ESRF	Experiment title: Competition between charge density wave and superconductivity in $ZrTe_3$	**Experiment number**: HS-3704
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Report:

At ambient pressure $ZrTe_3$ shows a transition to a charge-density wave (CDW) modulated ground state at T_{CDW} = 63 K. The incommensurate propagation vector q_{CDW} = (0.07,0,0.3333) lies in the *a**-*c** plane of the reciprocal lattice. Previous resistivity measurements [1] have shown that the filamentary superconductivity found at temperatures below $T_c \approx 4$ K is quickly suppressed by applying hydrostatic pressure. At the same time the CDW transition temperature rises to 100 K around 2 GPa and then decreases again before the CDW signature is lost around 5 GPa. We have measured the CDW related incommensurate superstructure reflections by single crystal diffraction at high pressure and low temperatures.

Single crystals of this two-dimensional material form platelets of several mm lateral size and up to 200 µm thickness. Small discs of 50 – 150 µm diameter were cut using laser-cutting and captured by scotch tape, which also served to further cleave the samples down to thicknesses of ~30 µm. These platelets were loaded into a diamond anvil cell with 600 µm cutlet size and 300 µm diameter holes in a stainless steel gasket. The pressure medium was He and the hydrostatic pressure was measured by fluorescence of a ruby chip.

The cell was mounted in a He flow cryostat with an attached gas membrane for pressurizing the sample *in situ*. Precise control of the temperature and pressure in the range of 15 K < *T* < 300 K and 0.2 GPa < *P* < 6 GPa was employed. Diffraction data were acquired using the MAR 3450 image plate detector in the forward scattering direction with the focused x-ray beam of 2x2 μm^2, which served to choose a spot of good crystallinity in the single crystal samples. The *c** axis is naturally aligned to being close to parallel to the incoming beam, while the *a** axis was chosen close to perpendicular to the φ rotation axis. In this way the *a**-*b** plane is readily spanned on the detector in oscillations of φ, while different *c** components are accessible within the opening of the cell of ±20°. The data were indexed and reconstructed high symmetry planes were extracted using the CrysAlis software.

Figure 1 shows the reconstructed *a**-*c** diffraction plane of $ZrTe_3$ at pressures of 0.2 GPa, 2 GPa and 5 GPa. The pictures have been taken with varying degree of over-exposing thus the different gray-scale contrast. In all cases the superstructure spots are clearly visible near (4 0 -1) in the center of each picture. The component q_b of the CDW modulation remains zero, while the components q_a and q_c change with pressure, thus changing the angle of the CDW modulation within the reciprocal lattice. The lattice itself shows a slight, anisotropic compression with pressure, but no change of the monoclinic angle is observed. The data shown here were taken at $T = 40\ K < T_{CDW}$ for each case. Increasing the temperature toward T_{CDW} reproduces the phase boundary reported in [1] and shows no change of the CDW modulation, which remains incommensurate at all temperatures. Also above *P* = 5 GPa, the CDW is lost as reported in [1].

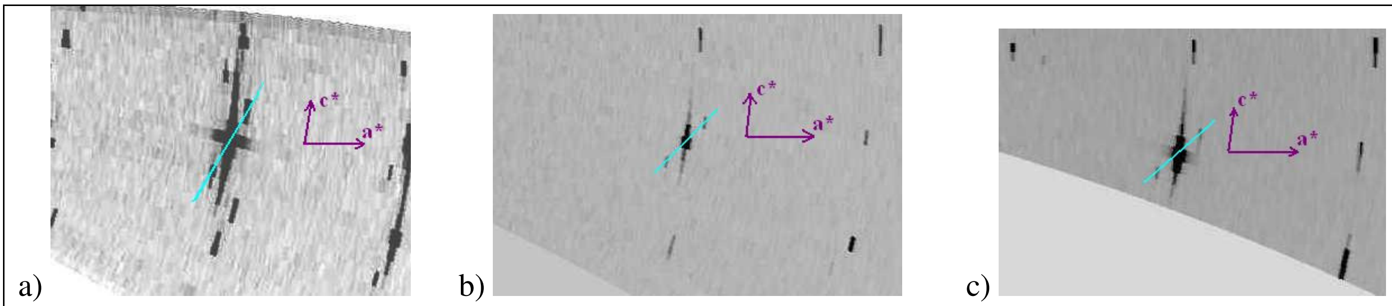

Figure 1: Reconstructed a^*-c^* planes of diffraction from ZrTe3 at T =40 K and pressures P of (a) 0.2 GPa, (b) 2 GPa and (c) 5 GPa. The (4 0 -1) Bragg spot in the center of each picture is strongly over-exposed and the CDW superstructure spots are marked by a light blue line. The a^* and c^* star axes run horizontal and nearly vertical as indicated.

