

## 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://www.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.



<b>Experiment title:</b> Charge density wave order, collective excitations, and the superconducting phase of 1T-TaS <sub>2</sub>	<b>Experiment number:</b> <b>HS-4464</b>
<b>Beamline:</b> ID09A and ID28	<b>Date of experiment:</b> from: 04/11/2011 to: 08/11/2011 and from: 23/11/2011 to: 02/11/2011
<b>Shifts:</b> 12 + 18	<b>Local contact(s):</b> Michael Hanfland and Alexei Bossak

*Received at ESRF:*

**Names and affiliations of applicants (\* indicates experimentalists):**

Jochen Geck\*<sup>1</sup>, Tobias Ritschel\*<sup>1</sup>, Jan Trinckauf\*<sup>1</sup>, Alexei Bossak\*<sup>2</sup>, Gaston Garbarino\*<sup>2</sup>,  
 Michael Hanfland\*<sup>2</sup>, Helmuth Berger<sup>3</sup>

<sup>1</sup>IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

<sup>2</sup>ESRF Grenoble, France

<sup>3</sup>Ecole polytechnique Federale de Lausanne, Switzerland

**Report:**

**High-Pressure XRD at ID09:**

At ID09A we conducted a high pressure X-Ray study of 1T-TaS<sub>2</sub> at room and low temperatures. We used a membrane driven diamond pressure cell mounted in a continuous flow helium cryostat. The beam energy was about 30 keV. The used single crystals were of typically size of about 80 micron.

At room temperature the nearly commensurate (NC) wavevector  $q_{NC}$  was found to move slightly towards the incommensurate (IC) position  $q_{IC}$  but at 18 kBar a first order like transition to an IC-Phase was observed. This high pressure IC Phase differs from the high temperature phase by a three fold splitting of the super lattice reflection, consistent with earlier observations. This successive process is illustrated by reciprocal space maps of the  $hk$ -plane in FIG. 1.

At 15 K the commensurate (C) Phase was found to be supercooled up to 42 kBar, where the C-to-NC-transition was observed. Similar to the room temperature measurement the NC wavevector moves to the IC position. Between 65 and 80 kBar a transition to the high pressure IC-Phase was found. On lowering the temperature to 3.5 K to reach the potentially superconducting phase no apparent change in the diffraction pattern could be observed.

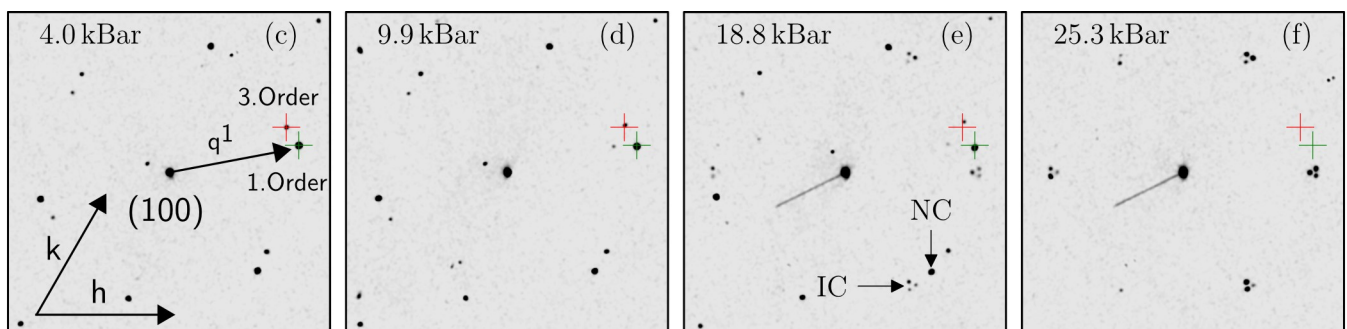


FIG. 1: Reproduced reciprocal space maps for different pressures at room temperature. These maps represent cuts through the reciprocal space parallel to the  $hk$ -plane, while they are integrated along the  $c^*$ -direction (from  $l = -1/3$  to  $l = 1/3$ ) to show all super structure reflections. These images illustrate the effects of pressure on the NC-Phase. The green and red cross mark the first and third order NC-vector at ambient pressure, respectively.

