ESRF	**Experiment title:** Phonon spectra of 2H-NbS_2	**Experiment number**: HS3996
Beamline: ID28	**Date of experiment**: from: 27/01/2010 to: 02/02/2010	**Date of report**: 1/04/2010
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Report:

The main aim of this experiment was to study the phonon spectrum of 2H-NbS_2. 2H-NbS_2 is the only 2H superconducting dichalcogenide (Tsc~6K) which doesn't develop any charge density wave at low temperature. Comparing the phonon spectrum, with that of the well known iso-electronic compound 2H-$NbSe_2$ which shows the coexistence of a charge density wave (CDW – T_{CDW}~33K) and superconductivity (Tsc~7K), 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.

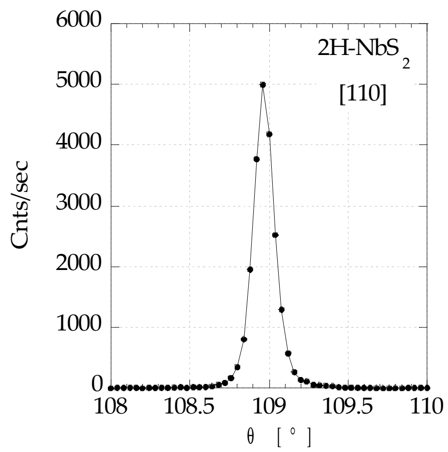

Fig. 1 : rocking curve of the bragg peak [110]

In 2H-$NbSe_2$ the CDW which is formed below T_{CDW} is associated above T_{CDW} with the softening of the longitudinal Σ_1 phonon mode with a wave vector Q=2/3ΓM [Moncton77, Ayache92]. The temperature dependence of the softening follows a critical exponent of ¼ smaller than ½ expected by the mean field theory . In the iso-electronic compound 2H-NbS2, a strong softening at the same Q vector is expected[Nishio94].

A high quality single crystal of 2H-NbS_2 has been carefully characterised by magnetic and thermodynamical probes (specific heat, AC susceptibility …) and crystallographic probes. The rocking curve confirms the excellent crystallographic quality of the crystal. The Phonon dispersions were measured with inelastic x-ray scattering (IXS). The experimental configuration used a Si (11 11 11) monochromator offering an high energy resolution FORMTEXT of E=1.0 meV. Energy scan between -3meV up to 23meV were performed along the ΓM direction at different temperature.

The IXS spectra obtained at different temperature is shown Fig.2. Two main features are observed :

1) a strong enhancement of the elastic peak intensity at low temperature and around Q=2/3 ΓM. While the non temperature-dependent part of the elastic peak can essentially be associated to structural or surface defects, the temperature dependent part of the elastic intensity most likely originates from CDW fluctuations, and can be seen as a precursor of the superstructure spots that should appear in a "real" CDW state. This behaviour was for instance recently reported in $ZrTe_3$ above the temperature Tp below which appears a CDW [Hoesch09]. However, this experiment doesn't allow a quantitative analysis of this enhancement, since only a part of the scattered intensity is measured here.

2) A clear peak associated to the longitudinal Σ_1 phonon mode is observed. On Fig. 3, the dispersion curve of the longitudinal Σ_1 phonon mode is presented for different temperatures. A clear anomaly is observed at Q=4/5ΓM, where we observe a logarithmic softening the phonon energy between room temperature and 50 K.

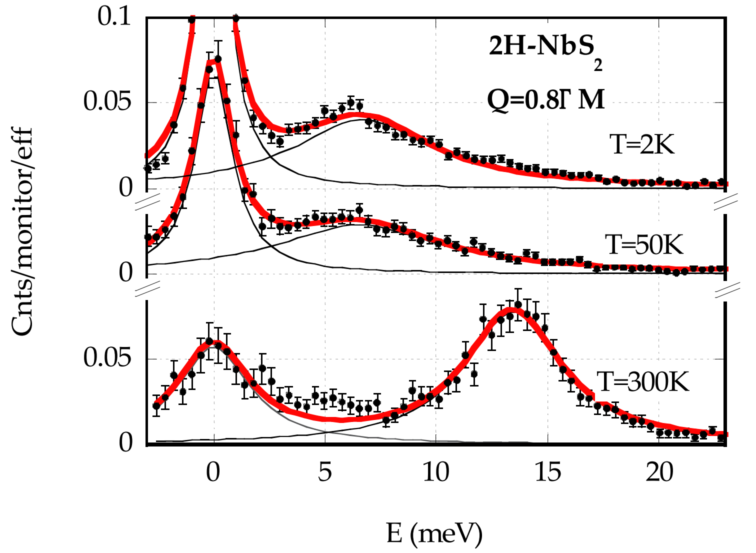

Fig. 2 : IXS spectra obtain at ID28 on single crystal of 2H-NbS_2 at different temperature for Q=4/5ΓM. The red curve is the sum of 2 Lorentzian centred at 0meV and at the phonon energy.

Interestingly, below T*~50K, close to the temperature where in $NbSe_2$ the CDW appears (at Q=2/3ΓM), the softening seems to *freeze.* This very unusual temperature dependence of the soft mode is compared to the case of $NbSe_2$ in the Figure 4.

Moreover, no modification of the phonon spectrum was observed above and below the superconducting critical temperature.

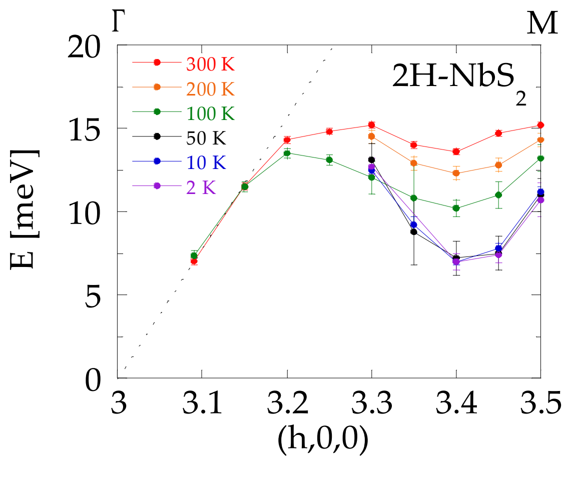

Fig. 3:The dispersion curve along ΓM. A clear softening of the Σ_1 branch is observed as calculated by Nishio & al [Nishio94].

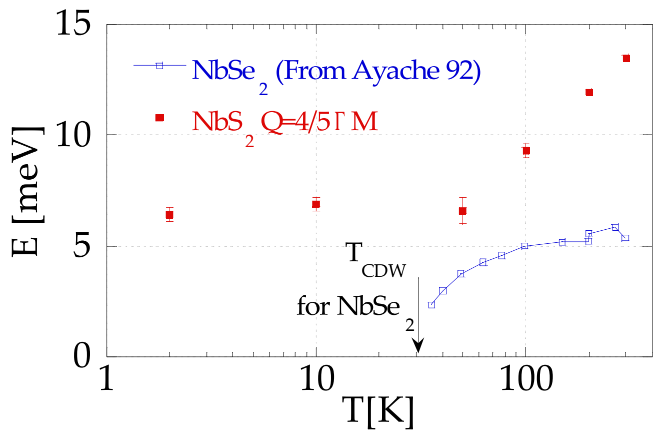

Fig. 4:Temperature dependence of the energy of the soft phonon mode at Q=4/5ΓM of NbS_2 compared to this of $NbSe_2$

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