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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.

Published papers

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:** Lattice Dynamics of the Superconducting monophosphate tungsten bronze P4W14O50 with two charge density waves	**Experiment number**: HC-2506
Beamline: ID28	**Date of experiment**: from: 20-04-2016 to: 25-04-2016	**Date of report**: 08/09/2016
Shifts:	**Local contact(s)**: Alexei Bosak	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

The family of monophosphate tungsten bronzes with pentagonal tunnels $(PO_2)_4(WO_3)_{2m}$ is a large family of low dimensional metallic oxides presenting an interesting lattice dynamics, with up to three Charge-Density Wave (CDW) transitions occurring at temperatures ranging from 730K to 30K. The transitions are accompanied by a periodic distortion of the atomic structure that induces the appearance of satellite reflexions on the diffraction pattern. During this experiment, we studied the member m=8, with formula $P_4W_{16}O_{56}$, presenting two commensurate CDW instabilities appearing at approximatively 260K (T_{CDW1}) and 160K (T_{CDW2}) with different nesting vectors coupling different parts of the Fermi surface. The crystal had been characterized by elastic X ray diffraction and diffuse scattering showing diffuse line at above T_{CDW1} which then condenses in satellite reflexions below the first transition at $T_{CDW1.}$

The aim of the experiment was to evidence the mechanisms of the CDW formation along the successive transitions using inelastic x-ray scattering on a single crystal of $P_4W_{16}O_{56}$ as a function of the temperature and by studying acoustic phonons and their eventual softening. We first checked the value of the two transition temperature T_{CDW1} and T_{CDW2} by monitoring the intensity near a CDW1 satellite position. As shown in figure 1 we observed two transitions at 250 and 140 K in agreement with previous experiment. Then, we have measured by IXS constant q energy scans along several directions at different temperatures. A first set of measurements was carried out with the Si (9 9 9) with resolution of 3 meV for longitudinal and transverse direction, in order to explore rapidly different Brillouin zone and locate the best q and T measuring conditions. We then switched to the Si(12 12 12) mono to get an energy resolution of the order 1.4 meV. Measurements were carried out mainly in almost transverse geometry around the strong (4 0 0) Bragg peak.

In particular we explored the dynamical response along the direction of strong diffuse scattering (-ξ 0 -10ξ) above T_{CDW1} at different temperature. Indeed this strong diffuse scattering intensity condenses in different CDW satellite reflections positional along the diffuse line, see figure 2.

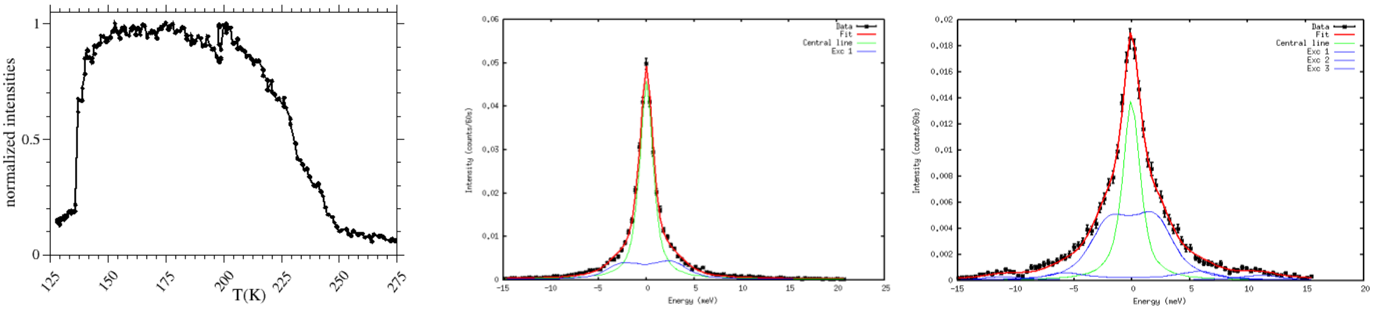
This experiment leads to two main results:

i) For scans along the direction (-ξ 0 -10ξ) we observe a clear phonon softening, with a minimum energy equal to roughly 3.8 meV when q is close to the strong elastic line at (3.5,0,5) as shown in the diffuse scattering in figure 2. The FWHM graph in figure 3b shows a tendency of the phonon to become larger near the softening;

ii) We did not observed, in the explored range (Tc=260K Tmax=400K), any significant temperature evolution of the soft phonon mode energy. We rather have observed a rapid decrease of the central elastic line intensity as the temperature is increased as shown in the Figure 1b and 1c.

