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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:** Structural characterization of topological insulators epitaxial layers	**Experiment number**: SI-2461
Beamline: BM-20	**Date of experiment**: from: 27.7.2012 to: 1. 8. 2012	**Date of report**: 28.8.2012
Shifts: 15	**Local contact(s)**: Carsten Baehtz	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

The topological insulators are recently found family of materials. These materials have in bulk a band gap so that they behave like ordinary insulators or semiconductors, but they exhibit in addition a gapless surface or edge states that are topologically “protected” and immune to impurities or geometrical perturbations (see the reviews [1,2]). The aim of the experiment was to study structural defects in the epitaxial layers of topological

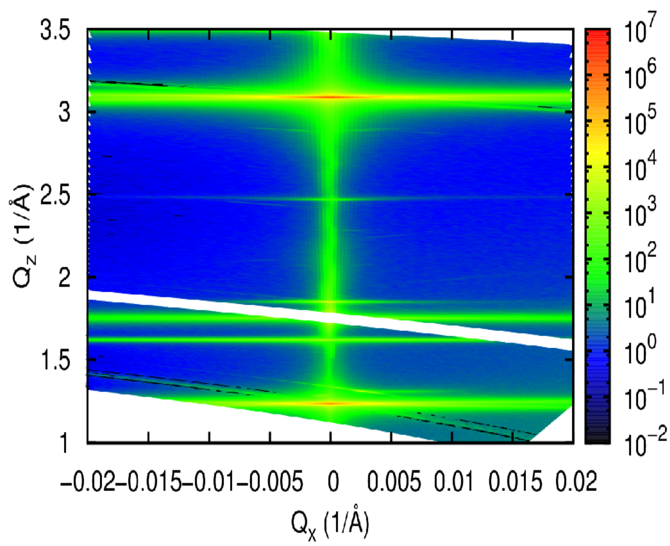

Fig. 1: Reciprocal space map along symmetric truncation rod measured on the 500 nm thich Bi_2Te_3 layer grown on BaF_2 substrate.

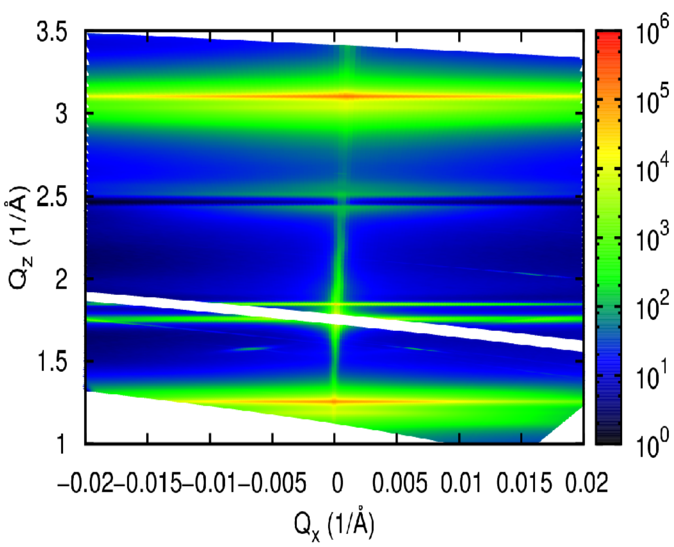

Fig. 2: Reciprocal space map along symmetric truncation rod measured on the 500 nm thich $(Bi,Mn)_2Te_3$ layer grown on BaF_2 substrate. The nominal Mn concentration is 3%.

insulators and to correlate the structural quality of the layers with the electronic structure of the layers studied using angle-resolved photo-electron spectroscopy measurements.

The samples were grown using molecular beam epitaxy on the cleaved BaF_2 (111) substrates. The thickness of the layers was 300 nm to 500 nm. We have studied the samples of pure Bi_2Te_3 and Bi_2Se_3 layers as well magnetic layers of $(Bi,Mn)_2Se_3$ and $(Bi,Mn)_2Te_3$ layers. The nominal Mn concentration of the layers was up to 10 %.

We have measured the x-ray scattered intensity in the vicinity of several symmetric and asymmetric x-ray diffractions as well as the intensity on the truncation rods between them in the symmetric and asymmetric along lines 0 0 0 L and 1 0 $\bar{1}$ L, respectively, where we have used the hexagonal notation of the unit cell.

The pure Bi_2Te_3 and Bi_2Se_3 layers has shown the nearly perfect crystalline structure, while the Mn doped samples present some deviations as shown in Fig 1, 2 and 3 for the Mn doped Bi_2Te_3. The most obvious are the shifts of 0 0 0 6 and 0 0 0 15 diffraction peaks and the split of the 0 0 0 12 diffraction peak in two distinct maxima. Very similar features were observed for the Bi_2Se_3 layers.

