ESRF	**Experiment title:** Pressure dependent X-ray diffraction study of the charge orbital density-wave in $Ir_{1-x}Pd_xTe_2$	**Experiment number**: HC1108
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Names and affiliations of applicants (* indicates experimentalists):
Tobias Ritschel*
Jan Trinckauf*
Jochen Geck*
Gaston Garbarino*

Report:

The aim of this experiment was to study the charge orbital density wave (DW) in the heavily spin-orbit coupled superconductor $Ir_{1-x}Pd_xTe_2$ by means of elastic X-ray diffraction (XRD) as a function of hydrostatic pressure. Surprisingly, resistivity measurements revealed that the DW transition is strongly stabilized with increasing pressure, whereas the superconducting phase is suppressed, which is very unconventional. Since no microscopic information about the DW phase under pressure is available our goal was to close this gap by conducting XRD as a function of hydrostatic pressure and temperature.

A small, high quality single crystal of pristine IrTe2 was loaded into a diamond anvil pressure-cell (DAC). The DAC was loaded with He as pressure transmitting medium. We mounted the DAC into an oven on a single axis (φ) diffractometer. The wavelength of the incoming photons was fixed to λ = 0.3738 Ang. The diffracted x-ray intensity was measured using a MARCCD detector. The pressure was changed and monitored in-situ via ruby fluorescence. For each pressure point we collected φ-oscillation images with an image width of 0.5 degree and acquisition time of 1s from φ = −31 degree to φ = 31 degree for two different spots on the sample. For 0.4 GPa we found a hexagonal unit cell with cell parameters a = 3.9226 Ang and c = 5.3644 Ang. At 1.44 GPa the transition into the density wave phase already took place, which is clearly indicated by the appearance of the corresponding super-lattice reflections. The observed reflections can be indexed with the following triclinic unit cell: a = 6.405(9), b = 7.883(13), c = 15.698(10), α = 72.36(12), β = 70.84(10), γ = 74.24(14). In this cell the reciprocal c∗ -direction points in the a∗ + c∗ direction of the hexagonal cell, i.e. along the superlattice reflections. In the figure below we show reciprocal space maps containing this direction (the c∗ -direction is marked with a red arrow in the figure. These diffraction pattern are in good agreement with previously reported electron diffraction data. Next we increased the temperature to 50 C which was accompanied by an increase of pressure to 3 GPa. Upon this increase of temperature the diffraction pattern became stripy. These

