ESRF	Experiment title: Kohn Anomaly in charge density wave $ZrTe_3$	**Experiment number**: HS-3304
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Report:

The charge-density-wave (CDW) in $ZrTe_3$ is driven by a Fermi-surface nesting of the quasi 1-dimensional Fermi-surface sheet derived from the Te p_x orbitals along the *a*-direction of the lattice [1]. The Peierls distortion of the modulated structure below T_{CDW} = 63 K runs perpendicular to the prismatic chains along the CDW wave-vector q_{CDW} = (0.07, 0 0.333) [2]. The nesting is expected to cause a giant Kohn Anomaly (KA) in the phonon dispersion around q_{CDW}.

We have investigated the temperature-dependent phonon frequencies around q_{CDW} by inelastic x-ray scattering (IXS) and thermal diffuse scattering (TDS). While IXS directly shows the frequency and intensity of the phonon modes *S(Q,ω)*, TDS measures the energy-integrated quasi-elastic scattering intensity *S(Q)*. TDS measurements prior to the IXS study at the single crystal diffractometer at the Swiss-Norwegian Beamline had allowed a complete survey of momentum space and shown that enhanced TDS intensity is observed around q_{CDW} close to the (-4 0 1) Bragg spot, thus pointing at the involvement of a low-frequency phonon with *a**-polarization.

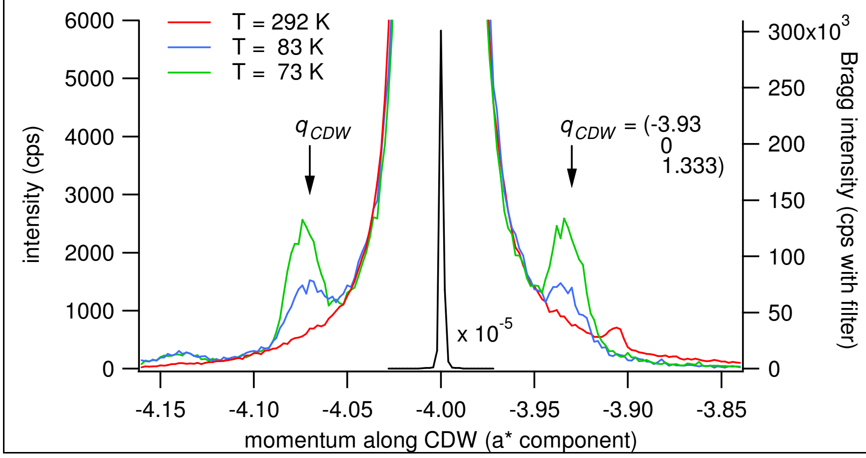

Figure 1: Thermal diffuse scattering at three different temperatures. The quasi-elastic total scattering intensity was recorded for a momentum direction along q_{CDW} from the (-4 0 1) Bragg spot. The data were measured using the energy integrating detector with x-rays of $h\nu$ = 15.82 keV. In the centre the intensity due to the (-4 0 1) Bragg scattering is shown on an intensity scale reduced by approximately 10^{-5} by attenuation of the incident beam.

Fig. 1 shows the measured quasi-elastic scattering intensity around the (-4 0 1) spot along q_{CDW} . In the tails of the Bragg spot a weak, broad shoulder is observed already at room temperature (~ $4.5 \cdot T_{CDW}$) on close inspection. At lower temperature, the shoulder develops into a strong bump. This feature is always weak compared to the main lattice Bragg scattering intensity. At temperatures below T_{CDW} it transforms into a superstructure reflection that is still broader than the main lattice reflections.