The detailed analysis of the obtained data is currently in progress. The preliminary analysis is based on the Monte Carlo simulation of the diffraction pattern on the random alloy of Bi_2Te_3 and Bi_3Te_4. Bi_2Te_3 crystals can be described as a stack of quintuplet layers (QL, two hexagonal Bi layers and three Te), whereas the unit cell of Bi_3Te_4 consists of seven monolayers (three Bi layers and four Te layers), i.e. the model calculates random combination of Bi2Te3 and Bi3Te4. The model shows similarity with the experimentally observed shifts of the diffraction peaks as well as splitting of the weak 0 0 0 12 diffraction maxima. Further improvement of the model will be based on the adding Mn atoms in the crystal lattice.

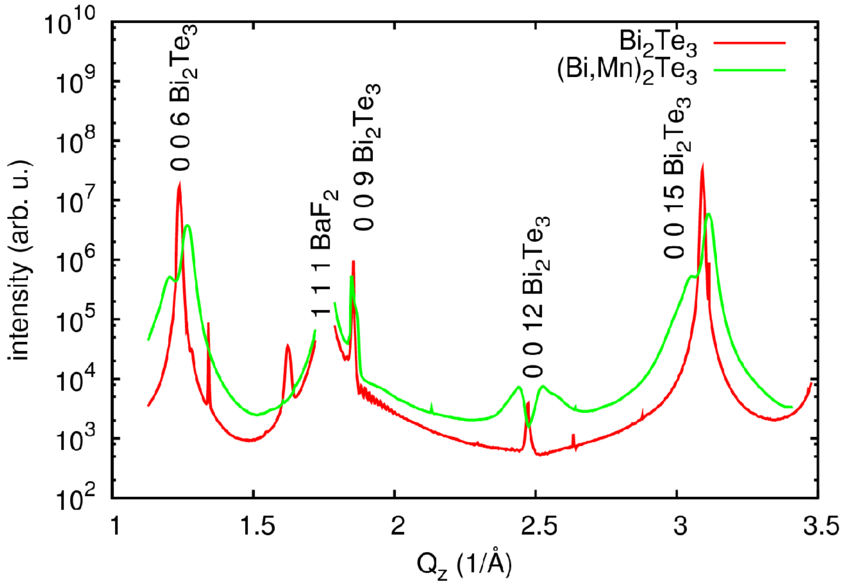

Fig. 3: Comparison of the symmetric scans along the symmetric truncation rod extracted from the previous figures 1 and 2 of the pure and Mn doped Bi_2Te_3 epitaxial layer grown on BaF_2 substrate. The vicinity of the substrate BaF_2 111 peak is skipped.

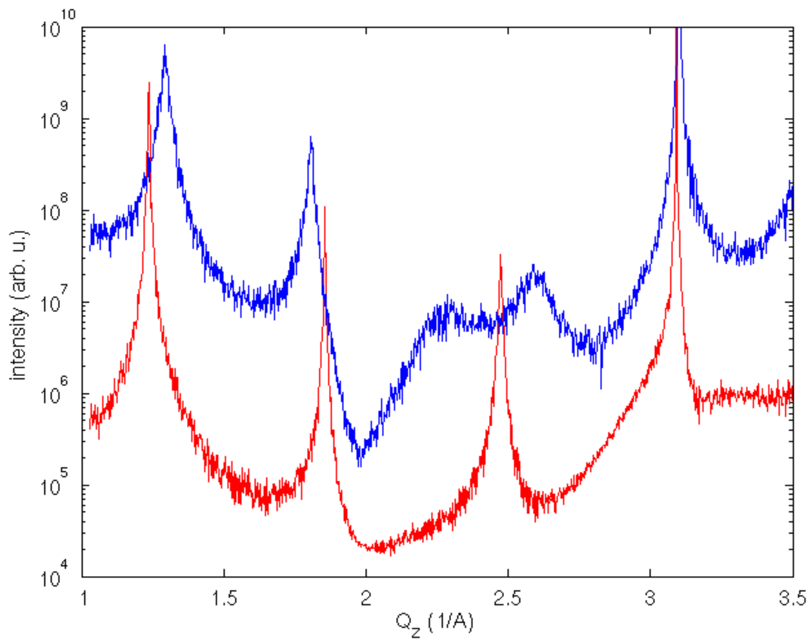

Fig. 4: Monte Carlo simulation of x-ray scattered intensity along symmetric truncation rod of pure Bi_2Te_3 (red curve) and the random alloy of Bi_2Te_3 and Bi_3Te_4 (blue curve).

References

[1] X. L. Qi and S. C. Zhang, Physics Today **63**, 33 (2010).

[2] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).