EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

	Experiment title: Investigation of the lattice dynamics on a CDW system, $PrPt_2Si_2$	**Experiment number**: HC 4523
Beamline: ID28	**Date of experiment**: from: 11.02.2021 to: 17.02.2021	**Date of report**: 12.09.2022
Shifts: 18	**Local contact(s)**: Alexei Bosak and Artem Korshunov	*Received at ESRF:*

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Report:

Twelve shifts were assigned to measure inelastic x-ray scattering on a CDW system, such as $PrPt_2Si_2$. This experiment was scheduled during the pandemic. For this reason, the diffuse scattering (DS) was done by the local contact in advance, using the rest of the allocated time. The purpose of this study was to understand the CDW phase transition on the system, looking at the electron-phonon coupling and the importance in the lattice and its dynamic through out the transition. Starting with a temperature measurement at the DS branch of ID28 beamline at the European Synchrotron Radiation Facility (ESRF, Grenoble – France), showing the region of interest for the phonon softening. The sample was a polished single crystal with the right thickness, and its good quality was checked by DS. The second part of the experiment was done at the other branch, where IXS could be done in the specific region of interest, as a energy-resolved experiment. Data were acquired at 17 keV with a energy resolution of 3 meV. The size and quality of the sample were enough to permit easy measurement on both branches. The experiment should have been done with a cryostream, since previous resistivity measurement showed two phase transitions: a slightly change of slope around ~200K and a clear transition at ~85K.

The plan of action for this experiment was quite straighforward:

1. Measure the two CDWs phase transition, looking at the temperature-evolution of the Kohn anomaly with the energy-integrated S(Q) obtained through diffuse scattering;
2. Look at the energy of the low-energy phonon related to the instabilities and the following phase transition.

DS Results:

DS maps were obtained at different temperature (RT, 150K, 120K, 100K and 80K). Two satellite are visible: q_1=(1/3,0,0) and q_2=(1/6,1/6,1/2). We see a clear peak forming ~200K, however the peak linked to the second transition was visible as diffuse but never as diffracted peak satellite. For this reason we decide to change to a cryostat measurement on the IXS branch. Diffuse scattering maps are shown in figure 1.

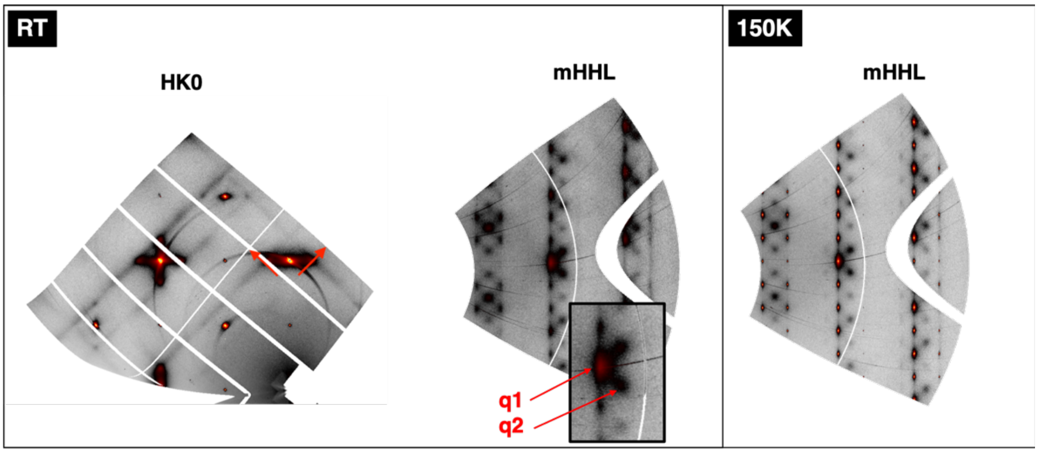
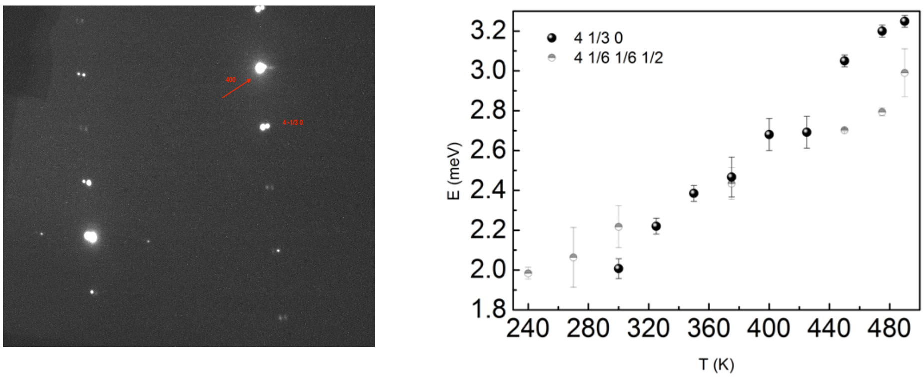


Figure 1. HK0 and mHHL (along the diffuse stripe visible on the HK0 plane) at RT and the same mHHL plane at 150K to show the formation of the first CDW peak q_1 at (1/3,0,0), where the diffuse on q_2 (1/6,1/6,1/2) does not seems to change significally.

<u>IXS Results:</u>

Thanks to the previous DS results, we decided to measured with a cryostat (able to reach 11K) on the inelastic branch. The sample was mounted with access on the H0L scattering plane, in order to measure near the 400 Bragg peak on the two CDW positions. We started on the q-points of the first CDW satellite, 4 -1/3 0, looking at simple rocking curve and checking the elastic evolution. The sample inside the cryostat was moving after every change of temperature and we had to stabilize its position waiting at least 20 minutes. We found the transition at 200K and we tried to do the same for the second satellite. It was never visible. Since the experiment with the cryostat was extremely challenging, we decided to only check if the satellite was visible at 11K looking with the CCD camera that we mounted directly after the sample. Also in this case, the satellite was not visible, as it can be seen in figure 2a. This could be an interesting result, which shows a transition that never occurred. More study should be done to confirm this hypothetic transition.

We decide to concentrate on the region around the satellites between RT and 100K, and we changed the set-up to a cryogenic gas stream system. The principal dispersions at RT were done along <010>, <100> and <001> directions near the 400 Bragg peak. Moreover, the scans done on the q-points around the satellites showed a soft-phonon region. Checking on the q-position of the two satellites, we found a phonon softening for both. The interesting results is that the instabilities and the linked Kohn anomaly are present also for the second transition, never fully reached, as shown in fig. 2b.



a) b)

Figure 2. Reciprocal space and satellites recorded at 11K through the CCD camera, the Bragg (400) and the satellite at (0,1/3,0) are marked in red; b) Temperature dependence of the phonon energy on the q-points of the two satellites.

<u>Conclusion:</u>

We obtained very satisfactory results that well described the first "hidden" phase transition. A secondary and unexpected result is related to the second transition, where the diffuse around q_2 does not seem to condense at any temperature (or at least till ~11K). However, the phonon beahaviour is quite similar in both positions. A Kohn anomaly associated with a phonon softening is present, obviosuly stronger on q_1, but visible also for q_2. Further experiment, expecially with a broader visual on the reciprocal space, will let us understand the second phase transition.