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

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal ("relevant report")

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a *"preliminary report"),*
- even for experiments whose scientific area is different form the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as "relevant report(s)" in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

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.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number 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:** **Structural and composition study of the roomtemperature metal-insulator transition in V_2O_3 thin film compounds**	**Experiment number**: 25-02-1000
Beamline:	**Date of experiment**: from: 26/10/2021 to: 01/11/2021	**Date of report**: 6 February 2022
Shifts:	**Local contact(s)**: Juan Rubio Zuazo and Jesús Lopez Sanchez	*Received at ESRF:*
Names and affiliations of applicants (* indicates experimentalists): *Dr. Mariela Menghini *Dr. Alvaro Muñoz Noval *Prof. Jean-Pierre Locquet		

Report:

Abstract

Cr-doped vanadium sesquioxide (V_2O_3) is a Mott insulator presenting an isostructural Mott metal-insulator transition (MIT) between paramagnetic metallic (PM) and insulating (PI) phases close to room temperature (RT) for a limited range of doping (0.5% - 1.7%). So far, this RT phase transition has been observed in bulk but has been elusive in thin films form. Very recently, a RT PM-PI transition both in pure and Cr-doped V_2O_3 thin films induced by strain engineering has been reported by the proposers (P. Homm et al., APL Materials **9**, 021116 (2021)). The controlled strain of the V_2O_3 layers was achieved by growing epitaxial layers on $(Fe_yCr_{1-y})_2O_3$ buffer layers with different Fe concentration. Novel intermediate states between the metallic and insulating phases, inaccessible in bulk materials, can be stabilized by a fine tuning of the engineered substrate lattice parameter. These results show that the control of the in-plane lattice parameter is extremely important to achieve a MIT at RT in V_2O_3 thin films. The detailed knowledge of the evolution of lattice deformations across this phase transition is therefore extremely relevant to gain a deeper understanding of the interplay between lattice degrees of freedom and the electronic properties in this Mott material.

Experimental results

The samples studied in this beamtime were:
- VCrO_021 (67 nm V_2O_3 on $(Fe_{0.75}Cr_{0.25})_2O_3/Cr_2O_3/Al_2O_3$)
- VCrO_021 (67 nm V_2O_3 on $(Fe_{0.5}Cr_{0.5})_2O_3/Cr_2O_3/Al_2O_3$)
- VCrO_021 (67 nm V_2O_3 on $(Fe_2O_3)/Cr_2O_3/Al_2O_3$)

High-angle diffraction and low-angle reflectivity measurements were performed in all samples. These were complemented by a comprehensive series of theta-scans at room temperature around different reflections: (0 0 L), (4 -2 0), (6 -3 0), (1 0 10), (2 0 8), (4 -2 6). All measurements were done at RT.

HAXPES experiments could not be performed as the substrates are highly insulating.

The aim of these experiments was to study the structural properties of V_2O_3 thin films subjected to different amount of strain induced by smart engineering of substrate templates. Preliminary analysis of the obtained

Reciprocal Space Maps show changes in V_2O_3 in-plane and out-of-plane lattice parameter accordingly to the different strain induced by the buffer layers.
Previous to the beamtime we have performed VESTA (Visualization of Electronic and Structural Analysis) analysis in order to determine what crystalline diffraction peaks could be more sensitive to change in atomic positions. We have selected a series of reflection planes (as mentioned above) based on these calculations.

Conclusions and future work

This experiment is related to experiment 25-02-956 where the aim was to study the structural changes across the low temperature metal-insulator transition in V_2O_3 films with different thickness. Due to the COVID-19 situation both experiments were allocated to take place one after each other from 26/10/2021 till 05/11/2021. During this period of time there were some technical issues at ESRF causing the beam to be down for two and half days. Due to this extended beam downtime it was not possible to complete all the planned experiments.
The analysis of the obtained results will represent a first approach to get a detailed picture on the relationship between structural and electronic properties in strained V_2O_3 thin films. Similar experiments in Cr-doped V_2O_3 films grown on different buffer layers can help to have a better understanding of the role played by structure in achieving a MIT at RT.
Future experiments can also include the study of the structural changes across the low temperature transition for films subjected to different amount of tensile and compressive strain.