	Experiment title: Study of the pressure-induced acoustic phonon softening in zinc metal by inelastic X-ray scattering	**Experiment number**: HS-1639
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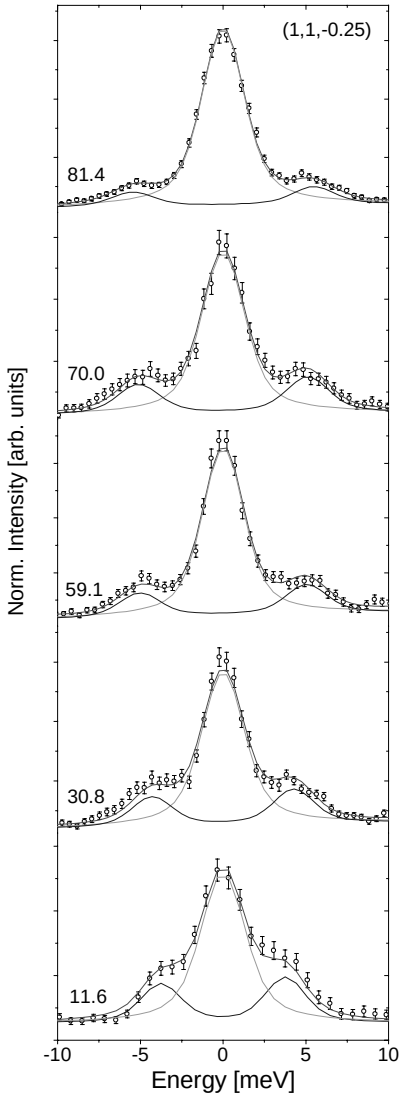
Report:

The pressure evolution of the transverse acoustic (TA) phonons along the c-axis (Δ_5-branch) in Zinc metal has been determined up to 81 kbar at room temperature. The single crystal sample of 200 μm diameter and 20 μm thickness was loaded in a diamond anvil cell (DAC) (700 μm culets) with helium as pressure transmitting medium. The pressure was determined in-situ by conventional ruby fluorescence technique, and independently, by determination of the lattice parameter a (following the Zn (110) reflection) and the known equation of state of zinc [1]. The crystal was aligned such that the [110] and [001] reciprocal lattice direction lay in the horizontal scattering plane. At each pressure point the crystal quality was checked by determining the rocking curve with of the (110) reflection. We observed an increase from 0.02º (P=11.6 kbar) to 0.046º (P=81.4 kbar), thus testifying that the excellent single crystal quality could be preserved up to the highest pressure, a prerequisite in order to correctly determine TA phonon energies. The experiment was performed with an overall energy resolution of 3 meV and a momentum resolution of 0.3 nm^{-1}. Spectra were recorded with a reduced momentum transfer q=(0;0;0.25) at Q=(1;1;0.25) in transverse geometry.

Figure 1 shows the pressure evolution of the Δ_5-TA phonon at five different pressures between 12 and 81 kbar. The experimental spectra are shown together with their best fits, obtained by the convolution of the experimental resolution function with a model function, composed of a pair of Lorentzians whose relative intensity was constrained by the Bose factor, and utilising a standard χ^2 minimisation routine.



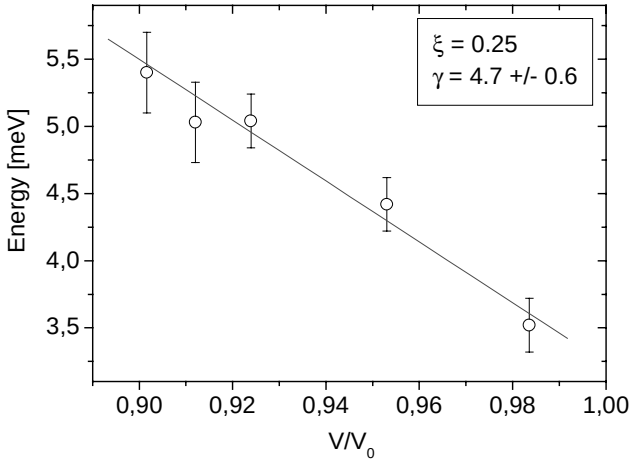


Fig. 1 (left). Representative IXS spectra of the TA Δ_5 phonon at q=(0,0,0.25) at the pressures indicated in the figure. The experimental data with their respective error bars are shown together with their best fits, obtained as explained in the text (red: total fit; green: elastic contribution; blue: phonon contribution).

Fig. 2 (top). TA phonon energies as function of reduced volume. The red line represents a linear from which the mode Grüneisen parameter, indicated in the figure, is derived.

Figure 2 shows the increase of the TA phonon energy as a function of reduced volume $V(P)/V_0$, where V_0 denotes the volume at ambient pressure. A linear fit to the experimental phonon energies reveals an approximately linear behaviour, from which we derived a mode Grüneisen parameter $\gamma(q)= 4.7+/0.6$. This value has to be compared with the ones obtained from previous inelastic neutron scattering (INS) results [2,3]. There, a value of 2.44 [2] and 2.9 [3] was obtained for the Σ_3-mode, corresponding to a TA mode propagating along [100] with polarisation along [001]. The larger value observed in the present study might be explained by the larger compressibility of the c-axis with respect to the a-axis [1].

Most importantly, we do not observe any anomalous phonon softening or stiffening, which would indicate the presence of an electronic topological transition (ETT). Our results might indicate that temperature reduces and/or shifts the ETT to higher pressures beyond the ones probed by the previous INS and IXS experiments. Future experiments should therefore extend the studies to higher pressures and low temperatures.

References

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[2] J.G. Morgan, R.B. Von Dreele, P. Wochner, and S.M. Shapiro; Phys. Rev. B 54, 812 (1996).
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