EUROPEAN SYNCHROTRON RADIATION FACILITY

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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:** Surface x-ray diffraction from crystalline topological insulators $Pb_{1-x}Sn_xSe$	**Experiment number**: HC1434
Beamline: ID03	**Date of experiment**: from: 1.10.2014 to: 7.10.2014	**Date of report**: 10.2.2015
Shifts: 18	**Local contact(s)**: Jakub Drmec	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

Crystalline topological insulators (CTI) are a new class of materials, in which the topological surface states are protected by the mirror symmetry of crystal lattice and not by the time-reversal symmetry, as for case of more intensively studied conventional topological insulators (TI) of the Z_2-class such as Bi_2Se_3 and Bi_2Te_3 [1-4]. During the beamtime, we have performed a systematic CTR-scattring study with the goal to determine the influence of the surface termination on the surface reconstruction and relaxation of the CTI compounds (PbSn)(TeSe), which are expected to affect the topological surface states as well.

Investigated samples $Pb_xSn_{1-x}Te$ and $Pb_xSn_{1-x}Se$ with various chemical compositions were grown by MBE at Institute of Semiconductor Physics, J. Kepler University in Linz, Austria, on BaF_2 (111) substrates. The surfaces of the grown layers were protected by 300nm Te or Se capping layers on Te- and Se-containing layers, respectively. The cap layers were removed in a UHV chamber at the beamline just before the CTR measurement by ion sputtering followed by heating to obtain clean surfaces. The heating temperatures and times as well as the sputtering duration slightly differ from sample to sample. Especially the sputtering rates are also expected to be very different due to the different electrical conductivity of the films and substrates. The removal of the capping was checked visually during heating. Selected samples were investigated also by Auger spectroscopy before and after decapping. Before decapping, carbon peaks in the Auger spectra were observed, however no signal of oxygen was present. After the decapping procedure, the carbon signal disappeared as well, which demonstrated a good chemical cleanness of the surface.

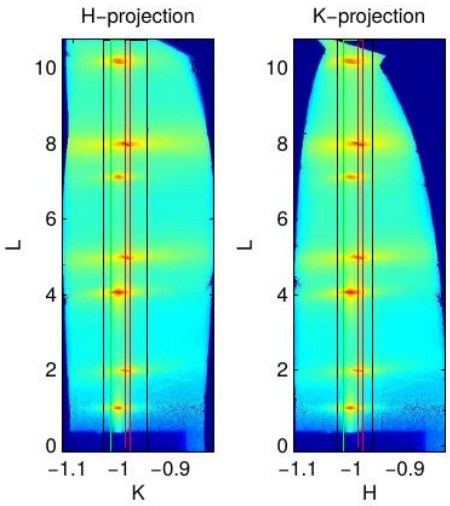

Fig. 1 Example of raw measured data projected to the 0KL (left) and H0L (right) reciprocal planes

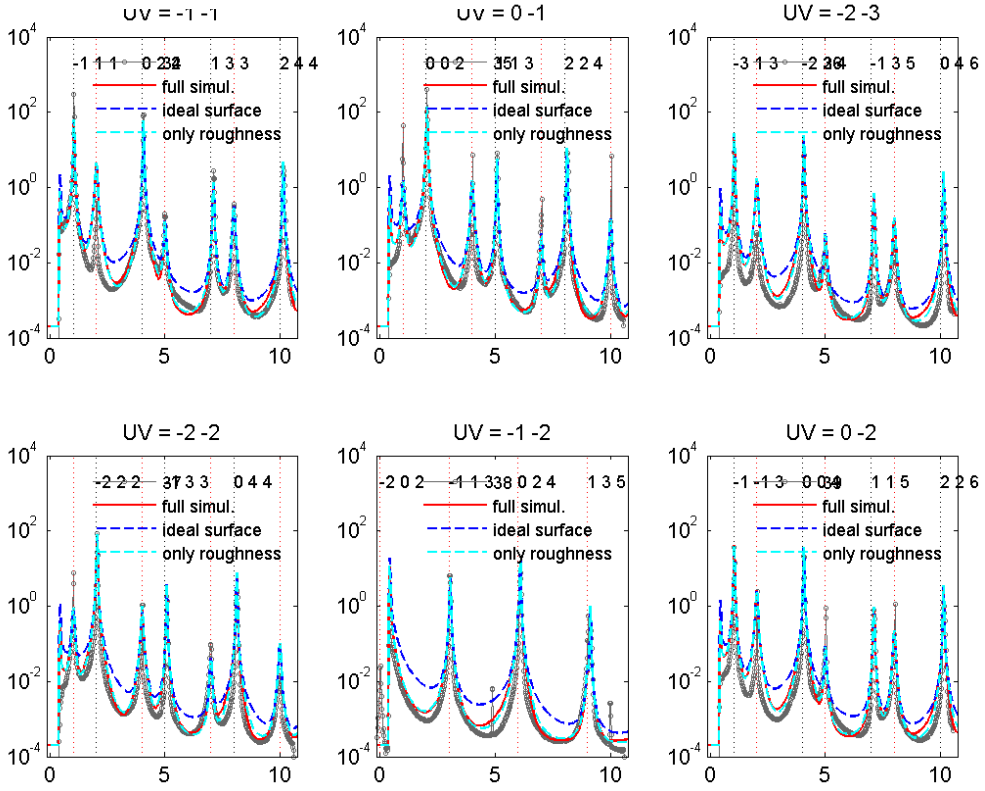

Fig. 2. Exaples of measured and simulated CTR scans measured along various non-symmetric CTRs. The vertical dotted lines denote the layer maxima (black) and the maxima of diffuse scattering from thensubstrate (red).

The crystal truncation rod (CTR) scans were carried out in the UHV chamber, using the photo energy of 24keV. The scattering geometry was vertical (i.e. the sample was mounted horizontally). The diffracted beam was measured by a two-dimensional detector. We used routines [5] for the extraction of specular and non-specular CTR scans from the measured data and for their conversion from the angular space to the reciprocal hkl-space; the routines were available at the beamline. The routines also corrected the experimental data for the limited experimental resolution and other experimental artifacts, like variable irradiated footprint etc.

Recently, the measured and corrected data are compared with simulations based on kinematical diffraction. In the simulations we took into account surface relaxation by introducing inhomogeneous vertical strain at the surface, the surface roughness was considered by using the standard beta-model of rough surfaces [6].

Figure 1 shows as an example raw data measured by a 2D detector and projected to the H0L and K0L planes. In Fig. 2 we present a preliminary comparison of the measured and simulated CTR scans.

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[4] P. Dziawa et al., Nature Materials **11**, 1023 (2012).
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[6] I. Robinson, Phys. Rev. B **33**, 3830-3836 (1986).