ESRF	**Experiment title:** **Anisotropy and temperature dependence of the Phonon spectra of 2H-NbS2**	**Experiment number**: HS4253
Beamline: ID28	**Date of experiment**: from: 27/10/2010 to: 02/11/2010	**Date of report**: 10/03/2010
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2H-NbS_2 and 2H-$NbSe_2$ are isostructural and pure superconducting dichalcogenides (Tsc~6K and 7K respectively), but only 2H-$NbSe_2$ shows the coexistence of a charge density wave (CDW – T_{CDW}~33K) and superconductivity. The origin of the CDW formation and the interplay between the CDW and superconductivity in 2H-$NbSe_2$ remain a highly debated issue after 3 decades of intensive studies [Kiss07, Borisenko09]. A comparison between the physical properties of these two compounds offers an unique opportunity to understand the origin of the development of a CDW instability, but also the influence of the CDW on the superconducting properties. The main aims of this experiment were to study the temperature dependence of the phonon softening that we observed in 2H-NbS_2 along the ΓM axis [HS3996] and the anisotropy of the phonon spectra.

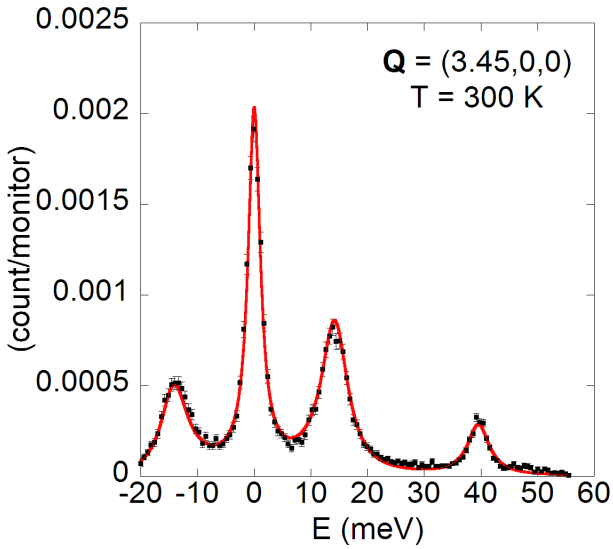

Fig. 1: Experimental scan with fit: DHO-Bose factor-Lorentzian experimental resolution convoluted

The high-resolution silicon backscattering monochromator was configured for the (9,9,9) reflection at an incident energy of 17,794 keV. The least-square fit to a Lorentzian curve of the elastic peak gave an experimental resolution (HWHM) of 1,3 meV. The incident beam of 280x160 µm (width x height) was focused by a multilayer mirror into a spot of 200x60 µm (width x height) on a single crystal of 2H-NbS_2 of 450x100 µm. Using the 5 pairs of detectors/analysers we were able to efficiently map the phonon dispersion along the ΓK and ΓM line at 14 different temperatures between 300K and 2K (pumped He^4 cryostat). On Fig.1 a typical spectra and fit is shown. The Stokes and anti-Stokes are clearly observed at 300K. We used least-square minimization with Levenberg-Marquardt algorithm and fitted phonons to a damped harmonic oscillator model (DHO) with Bose factor and convoluted by the Lorentzian experimental resolution function.

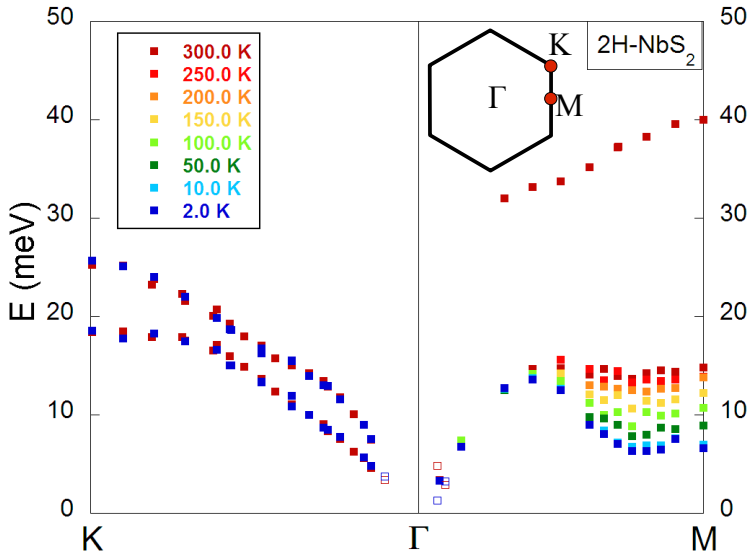

Fig. 2: Dispersion curves for several temperatures (open symbols correspond to transverse phonons and closed symbols to longitudinal phonons). Along ΓK: scans ranged from -5 to +31 meV at all temperature. Along ΓM: scans ranged from -5 to +25 meV at all temperature, except for the 300K scan which ranged from -20 to +55 meV.

