EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

	Experiment title: Electron-phonon interaction in the CDW-Weyl semimetal $(TaSe_4)_2I$	**Experiment number**: HC-4741
Beamline: ID28	**Date of experiment**: from: 22/09/2021 to: 28/09/2021	**Date of report**: 13/02/2022
Shifts: 24	**Local contact(s)**: Alexei Bosak	*Received at ESRF:*

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Report:

In the HC-4741 project, we have proposed to search for a **Weyl-Kohn anomaly** by measuring the low energy phonon spectrum of $(TaSe_4)_2I$, a compound recently reported to be a CDW-Weyl semimetal with charge modulations below 250 K. By studying the renormalization of the energy and linewidth of the longitudinal acoustic modes through the CDW transition, we wanted to observe the collapse of the soft phonon in $(TaSe_4)_2I$ driven by the nesting of the Weyl points and study the electron-phonon interaction in the CDW formation. Due to the slight improvement of the pandemic situation, the beamtime could have been carried out on-site.

First, our collaborators in Hamburg (Prof. Kai Rossnagel and Dr. Sanjoy Mahatha) have provided us with several $(TaSe_4)_2I$ single crystals with a different degree of disorder. This was achieved by varying the growth conditions, which allows to obtain crystals with I_2 deficiency. It turns out, as reported experimentally in the literature, that the degree of disorder strongly affects the onset temperature and propogation vectors of the CDW modulations. The degree of disorder and the quality of the $(TaSe_4)_2I$ single crystals was checked by x-ray diffarction and Raman scattering (see figure 1 a) and b)). We see that the crystal with T_{CDW}=240 K and $\mathbf{q}_{CDW}$=0.5 0.5 0.1 rlu (batch 127-6R) shows the highest degree of order and was used for the IXS measurements. Nevertheless, we have measured a total of 4 single crystals with thermal diffuse scattering and the best 2 were selected for the inelastic x-ray scattering data. Only the best data is shown in this report.

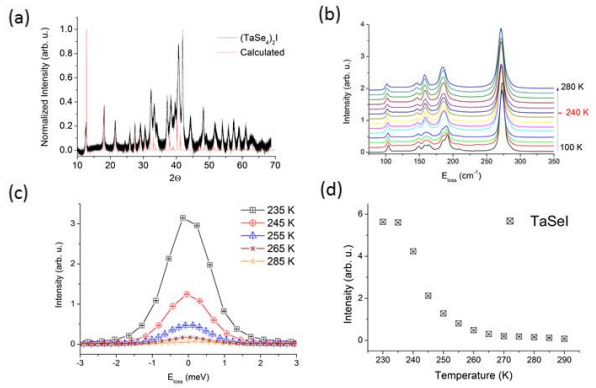

Figure 1: (a) Powder x-ray diffraction and (b) Raman scattering of $(TaSe_4)_2I$. (c) and (d) temperature dependence of the elastic signal, with T_{CDW}=240 K.

With a set of $(TaSe_4)_2I$ crystals, we have first dedicated 2 days of beamtime to obtain thermal diffuse scattering maps and locate the positions of the reciprocal space to better search for phonon anomalies. As expected, the sample labeled 127-6R shows the higher degree of order, with CDW propagation vector 0.05 0.05 0.1 rlu, alowing to measure phonon anomalies away from the nearby Bragg point. It turns out that higher degree of disorder reduces the $\mathbf{q}_{CDW}$ and merges the CDW peak with the Bragg spot, precluiding the observation of the low energy phonons in some of the other 3 crystals. Although, we have dedicated IXS beamtime to measure the 4 single crystals prepared, we are only reporting the results of the 127-6R sample, which gave the best data. This crystal, with the largest $\mathbf{q}_{CDW}$, shows an onset of the CDW modulations of 240 K (see figure 1c and d).
A care view of the reciprocal mapping of the thermal diffuse scattering maps allowed us to find the G=1 0 7 reciprocal lattice vector as the best postion to search for the phonon anomalies, see figure 2a, where 4 CDW Bragg spots are seen at 100 K. Here, the intensity of the thermal scattering is more clearly visible due to the low scattering form factor of the 1 0 7 Bragg peak, allowing to detect the transverse phonon softening, figure 2 b.

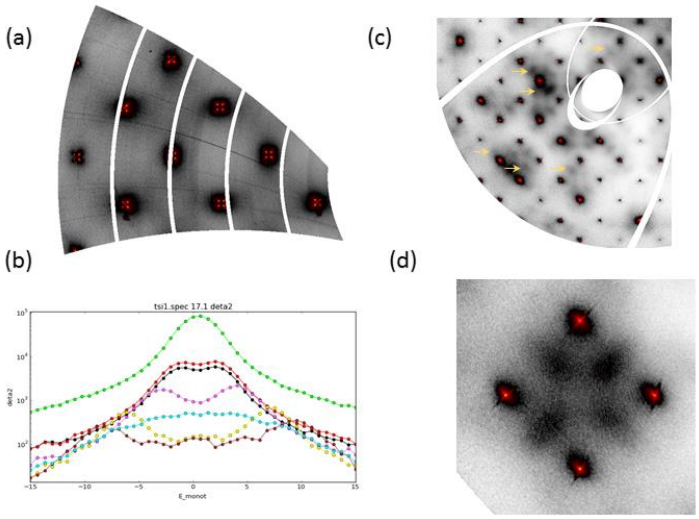

Figure 2: (a) Thermal diffuse scattering maps of the 127-6R sample at 100 K, observing the four fold symmetry of the CDW (red spots). (b) Temperature dependence of the IXS spectra at 0.05 1.05 6.9, observing a softening of the transverse branch. (c) and (d) TDS maps around the 1 0 7 region, highlighting the new difusse features at 0.5 0.5 6.9 (yellow arrows).

Moreover, the high quality of our 127-6R batch of crystals and the clean thermal diffuse maps we have obtained, allowed us to detect diffuse signals with different propagation vectors as the $\mathbf{q}_{CDW}$ (figures 2c and d), overseen by any other techniques like inelastic neutron scattering, and relevant for the low energy lattice dynamics of $(TaSe_4)_2I$. As a follows up of the project, we are resubmitting the proposal to continue with the scientific case and carry out the a comprehensive study of the phonon anomalies associated with the TDS scattering we found and highlighted in figure 2 c and d.

Overall we rate the beamtime as very succesful regarding its outcome, the amount data and the relevance of our results, which is very much appreciated taking into account the pandemic situation in September 2021.