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:** Time-resolved X-ray study of the newly discovered hidden quantum state in 1T-TaS_2	**Experiment number**: HC-3152
Beamline: ID09	**Date of experiment**: from: 27 Apr 2017 to: 02 May 2017	**Date of report**: 27.02.2018
Shifts: 15	**Local contact(s)**: Norman Kretzschmar	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Jochen Geck[1], Tobias Ritschel*[1,2] Quirin Stahl*[1], Maximilian Kusch*[1], Florian Heinsch*[1,3], Norman Kretzschmar*[4]

[1]TU Dresden, Institute of Solid State and Materials Physics, Germany
[2]UBC Vancouver, Stewart Blusson Quantum Matter Institute, Canada
[3]Helmholtz-Zentrum Dresden-Rossendorf, Germany
[4]ESRF Grenoble, France

Report:

The aim of this experiment was to study the microscopic structure of the newly discovered hidden (H) quantum state of 1T-TaS_2 by means of elastic X-ray diffraction XRD. Electrical resistivity and optical reflectivity measurements revealed that in thin single crystals of 1T-TaS_2 ultra-short laser pulses induce a semiconductor-to-metal transition into a new metastable charge density wave (CDW) phase [1]. Up to now the microscopic structure of this new laser-induced CDW remains widely elusive. Hence, our goal was to employ XRD in order to determine the modulation wave vector (q-vector), the correlation length and amplitude of the hidden CDW state.

Thin films with a thickness of about 50 nm and typical lateral dimensions of up to 100 µm were prepared by mechanical exfoliation from high-quality 1T-TaS_2 bulk single crystals. In order to optically pump the sample and subsequently probe their microscopic CDW structure, the exfoliated flakes were deposited on 200 nm thick Si_3N_4 membranes spanning a 1x1 mm^2 hole in a silicon wafer. The silicon wafer was clued on a sample holder, which was mounted on the coldfinger of a tailor-made continuous He-flow cryostat. The cryostat was attached to an one-circle goniometer. Following a quick assessment of the crystal quality at room temperature we cooled the samples down to 4K.

In order to induce the H-state the 1T-TaS_2 flakes were photo-excited with a 1.6 ps pump pulse from a Ti-sapphire laser with a wavelength of 800 nm. The laser beam had a diameter of 400 µm (FWHM). The CDW structure of the persistent photo-induced state was then studied by means of XRD. To this end, the sample was exposed to a 60x100 μm^2 X-ray beam with a photon energy of 18 keV. Single crystal datasets consisting of 120 frames measured over a sample rotation of 60 degree were collected using a Rayonix MX170 detector. We used four different pulse fluencies $F_{1,2,3,4}$ = 0.04, 0.09, 0.24, 0.60 mJ/cm^2 and studied two different samples.

In addition, we conducted XRD at ID27, in order to investigate the relationship between the H-state and the structurally closely related supercooled nearly commensurate (NC)-CDW state [2].

Most importantly, our work shows that the photo-induced transition into the H-state is associated with a marked change of the CDW stacking, as shown in the Figure. The stacking of the CDW in the hidden state is similar to the stacking found in the room temperature NC-CDW phase and the super cooled NC-CDW phase. Apart from the CDW layer stacking also the in-plane structure changes upon entering the H-state in a way that discommensurations form which yields a change of the in-plane q-vector and the appearance of higher order reflections. These results strongly suggest that the H-state is very similar to the supercooled NC-CDW. However, details of the discommensurations lattice differ for all three NC-CDW phases, and may thus explain different physical properties observed so far.

