ESRF	**Experiment title:** Competition between charge density wave and superconductivity in $NbSe_2$ under pressure	**Experiment number**: HS-3944
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Report:

2*H*-$NbSe_2$ was one of the first studied charge density wave (CDW) layered dichalcogenides. At ambient pressure the periodic CDW distortion is formed below T_{CDW} = 33 K and superconductivity is found in this ordered state with an unusually high T_c = 7 K. The structure is composed of layers of one sheet of Nb atoms between two sheets of Se atoms Se-Nb-Se. Adjacent layers are bonded with weak van der Waals forces, which leads to a pronounced two-dimensional character, making this compound the archetypical case of superconductivity in layered materials.

The particularity of this material is that the CDW and the superconducting state appear at very similar transition temperatures, causing a strong interaction between both states. The interplay between these two states was further exemplified by the evolution of both states with pressure, shown on Fig. 2[1]. As T_{CDW} decreases with pressure, T_c increases, showing that carriers from sections of the Fermi surface under the CDW gap are gradually released and made available for the superconducting state. However, recent measurements[2] of the T_c under pressure have given slightly but crucially different results, as the maximum of T_c is found beyond the previously reported disappearance of the CDW. It is vital for the understanding of the fundamental properties of this widely studied material to verify directly if the CDW distortion actually disappears at the pressure reported by Ref. 1 (3.7 GPa) or at the higher one that can implicitly be extracted from Ref. 2 (5 GPa).

The CDW distortion shows up as incommensurate superstructure reflections in the *a*-b** plane of the hexagonal lattice. The reduced wave vector q_{CDW}, representative of the Fermi surface nesting $2k_F$, is characterized by $q_{CDW} = 2/3\, \boldsymbol{a}^* (1 - \delta)$, with a small incommensurability $\delta \approx 0.02$ that shows a slight temperature dependence but remains incommensurate to low temperatures. The absence of a lock-in is an indication of a the strong role played by the Fermi surface. The evolution of $2k_F$ with pressure can thus readily be studied by x-ray diffraction.

Exprimental data and results

Small single crystals of $NbSe_2$ were mounted in a diamond anvil cell with 600 μm cutlet size and loaded with Ne as pressure transmiting media. The hydrostatic pressure was measured by fluorescence of a ruby chip. The cell was mounted in a He flow cryostat with an attached gas membrane for pressurizing the sample *in-situ*. Precise control of the temperature and pressure in the range of 10 K < *T* < 300 K and 0.2 GPa < *P* < 5GPa was employed. Diffraction data were acquired using a MAR CCD detector in the forward scattering direction with the focused x-ray beam of 2x2 μm2. The *c** axis is naturally aligned to being close to parallel to the incoming beam, while the *a** axis was chosen close to perpendicular to the φ rotation axis. In this way the *a**-*b** plane is readily spanned on the detector in oscillations of φ, while different *c** components are accessible within the opening of the cell of ±30°. The data were indexed and reconstructed high symmetry planes were extracted using the CrysAlis software (see figure 1).

We were able to measure the CDW superstructure peaks (see fig.1 upper panel). Using the reciprocal space reconstructions (fig 1 upper panel), we determined the incommensurability parameter δ ($0<\delta<0.02$) measuring the separation of the CDW peak respect to $\frac{1}{3}a^*$ and $\frac{2}{3}a^*$ normalized by a^* (lower panel of fig. 1). We showed that δ tends to zero at 4.5GPa, while the CDW transition is supressed at 3.5GPa (see fig.2). This results shows that the CDW modulation and thus the Fermi surface nesting condition slightly changes with pressure.

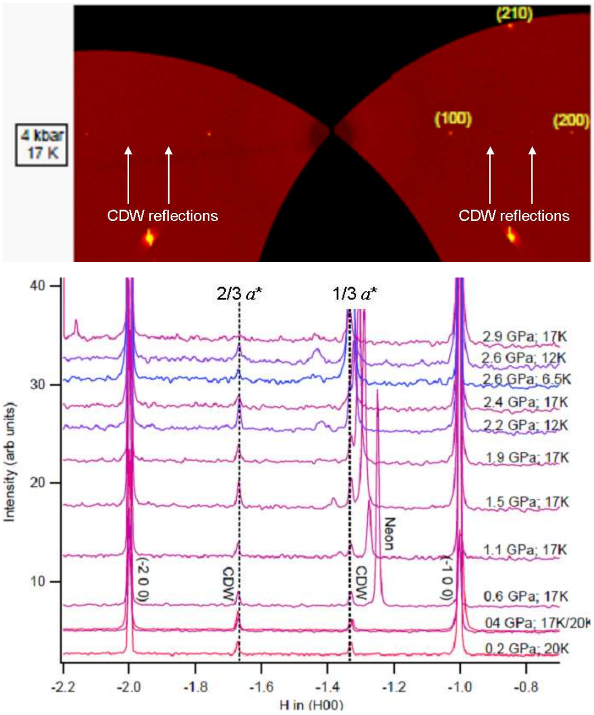

Fig. 1: Upper panel: Reconstructed (hk0) layer of the reciprocal space at the indicated pressure and temperature. Superstructure reflexions between the Bragg (100) and (200) peaks are clearly visible, demonstrating the occurrence of the charge density wave superstructure. **Lower panel:** Integrated intensity in a rectangular region between (-1 0 0) and (-2 0 0) reflections.

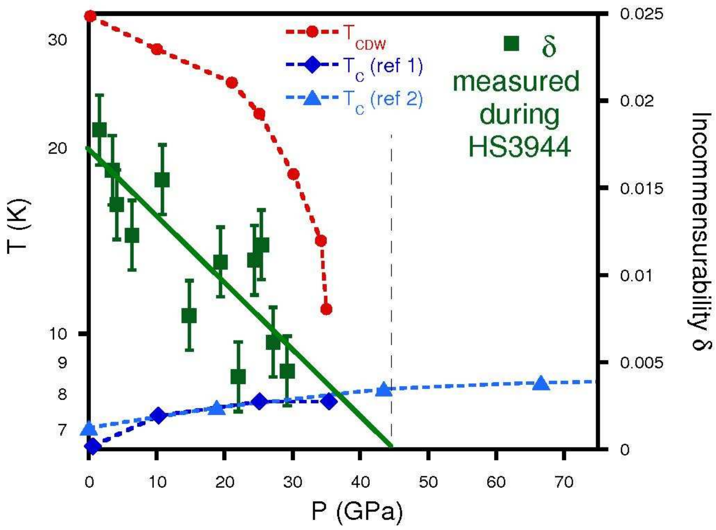

Fig.2: Incommensurability parameter δ (solid squares) and critical temperatures in function of pressure for 2*H*-$NbSe_2$ as obtained form this experiment (δ) and from resisitvity data (from Ref. 1 and 2). The solid line is a linear fit of the X ray data, while the dashed lines are guide for the eye.

References

[1] C.Berthier, P.Molinié and D.Jérome, "Evidence of a connection between charge density waves and the pressure enhancement of superconductivity in 2*H*-$NbSe_2$", Solid State Comm. **18** p. 1393 (1976).

[2] H. Suderow, V. G. Tissen, J. P. Brison, J. L. Martínez, and S.Vieira, "Pressure induced effects on the Fermi surface of superconducting 2*H*-$NbSe_2$", Phys. Rev. Lett. **95**, 117006 2005.