EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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

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:** Probing three-dimensional magnetic excitation in strain-engineering $SrCoO_3$	**Experiment number**: HC-4813
Beamline: ID32	**Date of experiment**: from: 12 April 2022 to: 19 April 2022	**Date of report**: August 5 2022
Shifts: 20	**Local contact(s)**: Nicholas Brookes	*Received at ESRF:*

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Report:

Perovskite SrCoO3 is a ferromagnetic material with a transition at 250K. Theoretical calculation claim it is a negative charge transfer material that the Co atoms are mainly in d^6 high spin state. A previous transport study shows that $SrCoO_3$ thin film will undergo a metal to insulator (MIT) transition, by applying tensile strain from 1% to 3% with different substrates [1]. Interestingly, its ferromagnetic property is not affected during the MIT transition. This robust FM order is unexpected considering that the spin state is correlated with the charge state. We proposed to use resonant inelastic x-ray scattering (RIXS) at Co L3-edge (~ 780 eV) to study the three-dimensional spin excitations in strain-engineering SrCoO3 on various substrates. The results will help to uncover the underlying spin mechanisms of SrCoO3 and provide valuable information on how to realize novel functionalities via stain engineering.

We prepared 4 samples for this beam time: three SrCoO3 thin films on substrate $La_{0.3}Sr_{0.7}Al_{0.65}Ta_{0.35}O_3$ (LSAT), $SrTiO_3$ (STO), and $DyScO_3$ (DSO), and a $Sr_2Co_2O_5$ thin film on substrate LSAT for comparison. We performed XAS at O K and Co L edge to determine the resonant energy. Resonant Inelastic X-ray scattering (RIXS) was performed at Co L3 edge (~780eV). The energy resolution of our measurements was about 30 meV with an exagap of 15 and 50 meV with an exagap of 30. The scattering plane approximately went along 111 and 101 directions.

We have performed energy detuning measurements on SrCoO3/LSAT and $Sr_2Co_2O_5$. Figure 1(a, b) shows the energy detuning measurement on SCO/LSAT at 25K and 270K. We can clearly see several Raman features at ~0.07 eV, 0.4-1.0 eV, and 1.5 eV at 25K, and the Raman features at 0.4-1.0 eV redistribute at 270K. Additionally, we can observe fluorescence features emerging from the resonant energy. Figure 1(c) compares directly the spectra at low and high temperatures. We notice that the intensity around 0.07eV increases significantly at high temperatures.

We also measured the momentum and polarization dependence on SrCoO3/LSAT at 25K and 270K. Figure 1(d) shows the momentum dependence in the 111 and 101 directions. We do not see any dispersive features. Figure 1(e) shows the spectra measured with different polarizations of the incident beam, which look very similar between horizontal and vertical polarizations. We also measured the strain dependence on SrCoO3 from 1% to 3%, as shown in Figure (f). They have similar features between 0.4 eV and 1.0 eV with a small intensity difference

To understand these results, we have performed multiplet ligand-field theory calculations with parameters estimated from DFT calculations [2]. Figure 1(g) shows the energy level diagram versus the crystal parameter 10Dq. The colors of the lines indicate the possibility of 1/2 (red), 3/2 (green), and 5/2 (blue) spin. The spin state results from the competition of the crystal field and the Hund rule, which is sensitive to the parameters used in the calculation. Our calculated spectra are shown in Figure 1(h, i) with high and low spin initial states respectively. These results correspond to RIXS spectra at low and high temperatures. Our calculations suggest a high spin ground state at low temperature and partly occupants at low spin excited states at high temperature by thermal excitation.