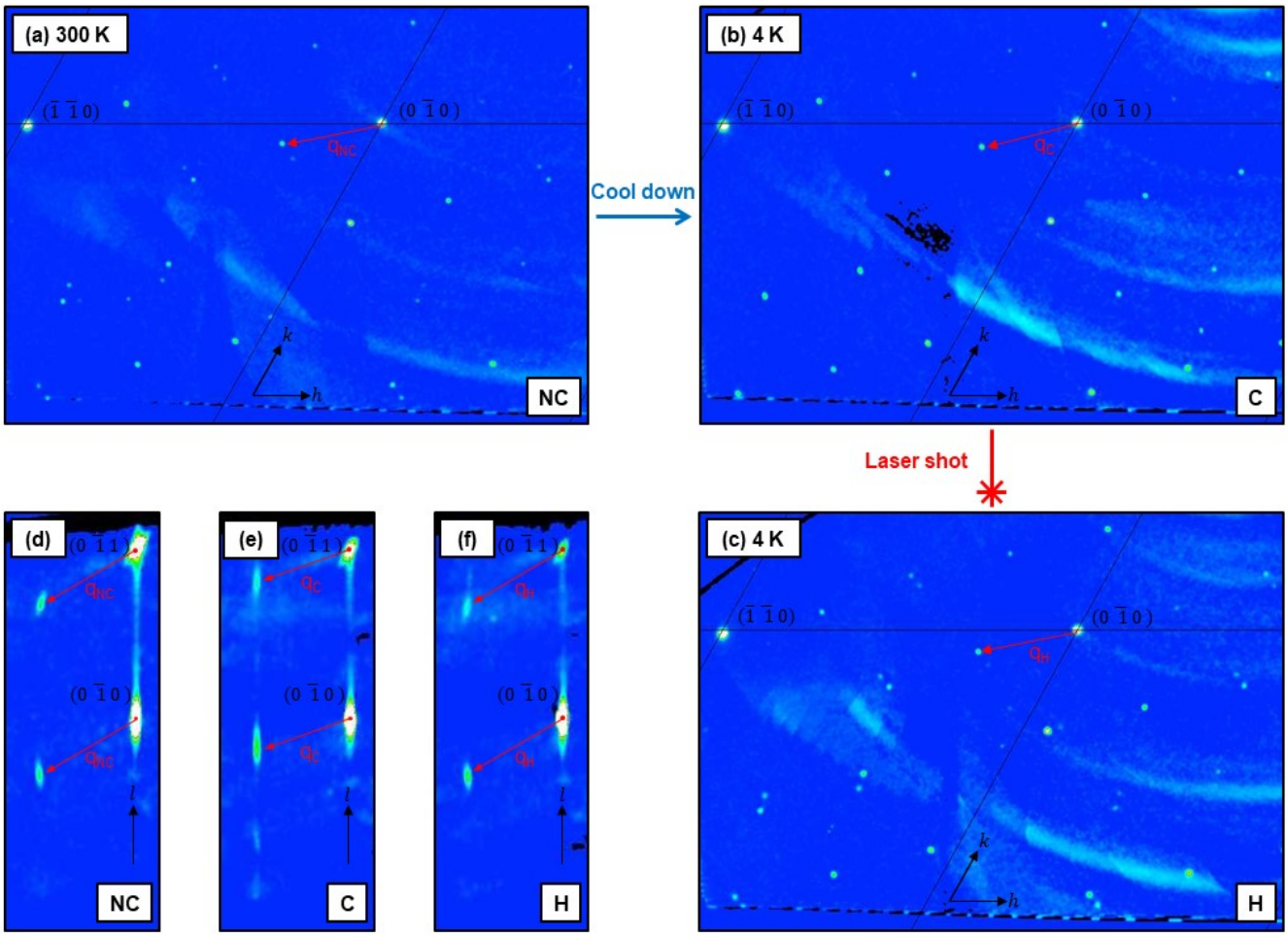

Figure: Reciprocal space maps of the XRD intensitsy for the NC phase (a), the C phase (b), and the photo-induced H phase (c), within a slice of thickness $\Delta l = 2/3$ onto the hexagonal *hk0* plane. The corresponding reciprocal-lattice region, along the modulation vector q and perpendicular to the *hk0* plane is illustrated in (d), (e) and (f). In all images the Bragg reflections are indicated by the Miller indices (*hkl*), and the axes of the reciprocal coordinate system, are shown by black arrows. (a) and (d) At room temperature 1T-TaS_2 exhibits a NC-CDW, with strong higher order peaks, arising from a domain like structure with sharp boundaries. Furthermore, the point-like satellite peak in (d), indicates a well-ordered stacking along *l*. In addition (c) and (e) illustrates the C-CDW order at 4K, characterized by broad peaks due to the presence of disordered stacking along *l*. (c) and (f) Keeping T at 4 K and inducing a 1.6 ps laser pulse at 800 nm, the H-phase is reached. The strong higher order peaks (c) and the sharp single peak along *l* (f), indicates that the electronic order in the H-phase is similar to the order in the NC-phase.

[1] L. Stojchevska *et al.*, Science **344**, 177 (2014)
[2] M. Yoshida *et al.,* Scientific Reports **4**, 7302 (2014)