EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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:** Pressure dependent orbiatl textures in 1T-$TaSe_2$	**Experiment number**:
Beamline: ID27	**Date of experiment**: from: 27/10/2016 to: 01/11/2016	**Date of report**: 20/02/2016
Shifts: 15	**Local contact(s)**: Volodymyr Svitlyk	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

At ID27 we conducted a high pressure X-Ray study of 1T-$TaSe_2$ at room and low temperatures. Oriented samples of about 50 µm diameter were loaded in a membrane-driven diamond anvil pressure cell (DAC), mounted in a continuous flow helium cryostat. The data collection was performed using a wavelength of 0.3738 Å and a MARCCD detector. At each pressure point, we collected a data set of 120 images over a sample rotation of 60° with 0.5° scan width per image, with an exposure time of one second.

At room temperature (RT) and ambient pressure, 1T-$TaSe_2$ exhibits commensurate (C) charge density wave (CDW) order. Keeping T constant at RT and increasing p, the incommensurate (IC) phase is reached at 4 GPa, by a first order phase transition. The superlattice peaks can be indexed by q_1=0.276a*+1/3c* and q_2=0.276b*-1/3c*. Above 10.0 GPa, another phase transition to (IC_{HP1}) is observed, in which the superlattice peaks split along the l-direction and change their intensities dramatically. The IC_{HP1} undergoes a second order like transition to yet another new IC phase (IC_{HP2}) at about 20 GPa, which breaks the sixfold symmetry of the superlattice. The new monoclinic superstructure IC_{HP2} is found to be compatible with a (3+2)-dimensional superspace group C2/c, Z=2, whereas IC shows a trigonal P-3m1 symmetry, Z=1. The position of the new modulation wave vectors are described by q_1=0.277a*-0.277b*-2/7c* and q_2=0.277a*+0.277b*+2/7c*, with respect to the monoclinic reciprocal lattice parameters. Reciprocal space maps for the individual ICDW phases are shown in the figure.

In order to search for further possible changes of the CDW order, we also cooled the sample from RT down to 10 K at 10 GPa, within the IC phase. With deceasing temperature a broadening of the main-reflections and the corresponding superlattice peaks along the l-direction indicating the presence of a disordered stacking along c. Lowering the pressure at 30K does not show any significant change in the broadening of the peaks. 1T-$TaSe_2$ undergoes a phase transition at a pressure of 5.5 GPa and 30K towards a twinned C-CDW order.

It should be noted that due to technical issues concerning the loading of the DAC we could not measure a single sample over the entire pressure range. Instead, we were forced to measure different samples in the different pressure-temperature regimes, which hampers a clear discrimination between pressure effects and sample quality dependent effects. In addition, these technical issues consumed a significant amount of time and, therefore, we could acquire only one data set at each pressure point where the exposure time and primary beam intensity was chosen such that the superlattice-peaks are well observable but the main-reflections are strongly overexposed. Therefore, it is not possible to accurately and quantitatively extract changes of peak intensities as a function of pressure and temperature.

In summary, we could successfully identify several new CDW phases as a function of pressure and temperature in 1T-$TaSe_2$ on a qualitative level. Despite technical issues which hamper a quantitative analysis of the data, we could acquire key insides and important experience with respect to future experiments.

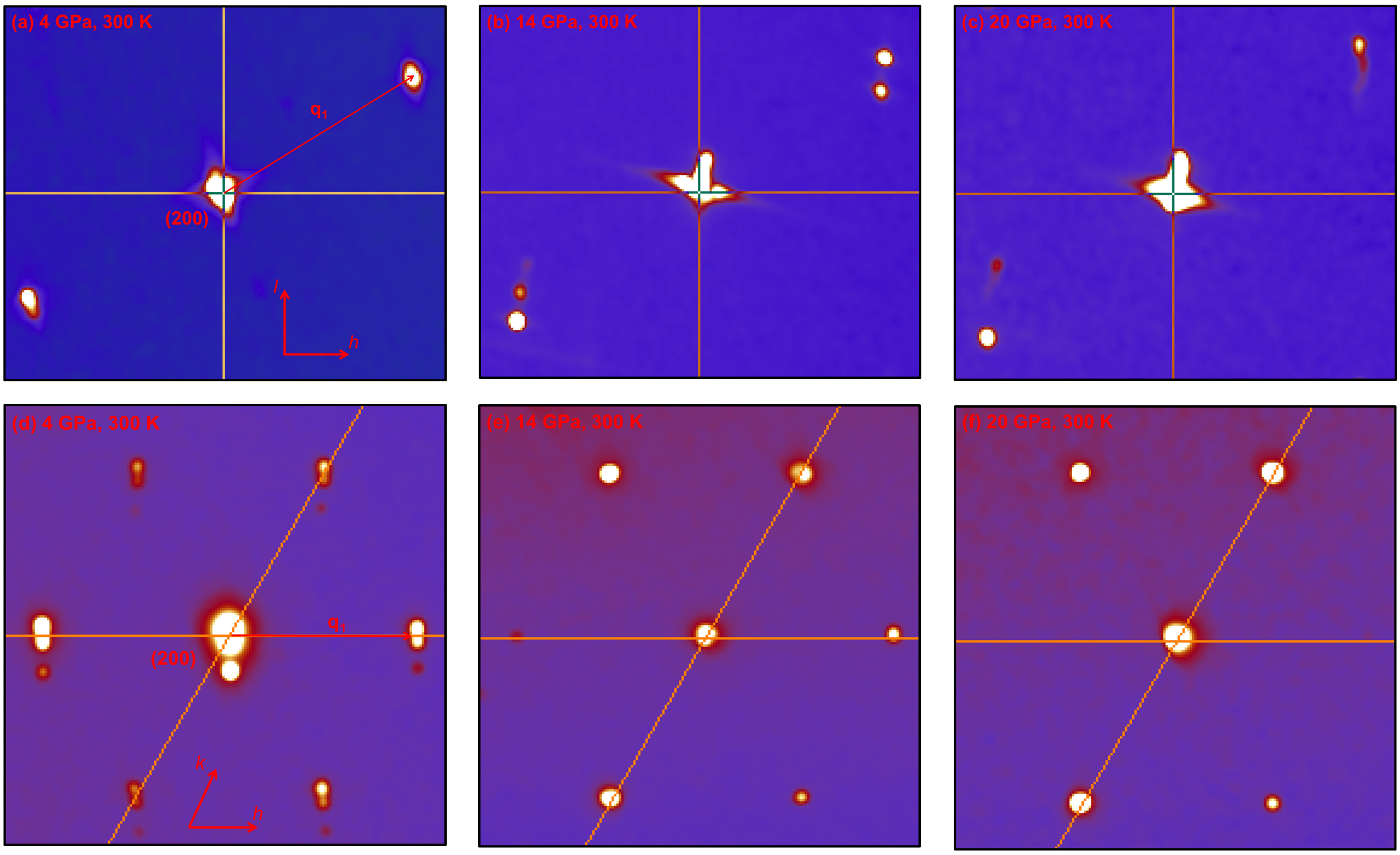

Figure: Reciprocal space maps of the XRD intensity for the various IC-CDW phases observed in 1T-$TaSe_2$. Reciprocal space maps of the *hl*-plane and *hk*-plane are shown in (a)-(c) and (d)-(f), respectively. The maps parallel to the *hk*-plane are integrated along the c*-direction ((d) from l=-1/3 to l=1/3; (e) from l=-0,3 to l=0.3; (f) from l = -2/7 to l=2/7).