EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

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.

	Experiment title: **The role of lattice dynamics in CDW BaVS3 metal-insulator transition**	**Experiment number**: HC3405
Beamline: ID28	**Date of experiment**: from: 25 oct 2017 to: 31 oct 2017	**Date of report**: 25/02/2018
Shifts:18	**Local contact(s)**: Adrien Girard	*Received at ESRF:*

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Report:

The plan of this experiment was to investigate the low temperature lattice dynamics of the system $BaVS_3$, which crystalizes at room temperature in the hexagonal structure with space group $P6_3/mmc$ and lattice parameters a=6.719 Å, and c=5.619 Å. Its structure consists of chains of V–S face sharing octahedra running in c-direction and separated by Ba. At T_S=240 K, BaVS3 undergoes a first symmetry lowering from hexagonal to orthorhombic symmetry through a displacive second order phase transition associated with a zigzag deformation of the V-S chains.

We started our investigations by conducting a Thermal diffuse scattering (TDS) survey in temperature on ID28 side station. 3D reconstruction of the diffuse signal around 301 reflection far above (T=330 K), just above (T=260 K) and below T_S (T=200 K) are gathered in Fig 1. A, B and C respectively. Upon approaching the transition, a strong diffuse signal was detected centered at the Γ point and disappears below the transition, indicating the softening of a zone-center phonon. This remarkable change in the TDS is a clear indication that the transition at T_S is driven by the softening of a phonon. However the soft mode could never be observed experimentally in Raman experiments. In view of these striking preliminary results, we decided to focus the IXS measurements on the transition at T_S, as it the meV resolution achieved at ID28 could allow to resolve the longstanding discussion about the soft mode character of the hexagonal-orthorhombic phase tranisition in $BaVS_3$.

The lattice dynamics in temperature was further investigated by IXS around q=(3.1,0,1). The dispersion of the soft mode was measured above T_S (Fig. 1D), and its softening is evidenced by the large variation of the central peak upon approaching the transition (Fig. 1E). Combined TDS and IXS experiments allowed to measure the soft mode and to identify it with a low energy optical mode, where the Raman experiments could clearly not allow its observation. Analysis of the DFT calculations are ongoing to identify the soft mode, the results will be summarized in a publication soon.

The combined use of the side station of ID28 with the IXS sepctrometer was decisive in the success of this experiment. We thank the ESRF and the referees for the acceptance of this proposal, and will communicate the publication to the ESRF database as soon as it is processed.

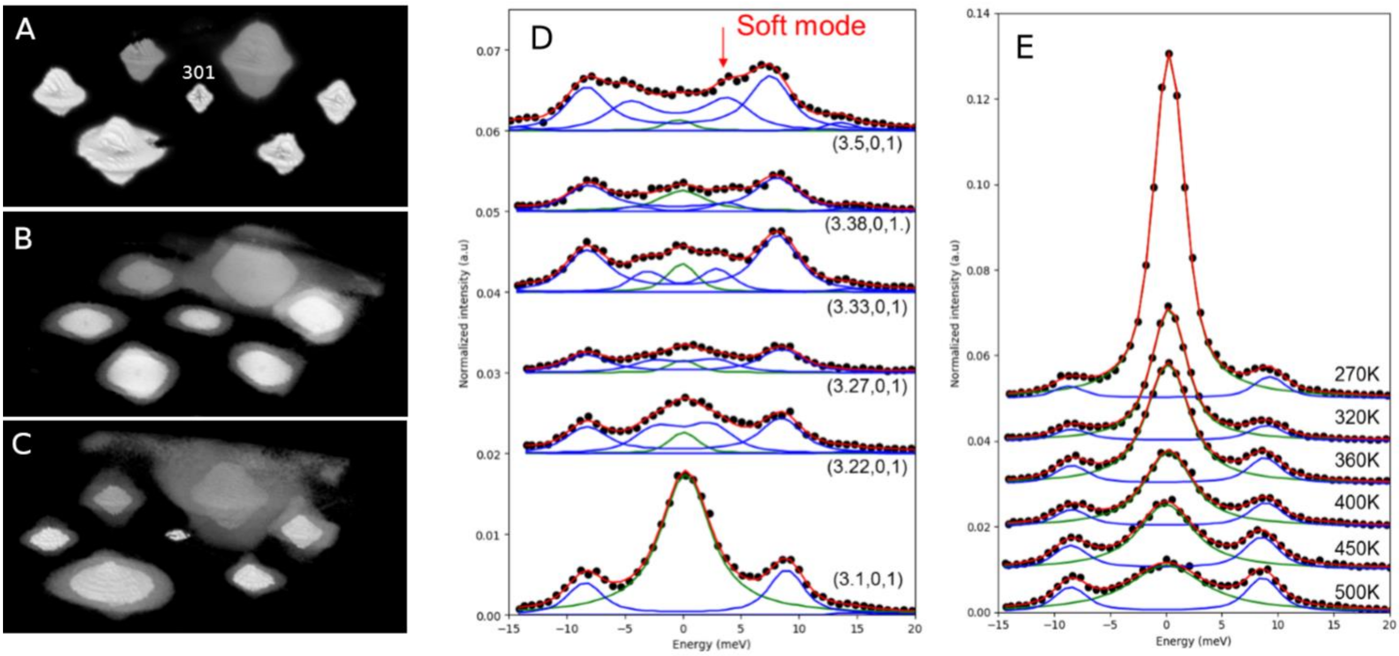

Figure 1. A, B, C: TDS signal around 301 reflection far above (T=330 K), just above (T=260 K) and below T_S (T=200 K). D: Dispersion of the soft mode measured by IXS. E: Temperature dependence of the soft mode across the transition.