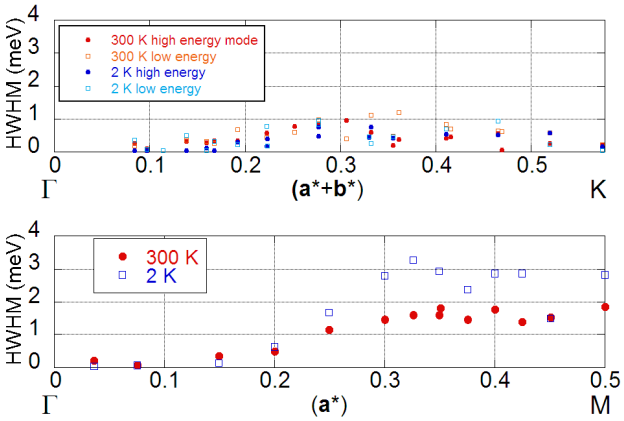

Fig. 3: linewidth of phonons after deconvolution from experimental resolution.Only the low energy mode is shown for ΓM.

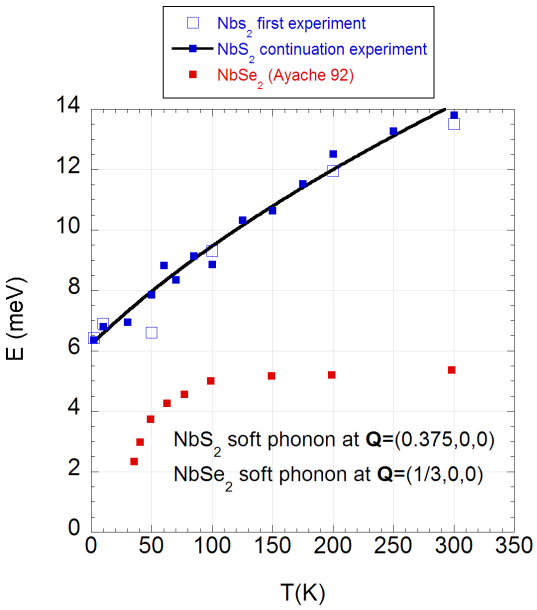

Fig. 4: Temperature dependence of the soft phonon mode in NbS_2 and $NbSe_2$

Fig.2 presents the low energy part of the phonon spectrum in the basal plane. The phonon dispersion curves along ΓK present little change between 300K and 2K : no softening is observed, whereas a strong softening of more than 6 meV appears along ΓM.

The temperature dependence of this softening (Fig.4) is in good agreement with mean field scenario which predicts a $T^{1/2}$ law. For comparison, in the isoelectronic compound $NbSe_2$ which develops a CDW for T<35K, there is also a soft mode at 2/3 of ΓM, but it follows a $T^{1/4}$ law [Ayache92]. This difference in the softening of both compounds is unexplained.

On Fig.3, one can see that the linewidth of excitations along ΓK are mainly due to the experimental resolution, and within the uncertainty due to this experimental resolution, no temperature dependence is observed. On the contrary along ΓM the linewidth can reach twice the experimental resolution, besides this linewidth decreases at high temperature, especially close to the soft mode. There are two main mechanisms which can broaden the deconvoluted linewidth: phonon-phonon interaction or electron-phonon coupling. [Calandra05,Aynajian09] Owing to the presence of a CDW in the parent compound $NbSe_2$, and since the phonon-phonon interaction usually increases linewidth at high temperature, we rather suspect electron-phonon coupling of playing an important role in the softening and the broadening of the linewidth.

An open question is if these soft phonon modes could be the evidence of the proximity to a quantum critical point (QCP), where the 2nd order phase transition is a CDW instability. In such a scenario $NbSe_2$ and NbS_2 would be on each side of this QCP. This requires to investigate the phase diagram tuned with an external parameter.

References

[Kiss07] T. Kiss & al Nature Physics 3 (2007) 720

[Borisenko09] S.V. Borisenko; Phys. Rev. Lett. **102** (2009) 166402

[Ayache92] C. Ayache, R. Curriat and P. Molinié, Physica B 180 & 181 (1992) 333-335

[Aynajian09] P. Aynajian, Ph.D Thesis: Electron-Phonon Interaction in Conventional and Unconventional Superconductors (Max Planck Institut, Stuttgart, 2009)

[Calandra05] M. Calandra, F. Mauri, Phys. Rev. B **71** (2005) 064501