ESRF	**Experiment title:** Bulk and surface inelastic x-ray scattering investigation of the charge density wave material $TaSe_2$	**Experiment number**: HS 3063
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Report:

Due to their van der Waals bonded layered structure, the layered transition metal dichalcogenides exhibit fascinating properties including: superconducting behaviour, nonlinear and anisotropic electrical properties, very large dielectric constants, charge density wave (CDW) instabilities and a wealth of dynamical features [1]. $TaSe_2$ is a member of this group of materials. As a result of its layer-like structure $TaSe_2$ displays almost two-dimensional behaviour, exhibiting a CDW and superconductivity [2]. The single crystal investigated in this work is predominantly of the 2H-polytype. 2H-$TaSe_2$ undergoes an incommensurate charge density wave (CDW) phase transition at 122.2 K. This transition has been the subject of previous neutron and X-ray studies and is considered second order within experimental accuracy [3]. Using inelastic neutron scattering, Moncton *et al.* measured the room temperature bulk phonon dispersion curve for TaSe2 and $NbSe_2$. They observed a phonon softening of the Σ_1 mode at the CDW satellite position in Q-space and a complete mode softening at the CDW phase transition in the bulk [2]. 2H-$TaSe_2$ bulk dispersion curve calculations are found in Wakabayashi *et al* [4] for the two dimensional Kohn anomaly and Motizuki *et al*. [5] who report a theoretical study of 2H-$TaSe_2$ and 2H- $NbSe_2$ lattice dynamics and phonon anomalies.

The aim of this experiment was to measure both surface and bulk temperature dependent dispersion curves of $TaSe_2$ in order to compare the mode softening for both cases.

This recent experiment(April 2006) was a follow up to our pilot grazing incidence geometry phonon measurements performed at the inelastic scattering beamline ID28 at the ESRF[6,7]. At ID28 a total flux of $2.70 \cdot 10^{10}$ ph/s (at 200mA) is available with an instrumental energy resolution of 3.0 meV in a beam of 15 µm(V) x .300 µm (H) at a photon energy of 17.794 KeV. The single crystal 2H-$TaSe_2$ sample - 2 mm thick, surface area of 4 x 6 mm^2 - was mounted with the surface normal (0,0,1) vertical in a vacuum chamber after cleaving using the sticky tape method. Grazing incidence geometry was achieved by inserting a Pt coated glass mirror before the sample to deflect the primary beam downwards. Surface sensitivity was achieved by combining this deflection with the sample ϕ rotation. An incidence angle and exit angle close to the critical angle of total external reflection (0.154°) was obtained, providing a penetration depth of ~40 Å. Following surface alignment, the sample was oriented at α_c - 0.05° for surface sensitive measurements and α_c +- 0.05° for bulk measurements.. These small changes of angle were chosen so that we had surface or bulk sensitivity, but still benefited from the enhancement in the transmission function close to α_c. The 200 in-plane surface reflection was aligned and constant-q scans on the longitudinal acoustic branch propagating along Γ-

M high symmetry direction were carried preformed at room temperature and at 150 K (figure 1). The data were collected with the standard analyser opening of 20 x 60 mm^2 (H x V) providing a q resolution of about $\Delta q = 0.0216$ $Å^{-1}$.