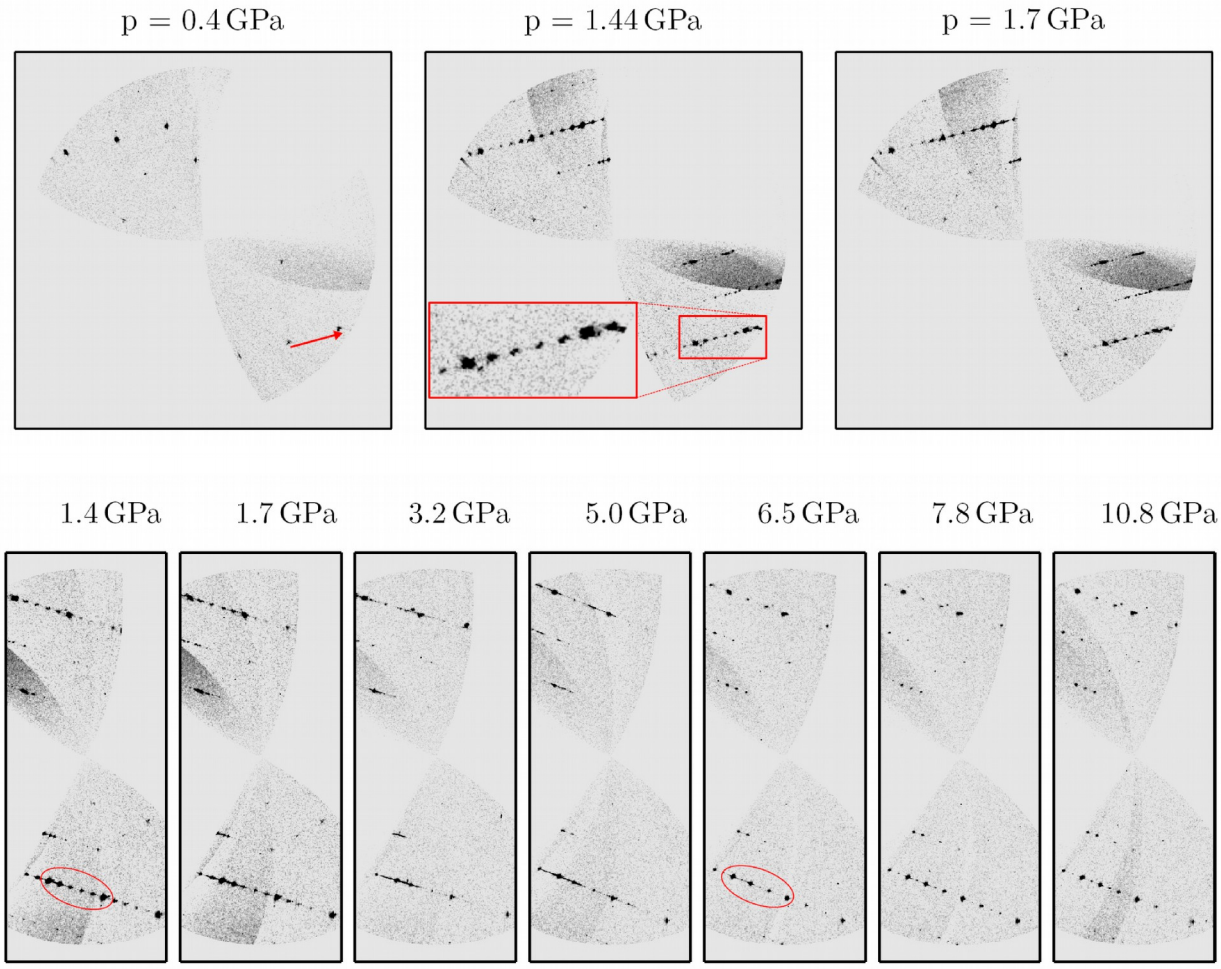

Figure: reciprocal space maps measured at different pressures.

smeared-out diffraction peaks indicate structural disorder. The diffraction peaks remain stripy up to 6.5 GPa where they become sharp again.

Moreover the unit cell changes to: a = 6.2828, b = 7.8605, c = 17.3639, α = 78.6842, β = 79.7326, γ = 73.7960. which is also directly visible in the reciprocal space maps. Comparison of the marked regions for 1.4GPa and 6.5GPa shows that the *q*-vector changes, i.e. for 1.4GPa 5 superlattice reflections fit between the two bright spots and for 6.5GPa only 4 superlattice reflections fit in-between.

In order to determine the transition temperatures and lattice parameters as a function of pressure we acquired so-called rotational images: Therefore the sample is rotated by 62 degree while the detector image is recorded. This type of data acquisition is very fast and therefore many pressure points can be measured and, hence, transition temperatures and lattice parameters can be analyzed precisely. Afterwards the 2D detector image is radial integrated to obtain powder-like diffraction data, i. e. diffracted intensity as a function of 2Θ. We did this for three different temperatures: 20, 150 and 250 degree Celsius. The transition into the density wave phase is clearly visible as a multitude of additional peaks appear. Upon increasing the temperature this transition is shifted to higher pressures in accordance with previous measurements.

We also measured samples doped with Pd (4%) and Pt (7%) at room temperature. For the Pd doped sample the transition into the ordered phase takes place already at around 0.6 GPa. A stripy phase is again reached at 2.9 GPa (fig5(c)). These stripes disappear upon further increasing the pressure. The Pt (7%) doped sample shows the transition only at about 7 GPa.