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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 structure is made of linear prismatic chains along the *b*-axis, similar to the prototype CDW-material $NbSe_3$, but the nesting leads to a Peierls distortion perpendicular to the chains. The CDW wave-vector $q_{CDW} \approx (0.05, 0\ 0.33)$ [2] corresponds well to the nesting-condition [3]. The nesting is expected to cause a giant Kohn anomaly and with the emergence of the CDW at below T_{CDW} = 63 K phonon modes near q_{CDW} should soften due to the electron-phonon interaction. The temperature-dependence of this softening is likely to follow a BCS-behaviour with first deviations from the high-temperature “undisturbed” lattice dynamics around the mean-field temperature $T_{MF} = 4\ T_{CDW} = 252$ K [1].

We have investigated the temperature-dependent phonon frequencies of various optical and acoustic modes both near and away from q_{CDW} in several scattering geometries for different phonon polarizations. Figure 1 shows representative data of for three momentum points around q= (-0.05 0 9.33) near q_{CDW}. In all three sets the temperature-dependence shows a strong increase of the central elastic-scattering peak as the temperature is lowered. Precise peak-fitting with a model function of δ-function sharp phonon peaks convoluted with the measured resolution function yields a reliable determination of the peak positions even as the central peak becomes the dominant feature. The peak positions of all three modes was found unchanged with sample temperature. Thus no softening was observed. This holds for all investigated modes, including high-frequency bond-stretching modes of the Te-atoms at 26.9 meV, various intermediate-energy optical modes polarized along a^* and c^* both at and away from q_{CDW}. It also holds for the acoustic modes polarized along a^* and c^* so long as their peak position could reliably be determined in the presence of a strong central peak at low temperatures. Equally, no change of the width of phonon peaks was observed within the resolution limit of 3 meV.

At the lowest temperature of T = 25 K the sharp CDW superstructure peak was observed in the q-dependent elastic scattering signal. With much higher precision than previous experiments [2] it was determined as q_{CDW} = (0.07, 0, 0.34) in agreement with the considerations of Fermi-surface nesting [3].

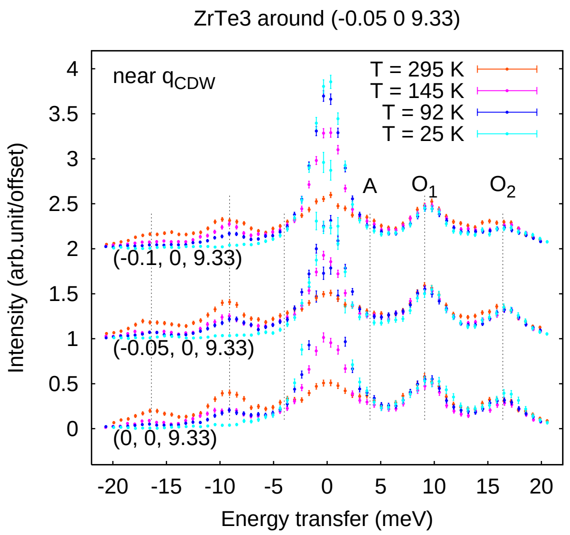

Figure 1: Temperature-dependence of the inelastic x-ray scattering spectra of ZrTe3 around q_{CDW}. In this scattering geometry phonons polarized along c^* are predominantly observed. One acoustic mode at ω_A = 4 meV and two optical modes at ω_{O1} = 9.1 meV and ω_{O2} 16.4 meV are determined by peak-ftting.
As the temperature is lowered, the detailed-balance shifts spectral weight from the anti-Stokes to the Stokes peaks and the central elastic scattering peak increases in intensity. The measured intensities were adjusted to yield the same peak height at ω_{O1} . Within the reliable bounds of the peak fitting of approx. 0.1 meV no shift of the peaks is observed for all three phonons.

In stead of either of these expected manifestations of electron-phonon coupling (softening and/or broadening), a new observation was made concerning the intensity of the phonon peaks. The acoustic phonon peaks are reduced in intensity at low temperatures beyond the changes of the peak heights due to the Bose-Einstein factor. This is clearly seen in Fig. 2 for three momentum points near and away from q_{CDW}. The total intensity of the spectra is again adjusted to the peak heights in the Stokes region. The strong increase of the elastic scattering is seen as a sharpening of the central peak. The acoustic phonon peaks almost vanish into this elastic peak at low temperatures. Compared to the optical phonon peaks the total intensity of acoustic phonon scattering is reduced. This reduction of intensity as well as the increase in elastic scattering is observed at all q points. The effect is slightly stronger near q_{CDW}, but a systematic trend in the q-dependence is not observed in the data set.

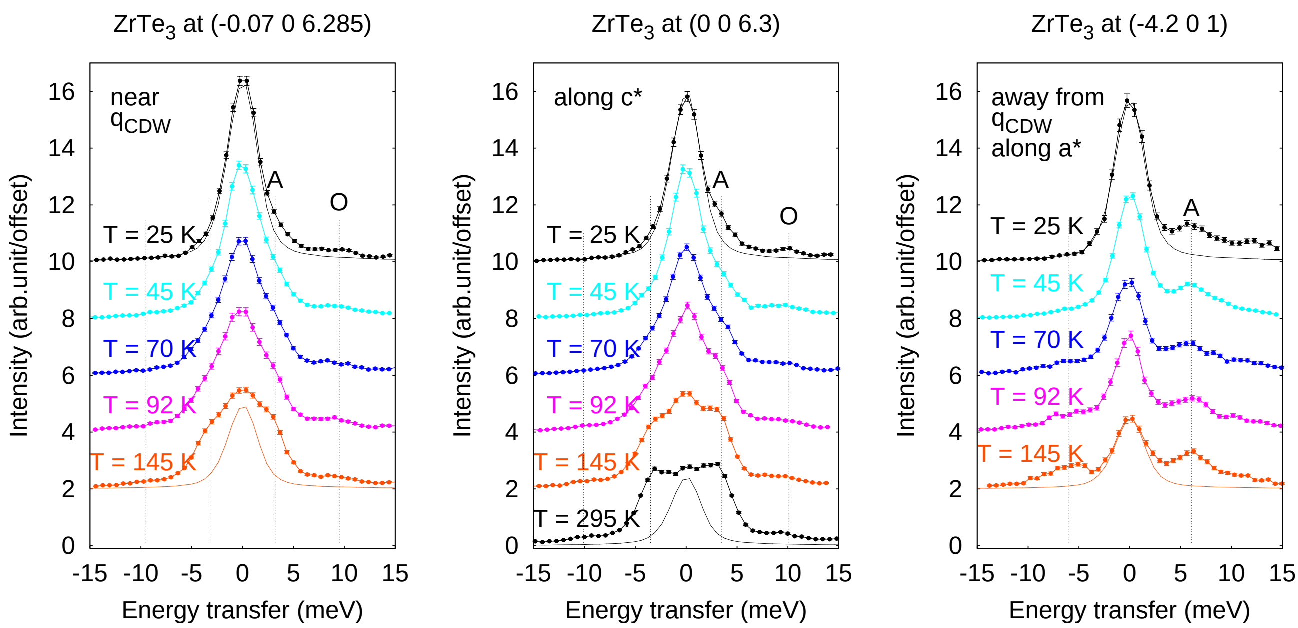

Figure 2: Temperature-dependence of inelastic x-ray scattering spectra at 3 meV resolution for 3 momentum positions as indicated. The spectra are adjusted in intensity to show the inelastic scattering peaks at positive energy transfer. At the lowest and highest temperature a measured resolution function is plotted to represent the contribution of elastic scattering.

References

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