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ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal:

https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do

Reports supporting requests for additional beam time

Reports can be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

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All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title: Pressure temperature dependence of the Phonon spectra of 2H-$NbSe_2$**	**Experiment number**: **HS-4536**
Beamline: ID-28	**Date of experiment**: from: 19/10/2011 at 08:00 to: 25/10/2011 at 08:00	**Date of report**:
Shifts: 18	**Local contact(s)**: BOSSAK Alexei	*Received at ESRF:*

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Report:

I - Context

At ambient pressure, the dichalcogenide 2H-$NbSe_2$ presents a charge density wave (CDW) below T_{CDW} = 33 K, and then becomes superconducting below T_c = 7.1 K [5, 8]. Under pressure, the CDW disappears between 3.5 and 5 GPa [1, 3], meanwhile T_c only slightly increases up to a maximum of 8.2 K at 10 GPa [10]. However, the superconducting gap has an intriguing feature, at least at ambient pressure, it is either anisotropic or multi-gap [4, 6, 7]. Previously, by comparing with 2H-NbS_2, a parent compound with no CDW, we showed that this particular superconducting gap is not directly related to the CDW [2].

Yet, 2H-$NbSe_2$ and 2H-NbS_2 both exhibit a very similar, deep and wide soft phonon mode [11, Leroux et al. (in press)]. These soft modes are expected to give a major contribution to the electron-phonon coupling constant [9] and may therefore have a strong influence on the superconducting properties. The main aim of this experiment was to investigate whether a soft phonon mode is still present in 2H-$NbSe_2$, above the critical pressure where the CDW is not the ground state.

II - Experimental setup

We used the (9,9,9) reflection on the backscattering monochromator with an incident energy of 17.794 keV, and corresponding energy resolution of 1.3 meV HWHM (lorentzian fit of the elastic peak). The incident beam was focused by a multilayer mirror into a spot of 100 x 60 µm (width x height). We used two single crystals of 2H-$NbSe_2$ synthesized by L. Cario, the size of which was 100 x 100 x 50 μm^3 (**a** x **b** x **c**). The x-ray beam was aligned along the c-axis. The diamond anvil cells were 400 µm in diameter, allowing to reach at most 40 GPa.

We measured the phonons dispersion along (2-h,0,0), since this selects only the optical soft phonon mode along GM, according to the phonon calculations. As illustrated in Fig. 1 we found that a small c-axis component (up to 0.3 c*) has no influence on the dispersion, owing to the 2D character of the compound. This allowed us to simultaneously use the 9 pairs of detectors/analysers, greatly enhancing the statistics.

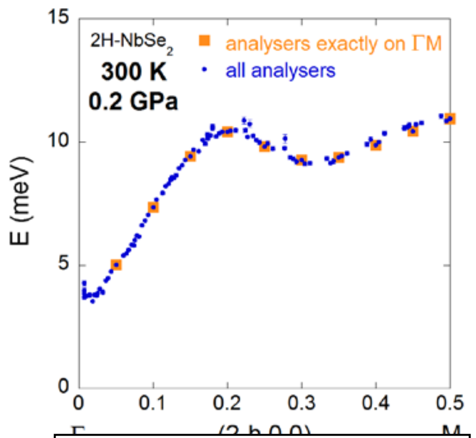

Figure 1 : *Phonon dispersion exactly along GM, and with a small c-axis component.*

III - Results

High quality data were obtained, that allow us to track the optical soft phonon branch at 6 pressures (0 to 16 GPa) and 7 temperatures (between room temperature and 20 K – the low temperature data were taken during the first session of measurements, from October 19 to 25, and completed with the room temperature data from November 2 to 4). Typical results of this experiment is presented in Fig. 3. We found a dip in the dispersion, characteristic of the soft phonon mode, at all measured pressures and temperatures.

At constant pressure, an increase of temperature only affect the depth of the dip: its energy increases as a $T^{1/2}$ exponent compatible with mean-field theory like at ambient pressure [11]. At constant temperature, an increase of pressure shifts up the whole phonon branch, with only a slight effect on the depth of the dip. It shows that strong anharmonic effects are present at all pressure. The main result of this experiment is that a soft phonon mode is still present at 16 GPa, far beyond the critical pressure where the CDW disappears. This strongly suggests that the soft phonon modes play a major role in the superconducting properties of both 2H-$NbSe_2$ and 2H-NbS_2.

Finally, this is the first time that a whole phonon branch is simultaneously measured under pressure and at low temperature, using Inelastic X-ray Scattering (IXS) on a submillimeter sized single crystal. This achievement emphasizes the great possibilities of IXS under extreme conditions: the combined use of a diamond anvil cell with an ^{4}He cryostat allows to reach pressures up to 40 GPa and temperatures down to 2 K, on a submillimetre single crystals.

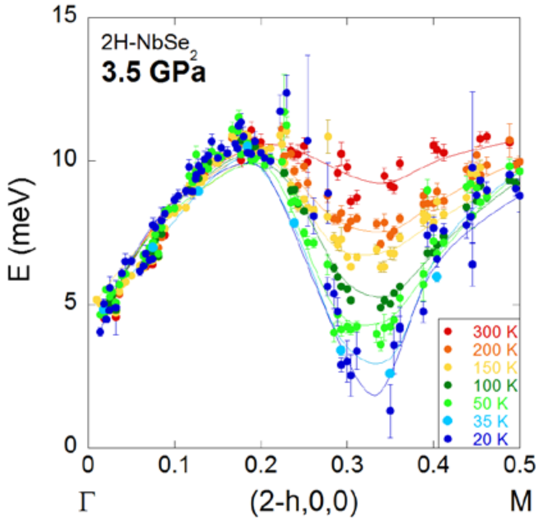

Figure 3: 2H-NbSe2: temperature dependence of the optical soft phonon branch at 3.. Lines are guide for the eyes.

References

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