This seems to be the signature of an order/disorder transition, as proposed in a polaronic model by Aubry *et al.* [1] in the context of strong coupling theory, rather than a 'classical' displacive soft phonon mode softening as in a Peierls transition, where the phonon goes to zero energy at Tc. Indeed in the case of strong coupling one expects a central elastic contribution to remain above T_{CDW1}, however accompanied by a ‘hardening’ of the soft phonon mode when T increases. The phonon dispersion along this direction at higher temperature should show this behaviour.

This experiment was successful, with the first measurements of lattice dynamics in this Bronze family. Whereas, the current data set do not allow us to give a decisive answer on the mechanism that plays for this particular transition and further measurements are required at higher temperatures. To complete this project, we plan to submit a new beamtime request to complete the temperature mapping and analysis of elastic vs inelastic contribution in the different CDW states.



a) **b)** **c)**

Figure 1: **a)** Intensity near the satellite spot (3.53, 0, -3.46) in function of the temperature, the two transition are visible at 260K and 160K; Satellite spot at (3.53, 0, -3.46) at temperature above T_{CDW1} at **b)** 263K and **c)** 400K.

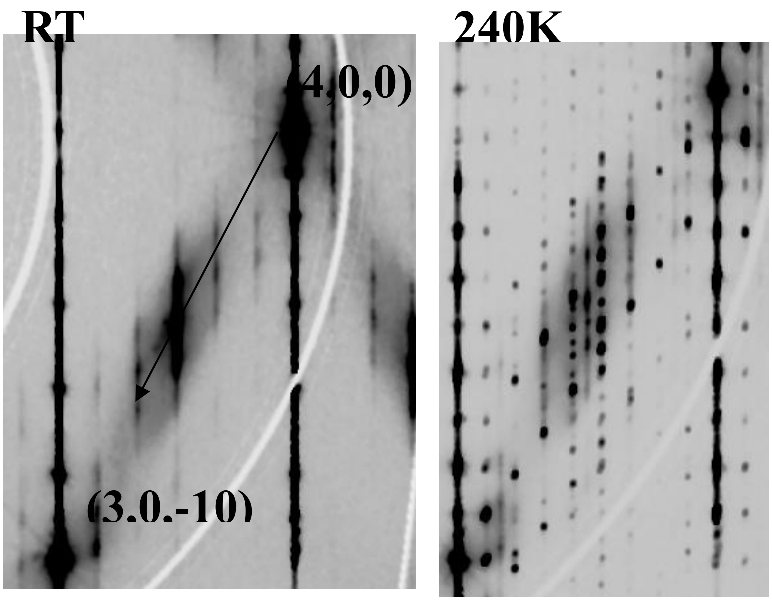


Figure 2: Diffuse Scattering in on the diffuse line along (-ξ 0 -10ξ) above and below T_{CDW1} where the spots condensation due to CDW are visible.

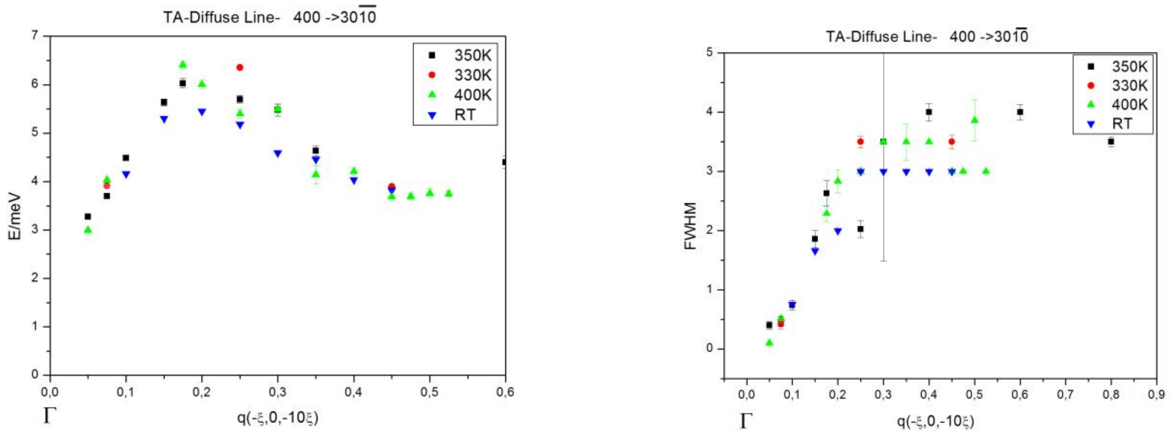


Figure 3: **a)** Transverse acoustic phonon dispersion **b)** FWMH of TA phonon along the diffuse line for T> T_{CDW}.

References: [1] S. Aubry et al., J. Stat Phys., 67 (1992), p. 675