From the data shown in Figure 1, the components q_a and q_c of the CDW modulation can be extracted. q_c = 0.3333 at ambient pressure corresponds to a tripling of the basic unit cell in the modulated ground state. The extracted components are shown in Fig. 2. Upon slight increase of the pressure P, the component q_c is quickly diminished. In an intermediate pressure range around 0.5 GPa, it is compatible with a value of q_c 0.25, i.e. a quadrupling of the unit cell along c. At higher pressures this component, like q_a, becomes incommensurate.

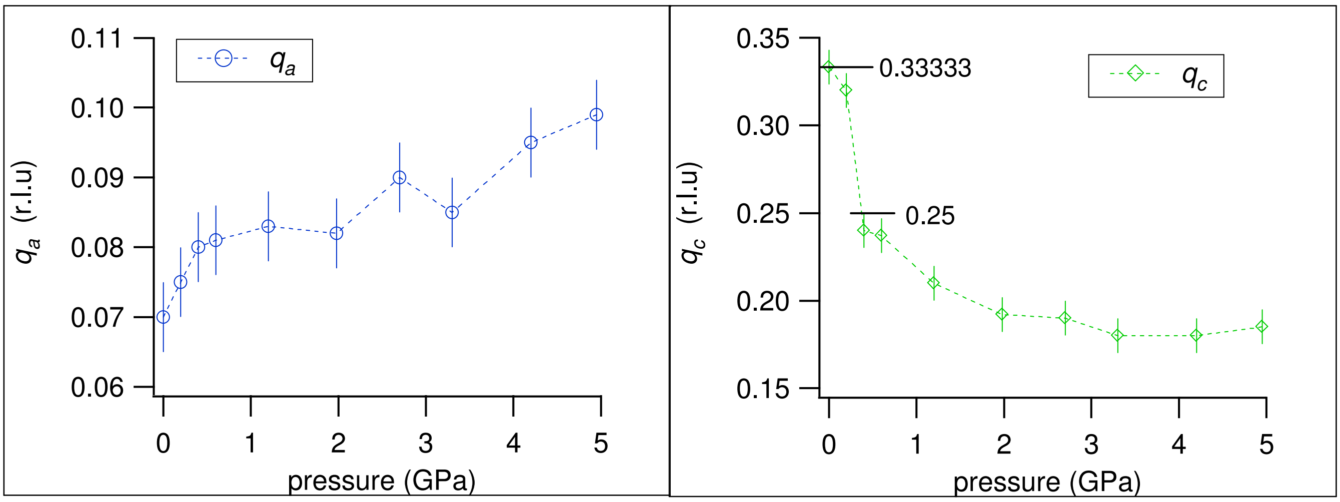

Figure 2: Pressure dependence of the components q_a and q_c of the CDW modulation vector as extracted from images as shown in Fig. 1. The components are shown in untis relative to the respective basic crystal lattice at each pressure.

This results shows that the CDW modulation and thus the Fermi surface nesting condition [2] changes with pressure. Upon slight compression of the lattice up to 0.6 GPa the locking of the component q_c to $^1/_3$ is released. At the same time, the component q_a is enlarged, thus corresponding to a larger opening of the Fermi surface. Effectively this change of components corresponds to a rotation of the CDW wave vector. This low pressure region is where resisitvity measurements have found a suppression of superconductivity and an increase of the CDW transition temperature. At pressures above 1 GPa, where the CDW transition is stable and then decreases until it is lost at 5 GPa, the diffraction data show a gentle continuation of the rotation of q_{CDW} in reciprocal space. The loss of CDW at 5 GPa is found in our data, too, but it is not related to any special re-configuration of the CDW modulation and thus the Fermi surface nesting.

References

[1] R. Yomo *et al.*, "Pressure Effect on competition between charge density wave and superconductivity in $ZrTe_3$: Appearance of pressure-induced reentrant superconductivity.", Phys. Rev. B 71 (2005) 132508.

[2] C. Felser *et al.*, "Electronic properties of $ZrTe_3$", J. Mater. Chem 8 (1998) 1787.