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 using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now 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:** **The geometric and electronic structure of the topological insulator Fe/$Bi_2(Te,Se)_3$ (0001)**	**Experiment number**: SI-2560
Beamline: **ID03**	**Date of experiment**: from: 22/10/2012 to: 31/10/2012	**Date of report**: *Received at ESRF:*
Shifts: **18**	**Local contact(s)**: **Dr. Juan RUBIO-ZUAZO**	
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Report:

It was the aim of the experiment to prepare a clean (0001) oriented surface of the topological insulator Bi_2Se_3 and to deposit submonolayer amounts of Fe followed by a thorough structure analysis by surface x-ray diffraction. Simultaneously high-energy x-ray photoemission (HAXPES) spectra were recorded. The experiments could be carried out successfully. Several unexpected results were obtained, one of them is discussed in the following:

Dosing of Fe on the clean Bi_2Se_3 (0001) surface at room temperature followed by mild (250°C) annealing leads to a reaction between Fe and the substrate, most likely involving an alloying of Fe with Bi. We found a complex superstructure.

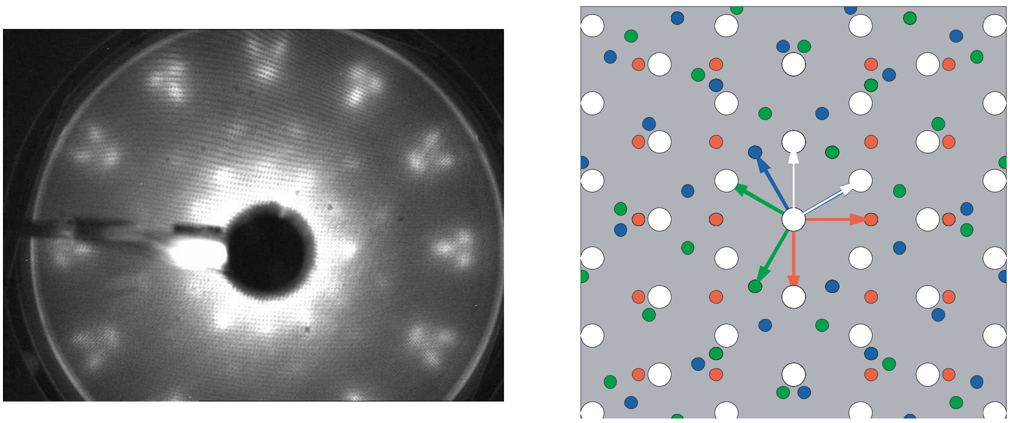

Figure 1: LEED pattern (E=92 eV) for about one monolayer Fe deposited on Bi_2Se_3(0001) (left) togther with simulation (right). The large white circles correspond to the (1x1) substrate reflections, the smaller colored ones to three different domain reflections of the superstructure. Note, that in the experiments not all reflections can observed (resolved) simultaneously at a given electron energy.

Fig.1 shows on the left side the LEED pattern (E=92 eV) together with the simulated pattern (right) revealing that the LEED pattern corresponds to a superstructure which forms three domains of a quadratic two-dimensional lattice (a_0=b_0=3.59 Å) which is related to the hexagonal lattice of the Bi_2Se_3 substrate by the matrix elements a_{11}=1, a_{12}=0, a_{21}=-1/√3, a_{22}=2/√3.

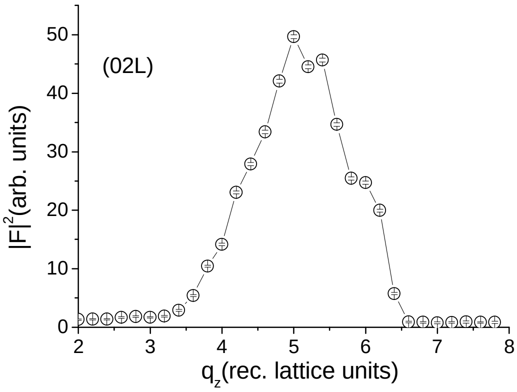

Fig.2: Experimental structure factor intensities along the (02L) superlattice rod of Fe/Bi_2Se_3 (0001). Other rods exhibit a similar shape with a maximum near 5 r.l.u.

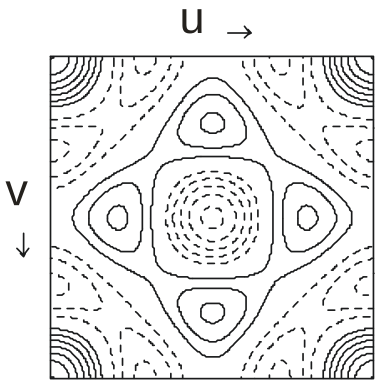

Fig.3: Projected Patterson-function [P(u,v)] of the superstructure derived from seven (near) in-plane structure factors. With the most prominent feature being the trivial maximum at (0,0), P(u,v) points to a simple structure.

Several superlattice rods (SLR's) were measured, one of them (02L) is shown in Fig.2. All SLR's show an overall similar shape along q_z with a maximum at around 5 rec. latt. Units with q_z referred to the Bi_2Se_3 c-lattice constant of 28.64 Å. This maximum corresponds to an interatomic correlation of about 5.7 Å along the c-direction. The similarity of all the rods points to a simple structure. This view is also supported by the projected Patterson function, P(u,v) which is shown in Fig. 3 and which was derived from seven in-plane superlattice reflections. Apart from the trivial maximum at the origin, there is only one weak (positive) peak at (u,v)≈ (0.20, 0.50), which even might be attributed to a truncation error.

In summary, we have investigated the structure of Fe deposited in monolayer amounts on the topological insulator Bi_2Se_3. Our results suggest that there is a strong interaction between Fe and the substrate involving a thorough reorganisation of the surface structure leading to an uniaxially incommensurate superstructure. The possible formation of an alloy structure even in the bulk has been reported recently [1]. In view of the widely discussed physical properties of the Fe/Bi_2Se_3(0001) interface [2-4] our results rises the question whether discrepancies in the results reported so far might be attributed to the formation (reaction) of different surface structures depending on subtle differences in the sample preparation (e.g. sample temperature). The analysis of the HAXPES data is in progress.

References:

[1] A. Adam, Mat. Res. Bull. 42, 1986 (2007)
[2] L.A. Wray, Su-Y. Xu, Y. Xia et al., Nat. Phys. 7, 32 (2010)
[3] M.R. Scholz et al., Phys. Rev. Lett. 108, 256810 (2012)
[4] J. Honolka, A.A. Khajetoorians, V. Sessi et al., Phys. Rev. Lett. 108, 256811 (2012)