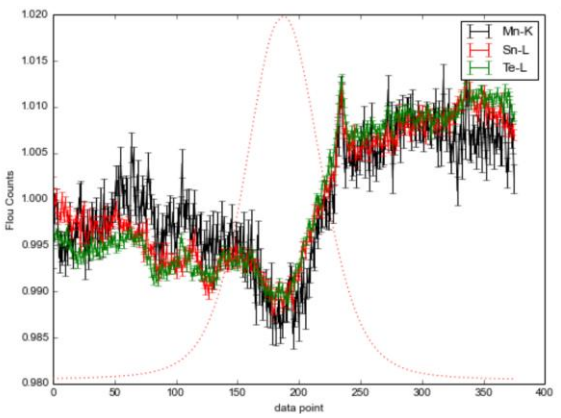

Fig. 3: X-ray fluorescence intensities from sample x_{Mn} = 4% as functions of the angular deviation from then diffraction maximum (XSW curves). The dotted line represents the measured diffraction maximum (not in vertical scale).

The analysis of the XSW curves is complicated by two facts: (i) the fluorescence detector was almost saturated by the $BaL_{1,2,3}$ fluorescence lines from the substrate, and (ii) the epitaxial layers consist of randomly rotated mosaic blocks caused by the mosaic structure of the substrate. The presence of the mosaic blocks is not apparent from omega/2theta diffraction scans, but it is obvious from the reciprocal space maps in Fig. 1.

The following analysis of the data will concentrate to a detailed comparison of measured diffraction data with simulations based on dynamical diffraction theory. We hope that from the structure factors of the layer in diffractions 111, 222, 333 and 331 it will be possible to determine unambiguously the Mn lattice positions. The XSW data will be analysed as well, however the analysis will not be straightforward, due to the facts mentioned above.

[1] Liang Fu, Phys. Rev. Lett. **106**, 106802 (2011).
[2] A.J. Nadolny *et al.*, J. Magnetism Mag. Mater. **248**, 134 (2002).
[3] P. Lazarczyk *et al.*, J. Magnetism Mag. Mater. **169**, 151 (2002); T. Story et al. Phys. Rev. Lett. **56**, 777 (1986).
[4] A.M. Black-Schaffer and A.V. Balatsky, Phys. Rev. B **86** 115433 (2012) and Phys. Rev. B **86**, 115433 (2012).
[5] J. Sanchez-Barriga et al., submitted.