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|  | <b>Experiment title:</b><br>Inelastic X-ray scattering study on the lattice- and charge-density-wave related dynamics in NbSe <sub>3</sub> | <b>Experiment number:</b><br>HS2218 |
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## Report:

Quasi-one-dimensional (Q1D) charge-density-wave (CDW) systems like K<sub>0.3</sub>MoO<sub>3</sub>, KCP or NbSe<sub>3</sub> undergo Peierls-transitions into a modulated low-temperature state. The phase-transition is related to an instability of the electron-density against a modulation with a wave number of  $2k_F$  ( $k_F$  the Fermi wave number) and is accompanied by a periodic lattice distortion with the same wave vector.

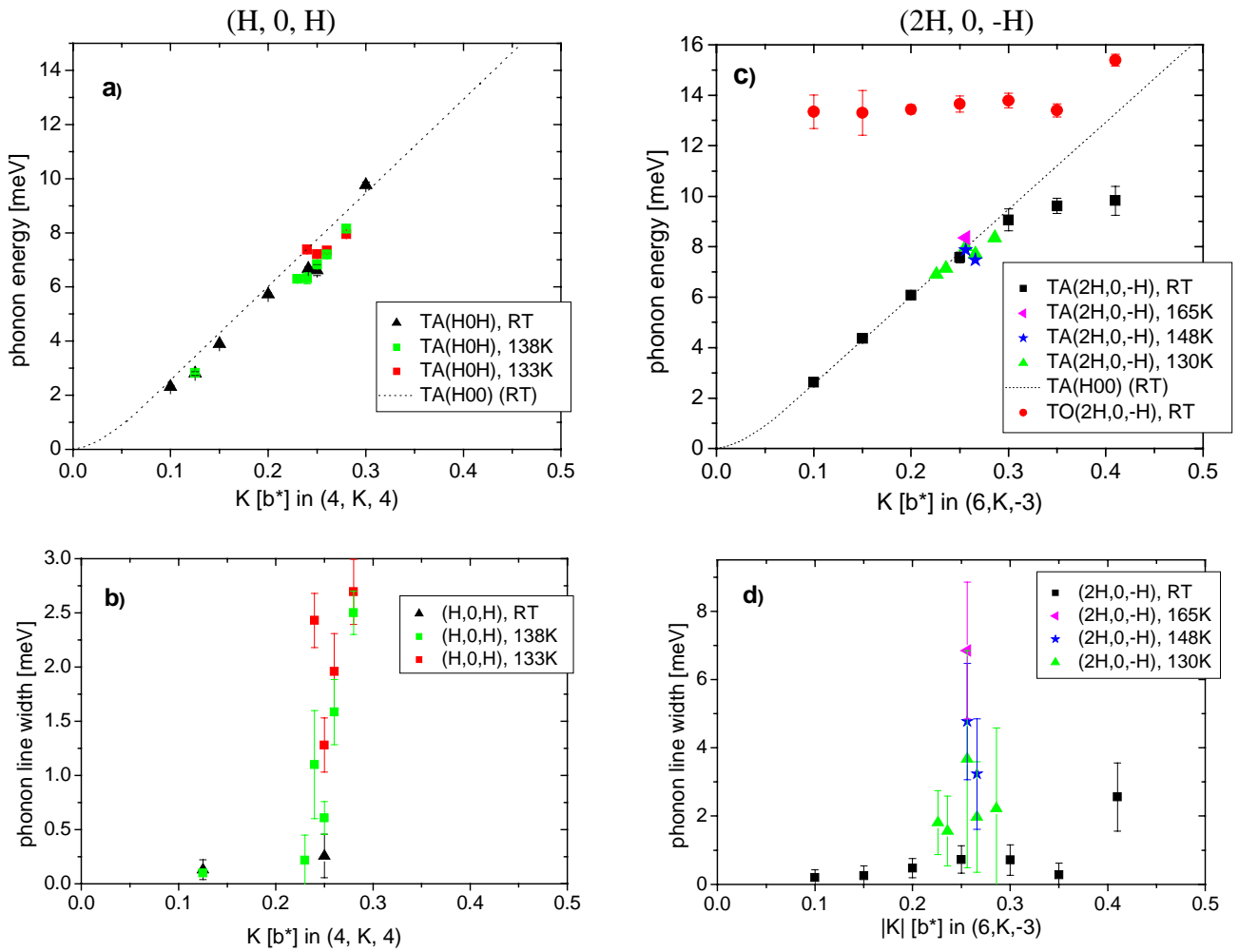
Models based on weak electron phonon coupling (Lee et al., Sol. State Comm. **14** (1974) 703) predict a steep softening of a phonon branch around the modulation wave vector precursor to the Peierls transition (Kohn anomaly) followed by a splitting into a phason- and an amplitudon-mode, corresponding to phase- and amplitude excitations of the CDW, respectively. Such a behaviour has been experimentally observed by inelastic neutron scattering in K<sub>0.3</sub>MoO<sub>3</sub> (Pouget et al., Phys. Rev. B **43** (1991) 8421) and KCP (Carneiro et al., Phys.Rev. B **13** (1976) 4258).

However, recent inelastic X-ray scattering (IXS) results on NbSe<sub>3</sub> have so far not revealed signs of phonon softening upon cooling down to the Peierls transition temperature nor of splitting of a phonon branch into phason and amplitudon modes (Requardt et al., Phys. Rev. B **66** (2002) 4303).

The purpose of the experiment reported here was to extend the low-temperature measurements on the transverse acoustic phonon branches propagating along the Q1D direction (0,K,0) in NbSe<sub>3</sub> to cover a wider range of directions of phonon polarization directions between the two crystallographic directions (0,0,L) and (H,0,0). This latter was the only transversal polarization projection studied so far.

The measurements have been carried out at the ID28 IXS-instrument using an incident photon energy of 17794eV, corresponding to an energy resolution of 3meV (provided by the Si(999) backscattering main-monochromator reflection). During the experiment the sample with lateral dimensions of 200 $\mu$ m x 3mm (VxH) and a thickness of about 3 $\mu$ m was mounted in two orientations: i) (2H, K, -H) and ii) (H, K, H) to

access to two more polarizations projections of the transversal acoustic phonon branches propagating along the Q1D direction (0,K,0). The data has been taken at several low temperatures down to and below the first Peierls-transition in NbSe<sub>3</sub> ( $T_{P1}=145\text{K}$ ). As visible in the Figs. a) and c), the low-temperature dispersion points do not show phonon softening. The corresponding room temperature data for these two transverse dispersions has been taken in the preceding experiment (HS1975), and serve here as reference for the metallic state of the system far from the CDW-state. The figures below show the dispersion curves and the corresponding phonon linewidths for the two directions of polarization projection: left hand side (H,0,H), right hand side (2H,0,-H). The dotted lines in the dispersion curves show the (H,0,0)-type transverse acoustic dispersion for comparison (see also Requardt et al.). The phonon line widths have been obtained from fits using a damped harmonic oscillator model convoluted with the experimental energy resolution profile.



*Figures:* Dispersion and line-width of transversal acoustic phonon branches with propagation direction along the quasi-one-dimensional direction (0,K,0).

In Fig. a) the dispersion with polarization projection along (H,0,H), in Fig.b) the corresponding phonon line width obtained from fits using a damped harmonic oscillator model.

Fig. c) and d) show the dispersion and linewidth, respectively, with polarization projection along (2H,0,-H). Note the absence of phonon softening in the dispersion curves.

The dotted lines in Figs. a) and c) show the dispersion of the (H,0,0) transverse acoustic phonon branch for comparison.