

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://www.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: Unusual vanadium arrangement in sodium layered vanadium oxides and its effect on their electronic properties	Experiment number: CH-3735
Beamline: ID31	Date of experiment: from: 15/02/2013 to: 18/02/2013	Date of report: 04/10/2018
Shifts: 9	Local contact(s): Andy Fitch	<i>Received at ESRF:</i> 04/10/2018
Names and affiliations of applicants (* indicates experimentalists): Dr Pierre Bordet Dr Claude Delmas Dr Marie Guignard*		

Report:

This successful ID31 experiment allowed to determine the structure of a series of sodium layered oxides with the general formula Na_xVO_2 which were used as positive electrode in sodium batteries.

For $\text{Na}_{1/2}\text{VO}_2$, we found that the ambient temperature structure was characterized not only by a sodium ordering (sodium ion occupy trigonal prismatic sites), but also by the existence of vanadium pseudo-trimers in the triangular lattice formed by the vanadium ions. The existence of short V-V distances was evidenced by pair distribution function (PDF) analysis obtained from the XRD data collected at ID31. We also found by PDF analysis that these pseudo-trimers disappear above 322 K.

As part of the complete composition-structure-property understanding for these materials, the ESRF data were combined with electrochemical measurements and magnetic measurement performed at the ICMCB. These results were used in 2 separate publications. Please refer to the publications listed below for details (and figures) of the results.

We thank Andy Fitch for providing assistance in using beamline ID31.

Publications incorporating ESRF, ID31 powder XRD data

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C. Didier, M. Guignard, M. R. Suchomel, D. Carlier, J. Darriet, C. Delmas “*Thermally and Electrochemically Driven Topotactical Transformations in Sodium Layered Oxides Na_xVO_2* ” Chemistry of Materials 28 (2016) 1462-1471.

M. Guignard, C. Delmas “*Using a Battery to Synthesize New Vanadium Oxides*” ChemsitrySelect 2 (2017) 2, 5800-5804.