The dispersion of the lowest two phonon modes along q_{CDW} close to (-4 0 1) is shown in Fig. 2. The lowest excitation corresponds to an acoustic phonon polarized along a^*. It is clearly resolved despite the emergence of a very strong central peak of elastic scattering at low temperatures. A subtle, but clear Kohn anomaly is observed already at room temperature. It develops into a very sharp giant KA that can be accurately traced down to $T = 68$ K $= 1.1 \cdot T_{CDW}$. A second excitation of a low-frequency optical phonon is not clearly resolved. Both dispersions correspond rather well to *ab-initio* calculations, except for the KA that is not represented by the theory. The optical modes shows no sign of a KA within the resolution thus pointing at the acoustic modes as a driving force of the CDW formation.

Two interpretations exist for the diffuse scattering intensity reported in Fig. 1. Truly thermal diffuse scattering by the phonons leads to an enhanced intensity of the low-lying phonons. The phonon dispersion is reflected in the TDS pattern as $I \sim \omega^{-2}$ [3]. The giant KA leads to a peak in the TDS because the softened phonons scatter more strongly. This effect is, however, not sufficient to explain the peaks at q_{CDW}. The alternative interpretation of the diffuse scattering relates the peak to fluctuating CDW order that develops in the pseudo-gapped region above the condensation temperature T_{CDW}. Indeed, the strongest enhancement of intensity in the IXS spectra is found in the central peak that is due to static diffuse scattering. The central peak intensities derived from the peak fitting closely follow the total diffuse scattering intensity. We thus conclude that fluctuating CDW order is present already at temperatures far above T_{CDW} that is driven by the Fermi surface nesting and the resulting giant Kohn anomaly.

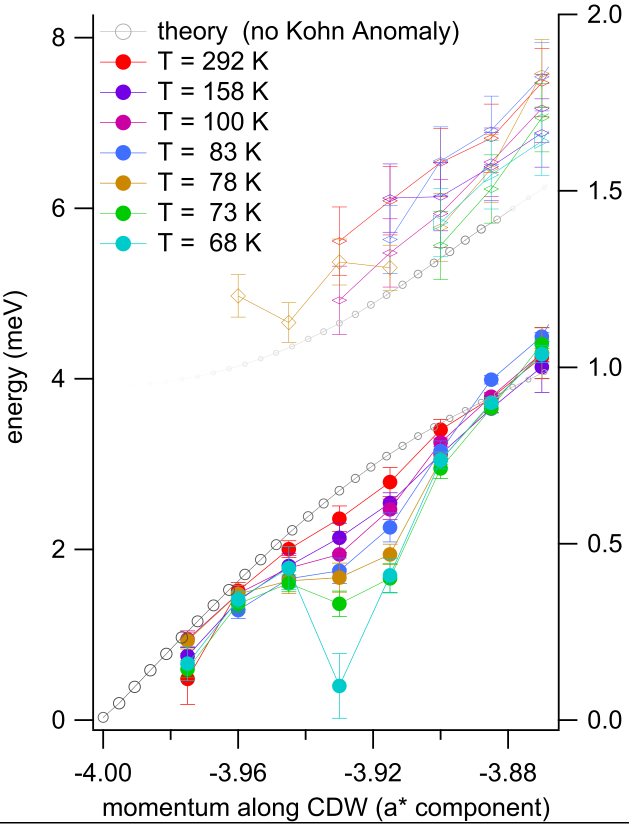

Figure 2: Dispersion of the lowest two phonon modes along q_{CDW} close to (-4 0 1). The momentum Q is represented by its a^* component, but the measurement is performed off the high-symmetry direction. Note the small range of momentum.
The phonon energies were extracted from IXS spectra at 1.6 meV resolution by peak fitting. At low temperatures and close to (-4 0 1), the intensity of the central peak exceeds the intensity of the phonon-scattering. A model of sharp, completely resolution-limited peaks was employed and found to represent the data well. The predicted phonon frequencies by *ab-initio* calculations are shown in grey.
In the lower part the acoustic branch polarized along a* is shown. The temperature dependent Kohn anomaly is discussed in the text.

References

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[3] M. Holt *et al.,* Phys. Rev. Lett. 86 (2001) 3799.