ESRF	**Experiment title:** Pressure-induced superconductivity in CrAs	**Experiment number**: HC 1936
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Report:

Single crystal inelastic X-ray scattering was carried out at ambient and 1.1GPa pressure at room temperature. The ambient pressure study was conducted from a needle like sample, see Figure 1a. For the high pressure part we have used a small single crystal embedded in a He loaded diamond anvil cell, see Figure 1b. The cell was of the cylinder piston-type with a gas driven membrane equipped with diamonds of 500μm culet. The pressure cell was mounted on a rotational stage and the pressure was determined by fluorescence measurement from Ruby crystals.

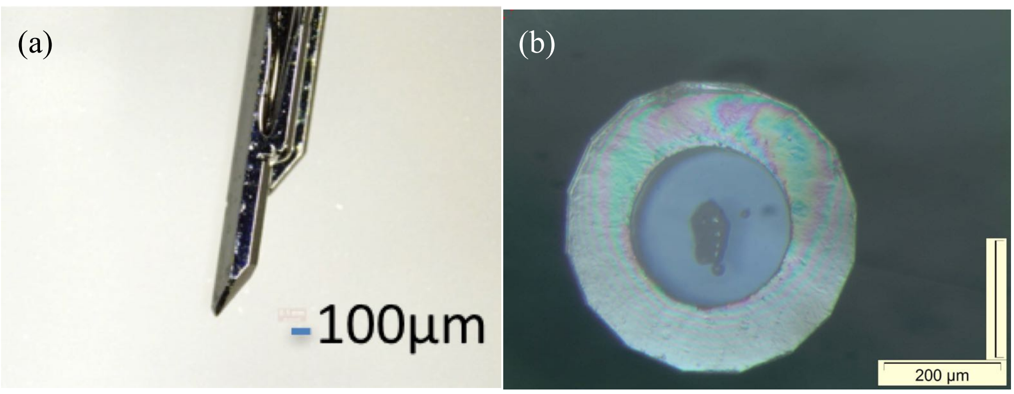

Figure 1. (a) Needle like single crystal used for measurements at ambient pressure and room temperature. (b) Loaded diamond anvial cell with a CrAs single crystal and two small Rubies for the pressure measurement.

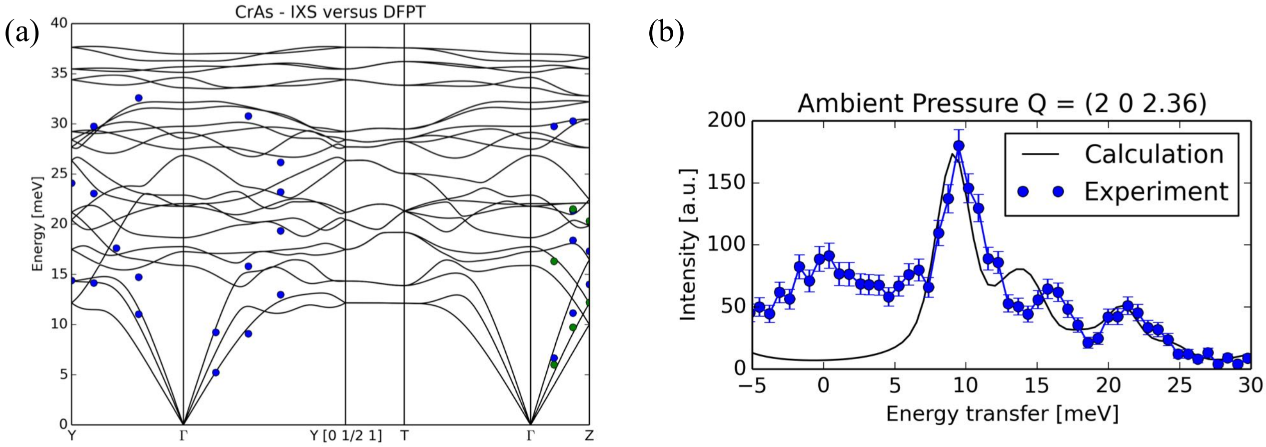

Figure 2. (a) Phonon band structure of CrAs, calculated by DFPT (full lines) and measured by IXS (295K) (circles). (b) IXS spectrum at Q = [2 0 2.36] compared to calculated intensities.

The spectrometer was operated at 17.794 keV incident energy which provides an energy resolution of 3.0 meV full width half maximum. The momentum resolution was set to 0.3 (horizontal) x 0.9 (vertical) nm^{-2}. Energy transfer scans were performed in transmission geometry at constant momentum transfer (Q), selected by appropriate choices of scattering angle and sample orientation.

