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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

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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.

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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 and interface structure of the clean and adsorbate (Cs, Fe, Ag) covered Topological Insulator Bi_2Se_3(0001)**	**Experiment number**: HC-906
Beamline:	**Date of experiment**: from: Jan. 22, 2014 to: Jan. 28, 2014	**Date of report**: Feb. 19, 2014
Shifts:	**Local contact(s)**: Juan Rubio-Zuazo	*Received at ESRF:*

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Report:

It was the aim of the experment to study the atomic structure of the clean and adsorbate covered (0001) surface of bulk Bi_2Se_3. As adsorbates we have chosen Cs, Fe and Ag due to the special interest concerning the adsorbate induced modifications of the topological surface state [1,2].

The experiments were the first to use the MAXIPIX two dimensional (2D) pixel detector at this beamline (BM25b). We could successfully carry out several experiments by collecting data from clean Bi_2Se_3(0001) and Cs covered Bi_2Se_3. Due to some technical problems with the vacuum in the diffractometer (≈5 shifts lost) there was no time left to collect data from Fe/Bi_2Se_3 and Ag/Bi_2Se_3. Although the experiments have been completed only three weeks ago we have already analyzed the atomic strcuture of the Bi_2Se_3(0001) surface, which will shortly be outlined in the following:

Fig.1 shows two representative crystal truncation rods (CTRs) each consisting of about 260 data points between L=2 and L=15 reciprocal lattice units. The whole data set including seven CTRs consists of more than 1500 reflections allowing an analysis of unprecedented accuracy. Symbols and lines correspond to experimental and calculated structure factor amplitudes, respectively. Integration and background subtraction of the raw (image) data were carried out by using the Python software. Excellent fits could be achieved using the structure model shown in Fig.2.

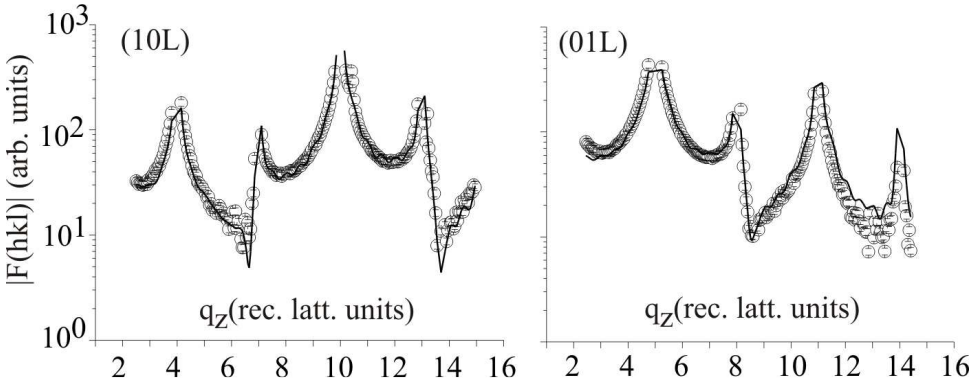

Fig.1: Experimental (symbols) and calculated (lines) structure factor amplitudes for the (10L) and (01L) CTR of bulk Bi_2Se_3(0001).

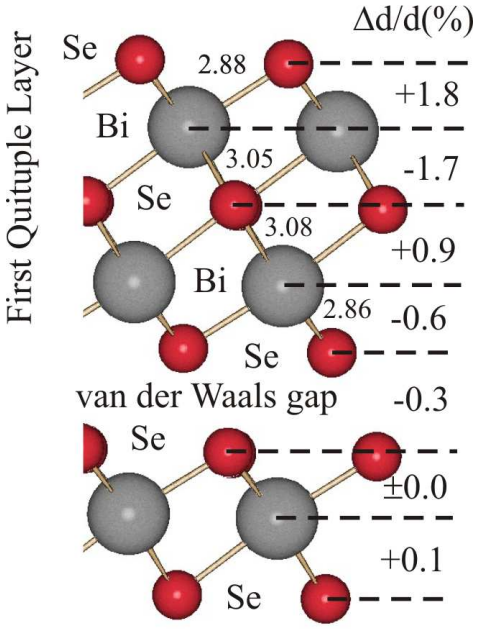

Fig.2. Structure model for Bi_2Se_3(0001). Numbers on the right label relaxations in percent of the bulk spacing or interatomic distances in Å.

The are some relaxations within the first quintuple layer. Most importanlty, we find a 2% *expansion* of the top interlayer spacing between the first Se- and the second Bi-layer. This unusual expansion is related to some contamination by small amounts of carbon which is also responsible for some modifications of the electronic structure as will be reported elsewhere [3]. Secondly, there is no substantial relaxation of the first van der Waals gap.

Based on this model we achieve an un-weighted R value in the 12% range. This can be improved by allowing for anisotropic disorder. We emphasize that the use of the 2D detector is essential, not only for the reduction of the measurement time but also for the proper integration of the reflection intensities in the presence of several crystalline grains which is typical for this class of materials.

In a second experiment we have dosed Cs in an amount of approximately one monolayer on the clean Bi_2Se_3(0001) surface. Notable changes of the intensities along the CTRs are observed. The data analysis is still in progress.

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References:

[1] T. Valla, Z.-H. Pan, D. Gardner, Y.S. Lee, and S. Chu, Phys. Rev. Lett. 108, 117601 (2012); [2] M. R. Scholz, J. Sanchez-Barriga, D. Marchenko,A. Varykhalov, A. Volykhov, L. V. Yashina, and O. Rader, Phys. Rev. Lett. 108, 256810 (2012); [3] S. Roy, H. L. Meyerheim, A. Ernst, K. Mohseni, C. Tusche, E. Chulkov, M.G. Vergniory, J. Schneider, and J. Kirschner, unpublished