ESRF	Experiment title: Study of phase excitations in the Charge Density Wave compound $K_{0.3}MoO_3$	**Experiment number:** **HC400**
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Report:

The purpose of this experiment was to explore the capabilities of this beam line regarding the study of phonon dispersion curves and its advantages and disadvantages with respect to inelastic neutron scattering techniques. The scientific case we have chosen is the problem of the measurement of phase excitations in incommensurate quasi-one dimensional compounds, as it has recently been measured in the compound $K_{0.3}MoO_3$ by inelastic cold neutron scattering techniques. As it can be seen in the figure of the proposal, the phase excitations are characterised by a very steep dispersion around the superlattice peaks, as the phase mode velocity is proportional to the Fermi velocity. Due to the poorer q-resolution of the neutron experiments this task is a real tour de force for neutrons.

We have used the Si(9 9 9) reflection of the monochromator which corresponds to an incident energy of 17 794 eV. The sample was mounted in a closed-cycle He refrigerator with a very limited angular range of the sample rotation (maximum 200). The scattering plane was the horizontal one, where the best energy resolution is achieved, and the maximum scattering angle was 14°. The sample was a ribbon 1.9*3 mm^2 in surface and 120μm in thickness (the best compromise between absorption and diffracted intensity at this wavelength). The sample was mounted with the (2x, m, -x) plane parallel to the scattering plane.

As a result of these severe constraints we only have access to one Bragg reflection 01=(0 2 0), and, below the phase transition temperature ($T_C \approx 1$ 83 K), to one superlattice reflection Q_2=(1, 1.264, *-0.5)*, with a measured intensities ratio $I(Q_1)/I(Q_2) \approx 1.5 \cdot 10^4$.

We first measured the low energy transverse acoustic phonon dispersion curve along the (2ξ, O, -ξ) direction, as it is shown in figure 1. In these constant-Q scans we see the progressive development of 2 peaks, that corresponds to phonon creation and phonon annihilation, whose energy increases as we go away from the Bragg peak position (O 2 O).

There is in addition a third peak centred at zero energy transfer which is attributed to diffuse scattering from the sample. The resolution profile was measured on the diffuse scattering and the line shape is found to be a distorted lorentzian, with a fwhm≈ 2.4 meV. The quality of the data and the low counting time needed to obtain reasonably good spectra shows that the capabilities of this instrument, working at the Si(9 9 9) reflection, can be compared with those of standard thermal neutrons three axis spectrometers. In figure 2 we have plotted the phonon dispersion curve and compared with similar data obtained with neutrons.

Encouraged by these results we set up to measure the soft mode above T_c along the (1, 1+μ, -0.5) direction. No trace of any extra intensity, other than diffuse scattering, was observed in our 5 minutes-a-point scans. The same occurred below T_c, and no trace of phase and amplitude modes appeared in our scans. This result must be taken with care, as the experimental constraints prevented us of searching the soft mode at optimum Q-positions. From our experience in neutron scattering studies on similar problems we expect variations of the phonon intensities of more than an order of magnitude from one Brillouin zone to the other.

As a conclusion of our experiment we have shown the adequacy of this instrument in measuring well defined lattice excitations down to 1 meV, However, and given the necessarily small scattering angle in the horizontal plane, we think these measurements should be performed in the vertical scattering plane, at the expense of energy resolution. This will allow phonon measurements at optimum Q-positions, i.e., where the phonon structure factor is the largest. Another important issue is the difficulty to deal with the lorentzian tails of the instrumental resolution that makes the diffuse scattering increase the effective background in the low energy part of the spectra. Finally the pure inelastic background is low (10 counts/60s) but not as low as in neutron scattering measurements (1 -2 counts/60 s).

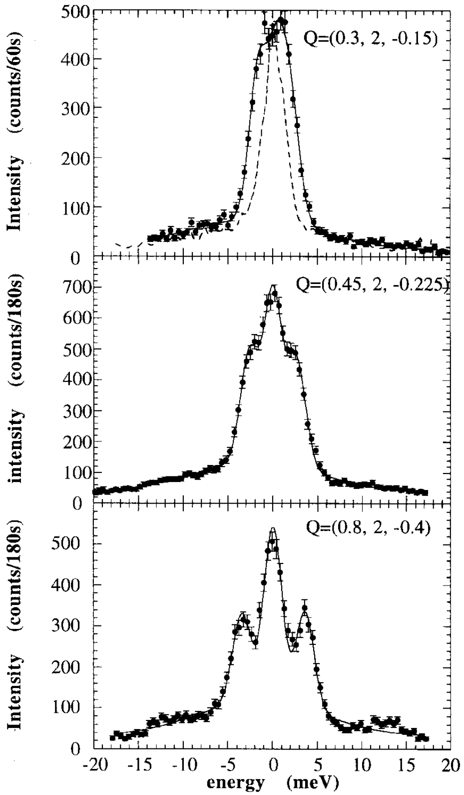

Figure 1. Inelastic x-rays scans at three Q-positions and T=290K. Solid lines are a fit of delta functions convolved with the experimental resolution line shape (dotted line in the first panel).

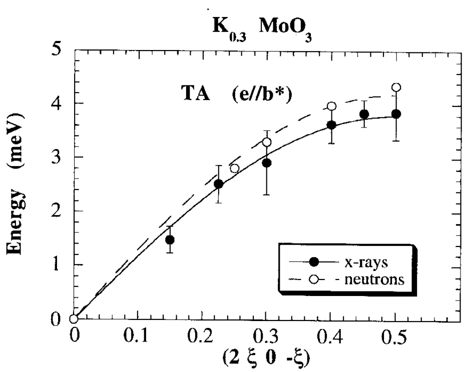

Figure 2. Phonon dispersion curve of a transverse acoustic mode polarised along b* and propagating along (2ξ, 0, -ξ) in $K_{0.3}MoO_3$ as measured by neutrons and x-rays.