Results at ambient pressure

Phonon dispersion relations along selected high-symmetry directions in the Brillouin zone are shown in Figure 2a. The measured points are compared to results from an ab initio calculation using density functional perturbation theory (DFPT). We note good agreement for most of the measured phonon branches. Scattering intensities were analyzed by direct comparison with calculated values for the single spectra. The *ab initio* calculated intensities are convoluted with the instrumental response function. An example spectrum at Q = [2 0 2.36] is shown in Figure 2b. The selected wave vector corresponds to the magnetic modulation determined by neutron diffraction [1]. We note that two phonon excitations at 9.7 and 22.5 meV are very well described whereas the excitation at 15.9 meV is underestimated in energy by the calculation. Intensities are well descried which shows that the phonon eigenvectors are correctly reproduced. The zero-energy transfer peak is due to elastic diffuse scattering and not taken into account by the calculation. The underestimation of the phonon excitation at 15.9 meV is currently investigated by comparing spin polarized and non-spin polarized calculations.

Results at high pressure

CrAs shows pressure induced superconductivity with maximal critical temperature T_c at a pressure of approximately 1.1 GPa [2,3]. In order to investigate the underlying mechanism creating the superconductivity at high pressure we investigate relevant phonon excitations at 1.1 GPa pressure.
IXS spectra at Q = [1.85 0 2] and Q = [2 0 2.64] are shown in Figure 3. Phonon excitations are clearly resolved, although the elastic contribution is increased compared to the ambient pressure data. The spectrum at Q = [2 0 2.64] has an equivalent reduced momentum transfer q as the ambient pressure spectrum at Q = [2 0 2.36]. We note that phonon energies are shifted to higher values. The most significant shift is observed for the phonon at 15.9 meV (P = 0), which appears at 16.9 meV for P = 1.1 GPa. The intensity ratio of the excitations is different due to the phonon selection rules at different absolute momentum transfer. Comparison with low temperature measurement at similar pressures are required to investigate if the shift is related to superconductivity. The experiment will certainly profit from better sample quality.
Attempts to measure at high pressures and low temperatures were unsuccessful due to technical reasons.

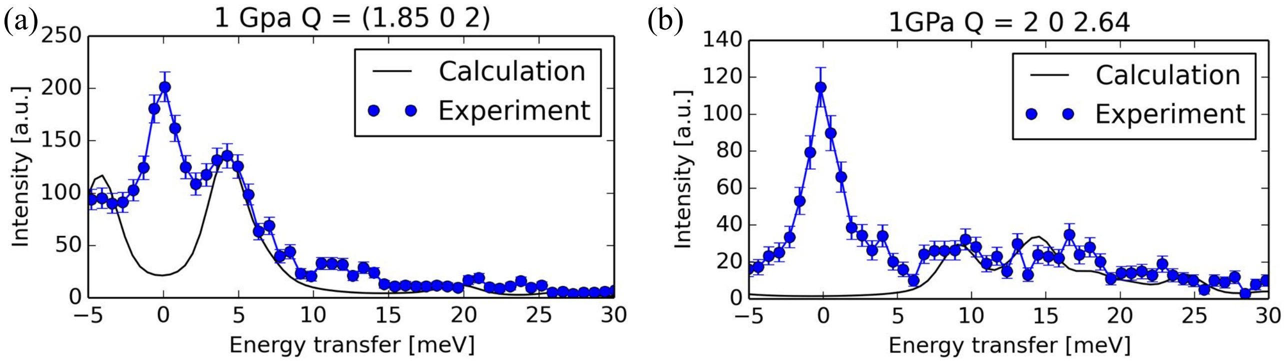

Figure 3. IXS spectra at P = 1.1 GPa from experiment (blue connected circles) and DFPT calculation (full lines) at (a) Q = [1.85 0 0] and (b) Q = [2 0 2.64].

References

[1] L. Keller, *et al.*, *Phys. Rev.* B 91, 020409(R) (2015)

[2] H. Kotegawa *et al.*, *J. Phys. Soc. Jpn.* **83**, 093702 (2014), "Superconductivity of 2.2 K under Pressure in Helimagnet CrAs".

[3] W. Wu, *et al.*, *Nat. Comm.* **5**, 5508 (2014), "Superconductivity in the vicinity of antiferromagnetic order in CrAs".