### High-Pressure IXS at ID28 and preliminary TDS at ID29:

In addition we conducted high-pressure IXS at room temperature along with temperature dependent IXS at ambient pressure at ID28 and some preliminary TDS experiments at ID29. For the high-pressure experiments we used the same pressure cell as at ID09. Since these experiments took place very recently the analysis of the data is currently in process. However, the raw data already clearly shows dramatic changes in the phonon dispersion as a function of external pressure, as exemplified in FIG. 2. We also find a Kohn-anomaly in the high-temperature IC-phase. Our data show that this Kohn-anomaly related to the IC-phase is strongly suppressed with increasing pressure.

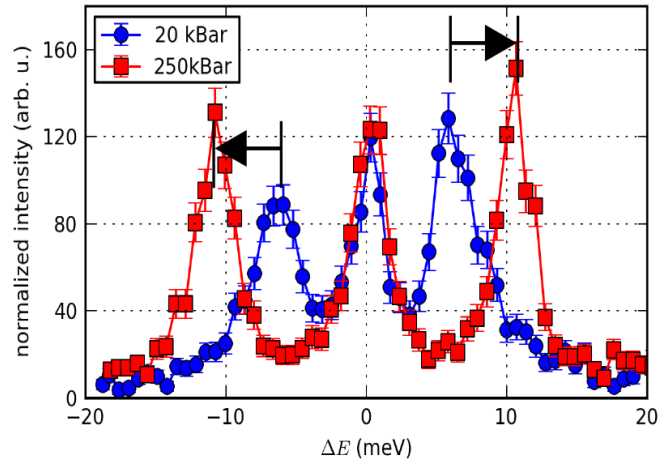


FIG. 2: IXS spectrum at the NC q-vector (1.689, 0.067, -1/3) for different pressures. A clear shift of the phonon peak is visible.

An equally dramatic change was observed in terms of TDS at ID29 as a function of temperature as shown in FIG. 3. Unfortunately, the temperature was more or less uncontrolled in this experiment. It is very important to perform systematic TDS studies as a function of temperature (from the low temperature C-phase at  $\sim 180$ K up to the high-temp IC-phase at  $\sim 400$ K).

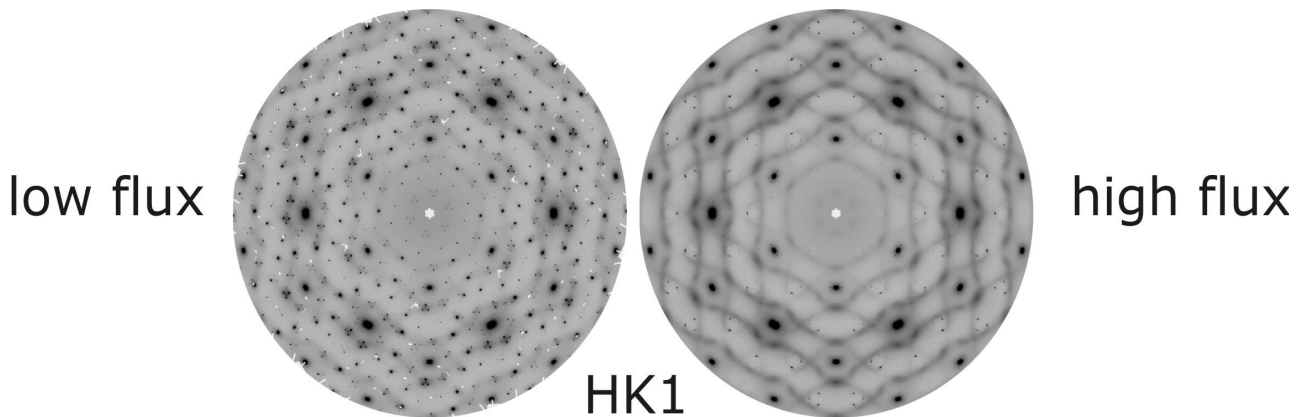


FIG.3: (HK1)-reciprocal-space-cuts measured with different beam heating. Left: low-flux measurement in the NC-phase. Right: high-flux measurement in the IC-phase