ESRF	**Experiment title:** X-ray diffraction study of the newly discovered hidden quantum state in 1T-TaS2	**Experiment number**: HC1957
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Shifts: 9	**Local contact(s)**: Michael Wulff	*Received at ESRF:*

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Report:

The aim of this experiment was to study the microscopic structure of the newly discovered hidden quantum state of 1T-TaS_2 by means of elastic X-ray diffraction. Using resistivity and optical reflectivity measurements it was found that ultra-short laser pulses induce a new charge density wave (CDW) phase in 1T-TaS_2, which is persistent and does not exist under normal equilibrium conditions. Up to now nothing is known about the microscopic structure of this new laser-induced CDW. Hence, our goal was to use X-ray diffraction in order to determine the modulation wave vector (*q*-vector), the correlation length and amplitude of the hidden CDW state.

Starting from high quality bulk single crystals we prepared thin films of 1T-TaS_2 by the exfoliation method. These samples were deposited on standard TEM grids. The thickness of the films was about 100nm and typical lateral dimensions were 500µm. The TEM grid was glued to a quartz capillary which was then attached to a standard goniometer head. A simple one-circle goniometer was used to rotate the sample. Cooling of the sample was provided by a Helium cryojet. The sample was exposed to a (60 x 100) μm^2 X-ray beam with a photon energy of 18keV. The X-ray diffraction from the sample was collected with a MAR CCD detector. In order to optically pump the sample a Ti-sapphire laser with a wavelength of 800nm and pulse lengths of about 1ps was used. The laser beam had a size of about (1 x 1)mm^2. At first we checked the crystallographic quality

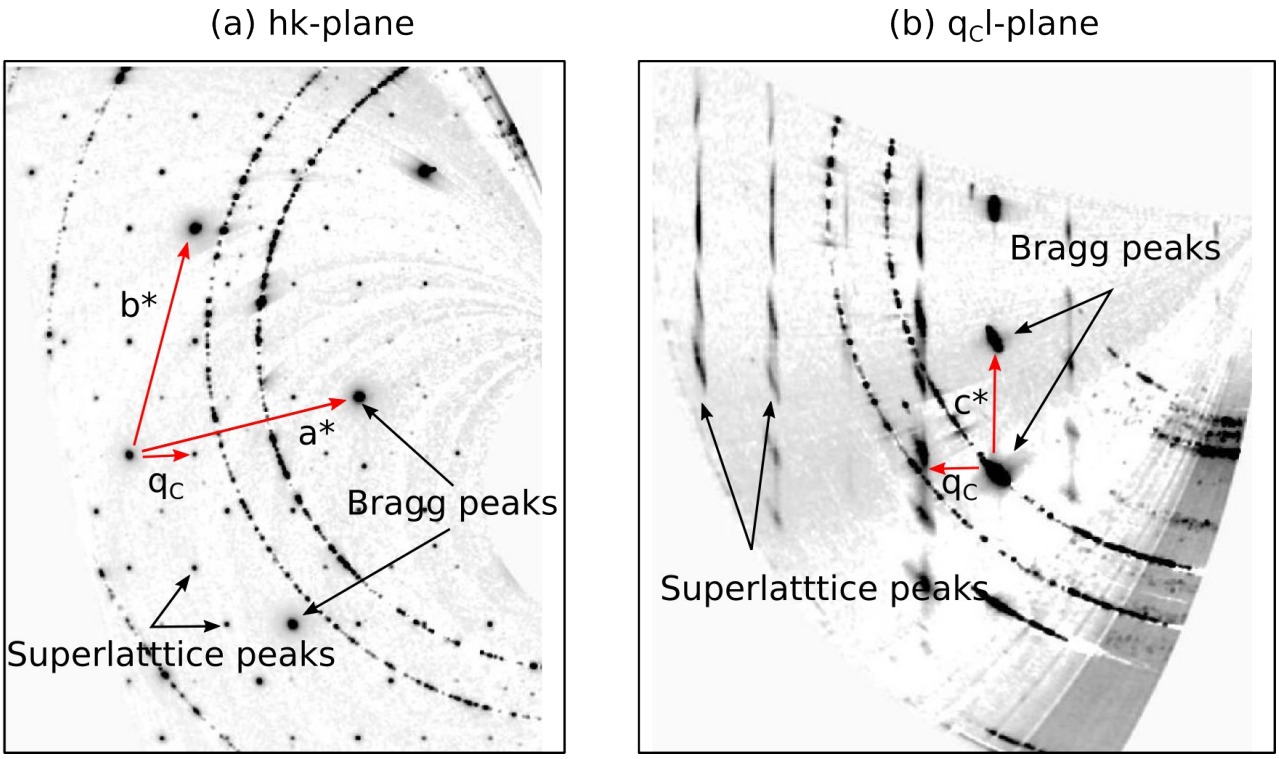

Figure: Reciprocal space maps parallel (a) and perpendicular (b) to the *hk*-plane measured at base temperature. The superlattice peaks are very sharp within the *hk*-plane (a) but smeared along the *l*-direction (b) which indicates the typical disordered CDW layer stacking of the commensurate CDW.

of our samples at room and low temperature. Therefore, we collected single crystal datasets consisting of 200 images measured over a sample rotation of 100 degree. Typical reciprocal space maps deduced from these datasets are shown in the Figure above. The data clearly confirm that the films are high quality single crystals which produce sharp and well defined diffraction peaks. Moreover, we could observe the expected superlattice peaks corresponding to the nearly commensurat CDW and the commensurate CDW at room and low temperature, respectively. The experiment indeed provided the expected *q*-space resolution which is much better than for comparable electron diffraction experiments. In particular the intensity distribution along the crystallographic *l*-direction, i.e. perpendicular to the TaS_2 -layers, is well resolved (see Figure (b)). These information are very important to elucidate the CDW layer stacking order and are commonly difficult to obtain from electron diffraction.

In the next step we kept the sample at base temperature and illuminated the sample with a 1.2ps laser pulse with varying laser fluence. In order to observe possible laser-induced changes of the CDW order we collected single crystal datasets after the optical pump pulse. However, we could not observe any changes of the diffraction pattern.

Due to technical difficulties with the beamline, the setup of this complex experiment took 3 shifts, which only left 6 shifts for the actual measurements. We decided to use a cryojet for cooling our samples, which unfortunately turned out to be inappropriate, as it could not provide a stable temperature below 30 Kelvin. We had no opportunity to replace the cryojet with the available cryostat due to the little time available to us. Nonetheless, this first attempt shows that the experiment is very well feasible. Most importantly, it will be possible to observe changes of the CDW order as well as changes of the CDW layer stacking order induced by the optical pump pulse.