ESRF	**Experiment title:** Study of the lattice- and charge-density-wave dynamics in the quasi-one-dimensional compound $NbSe_3$	**Experiment number**: HS1975
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Report:

Charge-density-wave (CDW) systems such as the blue bronze ($K_{0.3}MoO_3$), KCP or $NbSe_3$ undergo Peierls-transitions into modulated states at low temperature. This transition is driven by an instability of the quasi-one-dimensional conduction-electron density leading to an electron-density- as well as a lattice-modulation with a wave vector of $2k_F$ (k_F is the Fermi wave vector). Inelastic neutron scattering studies on $K_{0.3}MoO_3$ (J.P. Pouget et al, PRB **43** (1991) 8421) and KCP (K.Carneiro et al., PRB **13** (1976) 4258) have revealed an extremely steep phonon softening, the Kohn anomaly, of a low-energy phonon branch at the modulation wave vector, precursor to the phase transition, in agreement with theoretical expectations. However, inelastic X-ray scattering experiments carried out on $NbSe_3$ so far, did not show any sign of phonon softening upon cooling towards the Peierls transition (H.Requardt et al., PRB **66** (2002) 4303), as well as they did not present splitting of a phonon branch into distinct CDW-phase and –amplitude excitations below the Peierls-transition temperature, as it has been observed in $K_{0.3}MoO_3$ (J.P. Pouget et al, PRB **43** (1991) 8421, B.Hennion et al., PRL 68 (1992) 2374).

The purpose of this experiment was to extend the available phonon dispersion data to develop a basis for a more detailed understanding of the dynamics and its detailed features in the CDW-system $NbSe_3$.

The measurements were carried out at the ID28 inelastic X-ray scattering instrument at an incident photon energy of 17794eV (Si999 backscattering monochromator reflection, energy resolution: 3meV) on a sample of thickness 3μm and dimensions 200μm x 3mm (V x H) transverse to the X-ray beam. During most of the data collection the sample was mounted to have the (H, K, H)-plane in the horizontal scattering plane. The orientation (0, K, L) was tested but found poluted by intense phonon signal coming from the sample holder.
Low-energy phonon dispersion data was taken at room temperature in the (4, 0, 4)-Brillouin-zone along the propagation directions (H, 0, H), i.e. longitudinally polarized, and (0, K, 0), i.e. transversally polarized.

Phonons of mainly transverse polarization were recorded as well along the (0.5, K, 0.5) Brillouin-zone boundary.
Figure 1 presents two inelastic spectra taken at Q=(4, 0.15, 4) (Fig.1a) and Q=(4.53, 0.17, 4.53) (Fig.1b) showing the Stokes- and Antistokes-lines of the acoustic and, in Fig.1b, also a low-energy optic phonon excitation. The lines represent fits by damped-harmonic oscillator profiles to the data.
Figure 2 shows dispersion curves of longitudinally (Fig.2a) and transversally (Fig.2b,c) polarized phonon excitations. In the spectra taken closer to the Brillouin-zone centre than (0.1, 0, 0.1), Fig.2a, or (0, 0.1, 0), Fig.2b, the phonon peaks were too strongly merged into the intense elastic line to be separated by the fits.
The transverse acoustic branch shown in Fig.2b could not be followed beyond $\Delta K=0.3$ due to the strongly decreasing intensitity of the phonon signal which had already vanished to below the background level at $\Delta K=0.4$.
Furthermore, it is interesting to note the very low excitation energy over the complete Brillouin-zone of the longitudinal acoustic phonon branch along (H, 0, H), Fig.2a, a branch which corresponds to vibrations of entire $NbSe_3$-chains with respect to each other.