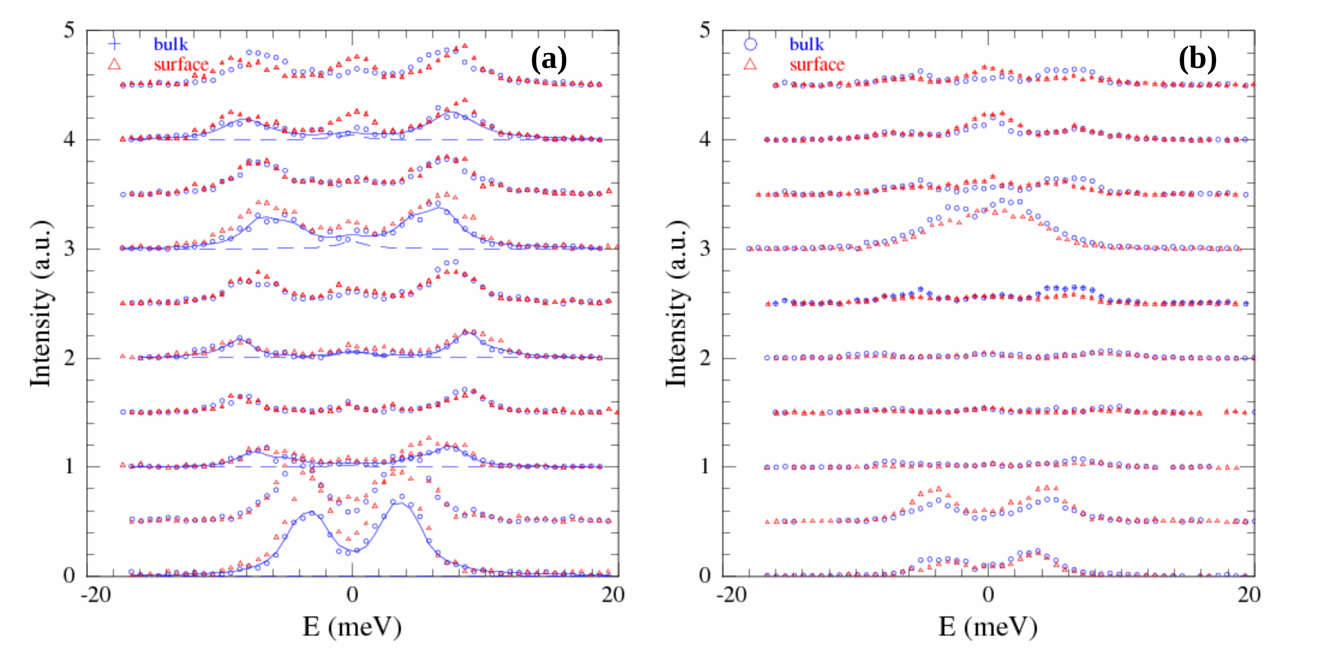

Figure 1: Surface and bulk IXS spectra of 2H-$TaSe_2$ at (a) room temperature and (b) 150 K measured on ID28, ESRF. (Surface-triangles, bulk-circles).

In conclusion we have successfully obtained surface and bulk sensitive data from a single $TaSe_2$ sample using grazing incidence inelastic X-ray scattering. We have observed phonon softening at the surface and in the bulk of $NbSe_2$ at room temperature and at 150 K. At room temperature there is considerable evidence that the sound velocity is lower in the bulk than at the surface. At room temperature behaviour at the surface and bulk behaviour is upon cooling to 120 K the degree of softening in the surface optical branch is greater for that in the bulk. Of particular interest is the behaviour at the M point where an unexpected softening in the acoustic branch was observed at room temperature (figure 2 a). At 150 K M point softening was observed in both surface and bulk $\sum_1\omega_1$ and $\sum_1\omega_2$ branches and was accompanied by an intensity increase in the elastic peak (figure 2 b). This may be evidence of additional ordering.

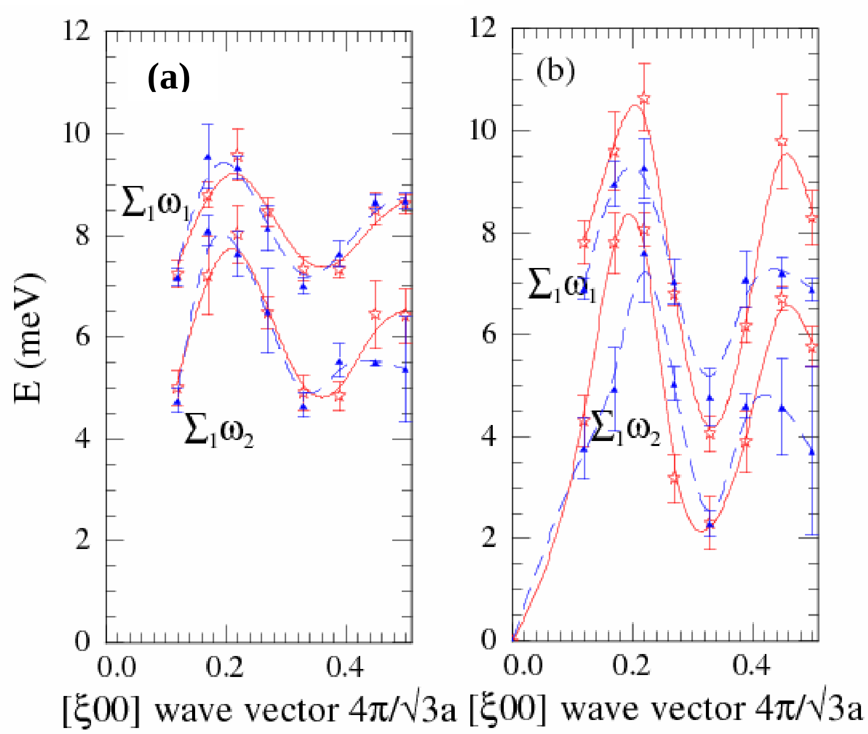

Figure 2(a)Temperature dependant Surface and bulk Despersion curve for 2H-$TaSe_2$.surface (continuous red line and open stars), Bulk (dashed line and closed triangles).

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