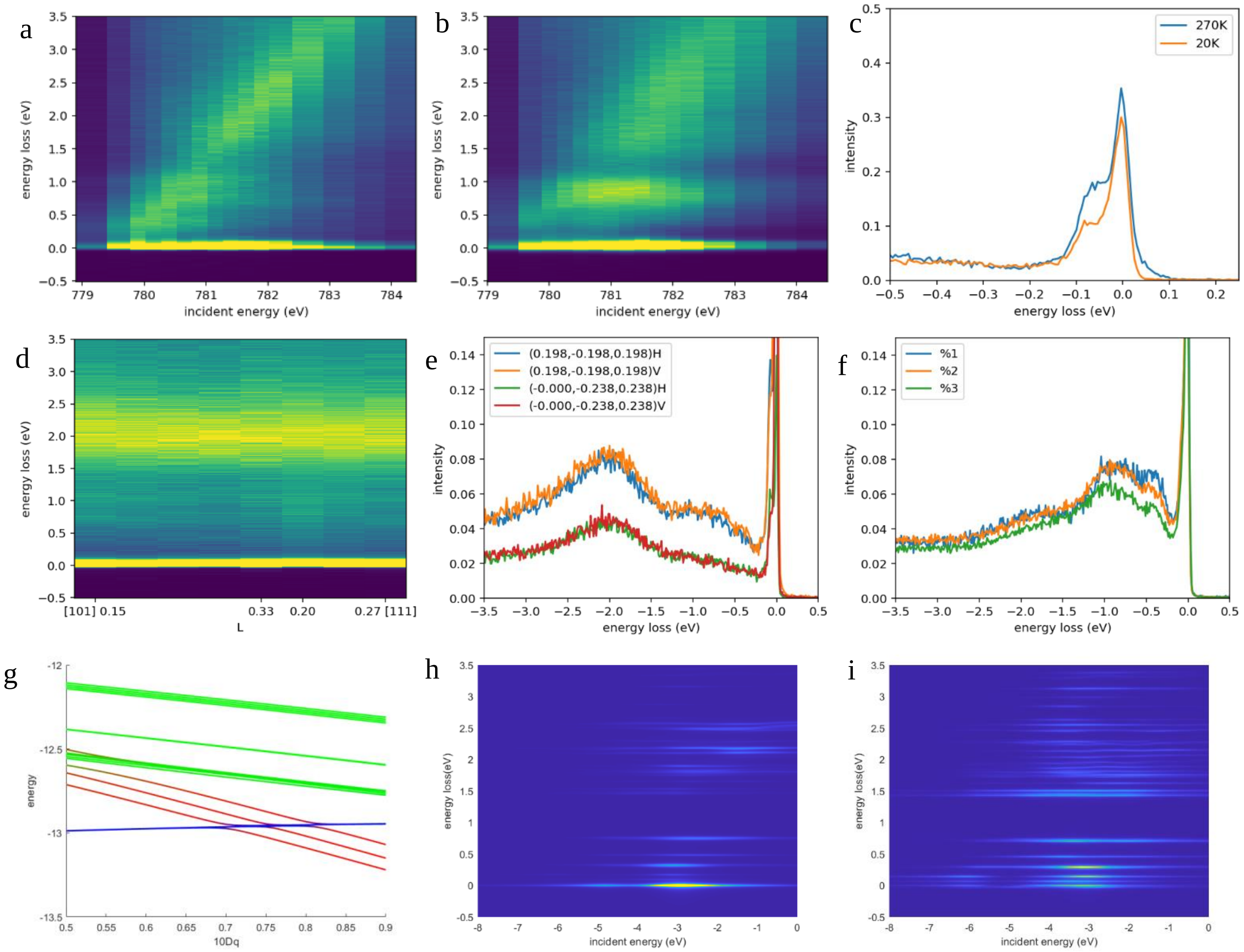

Figure 1: The detuning measurements on SCO/LSAT at (a) 25K and (b) 270K. (c) Comparison between 20K and 270K. (d) Momentum dependence along 101 and 111 directions. (e) Polarization comparison and (f) strain dependence on different substrates. (g) Calculated energy level diagram. Calculated RIXS spectra of (h) high and (i) low spin initial states.

References:

[1] Wang, Y. et al. Robust Ferromagnetism in Highly Strained $SrCoO_3$ Thin Films, Physical Review X. Phys. Rev. X. 10, 021030 (2020).

[2] Haverkort, M. W., Zwierzycki M. & Andersen O. K. Multiplet ligand-field theory using Wannier orbitals. Phys. Rev. B. 85, 165113 (2012).