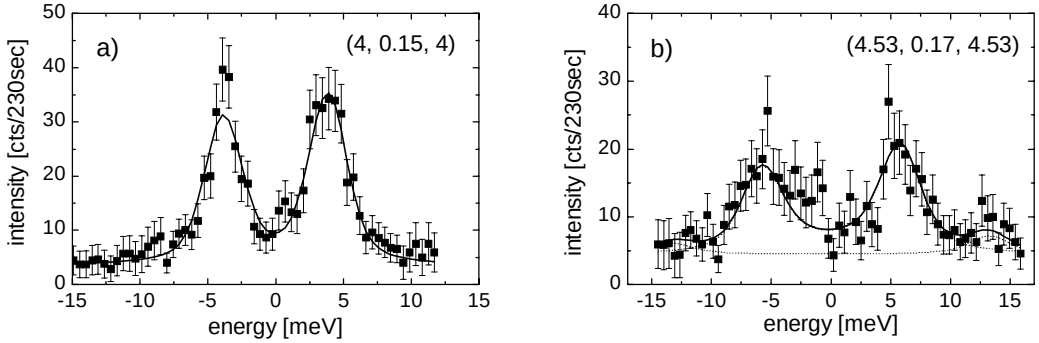

Fig.1: $NbSe_3$-phonon spectra (Stokes- and Antistokes-lines) taken at room temperature. The full lines indicate the fit to the spetra. a) Transverse acoustic phonon, Q=(4, 0.15, 4). b) Transversally polarized acoustic and optic phonon excitations at the Brillouin-zone boundary, Q=(4.53, 0.17, 4.53). The dotted lines indicate the corresponding fits to the two phonon contributions.

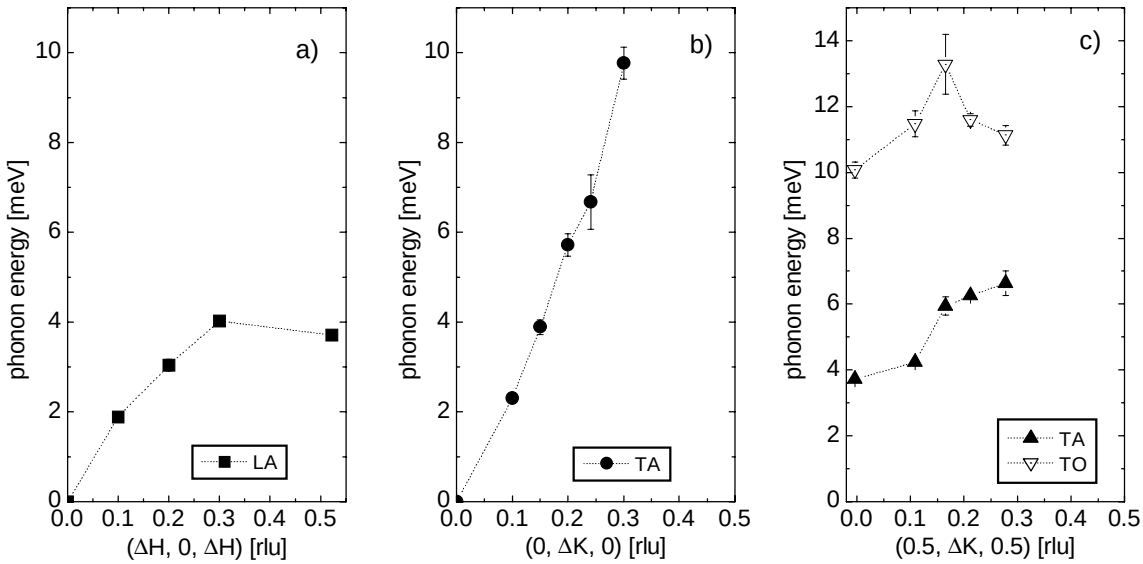

Fig. 2: $NbSe_3$-phonon dispersion curves with polarization principally along the (H, 0, H)–direction. The data was taken at room temperature in the (4, 0, 4)-Brillouin-zone: a) longitudinal acoustic (LA) branch, b) transverse acoustic (TA) branch propagating along the direction (0, K, 0) (quasi-one-dimensional direction). c) Dispersion of transversally polarized acoustic (TA) and low-energy optic (TO) phonon branches at the Brillouin-zone boundary along (0.5, K, 0.5). The dotted lines are guides to the eye.