EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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: Structure Analysis of the Ultra-Thin (BiSe)-TaSe2 Charge Density Intercalation Compound Prepared by Interface Reaction with Bi2Se3(0001).**	**Experiment number**: HC-3510
Beamline:	**Date of experiment**: from: 4.4.2018 to:11.4.2018	**Date of report**:
Shifts:	**Local contact(s)**: Dr. J. Rubio-Zuazo	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

(1) H. L. MEYERHEIM *(MPI f. Mikrostrukturphysik, D-06120 Halle (Germany)*
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Report:

It was the aim of the experiment to carry out SXRD experiments to study the atomic structure of an ultra-thin (BiSe)-$TaSe_2$ charge density intercalation compound prepared by interface reaction with Bi_2Se_3(0001).The experiments could be carried out very successfully. The data analysis has shown that an ultra-thin H-type $TaSe_2$ structure is formed rather than the intercalation compound.

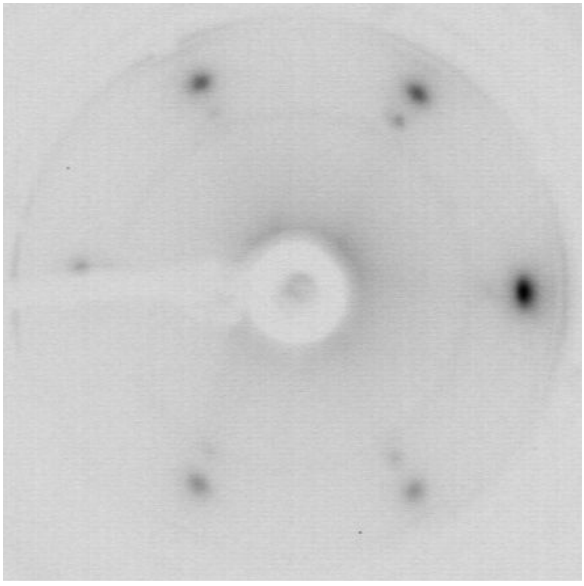

Fig.1 LEED pattern of $TaSe_2/Bi_2Se_3$(0001) The electron energy is equal to 44 eV.

Inner and outer spots correspond to Bi_2Se_3 and TaSe2, respectively. The in-plane lattice parameter are 4.14 Å for Bi2Se3 and 3.48 Å for $TaSe_2$ (bulk 2H TaSe2: 3.43 Å)

Tantalum was deposited in the sub-monolayer thickness range on a bulk Bi_2Se_3 (0001) single crystal prepared by sputtering and annealing [1, 2]. After tantalum deposition the sample was annealed to about 480°C to form the $TaSe_2$ film. The LEED pattern (Fig.1) shows extra spots related to the $TaSe_2$ film (outer ring) in addition to the spots related to the Bi_2Se_3(0001) surface (inner ring of reflections).

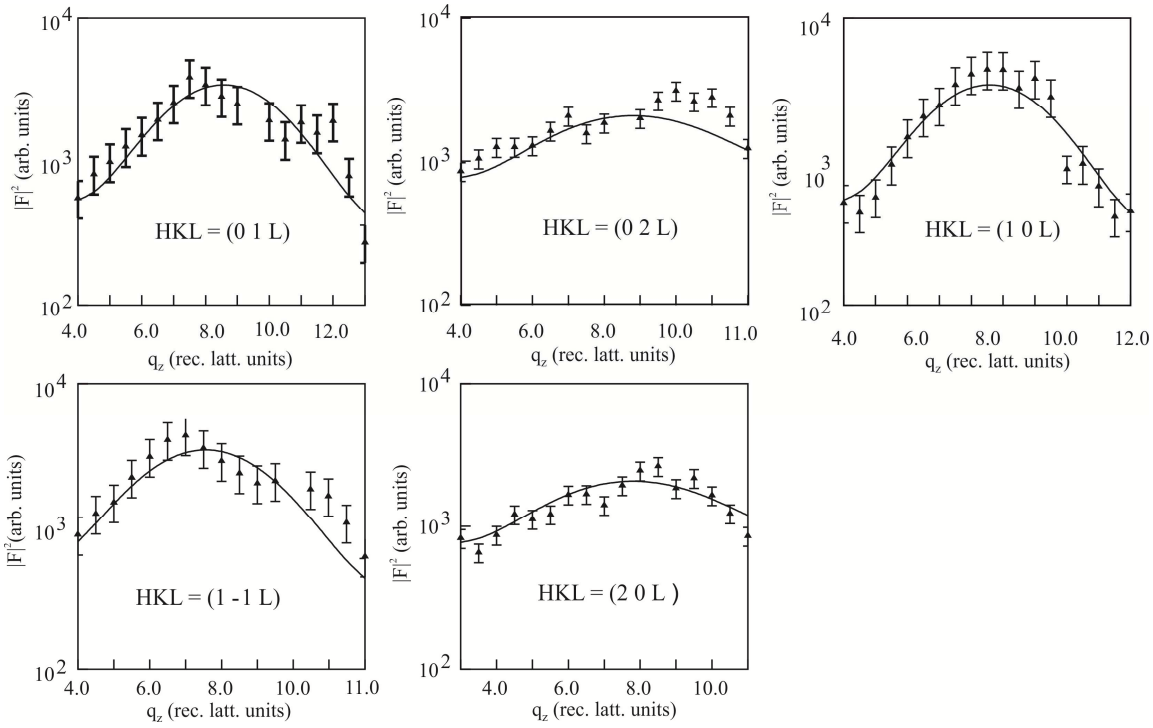

Fig.2: Measured (symbols) and calculated (lines) structure factor intensities along several reciprocal lattice rods of a H-type $TaSe_2$ monosheet grown on Bi_2Se_3.

X-ray diffraction intensities were collected along the lattice rods of the $TaSe_2$ film. An example is shown in Fig.2. The quantitative analysis (see solid lines as fits) shows that a single triple-layer sheet (Se-Ta-Se) of H type is formed, however as compared to the bulk structure there is conisderable vertical relaxation of the tantalum atom which involve a symmetry lowering of the structure. This has important implications with regard to the electronic structure of the $TaSe_2$ monosheet in the vicinity of the Fermi level. A publication is in preparation.

[1] Sumalay Roy, H. L. Meyerheim, A. Ernst et al., Phys. Rev. Lett. 113, 116802 (2014)
[2] H. L. Meyerheim and C. Tusche, Physica Status Solidi RRL, 1800078 (2018)