# Readme

The files provided in this data deposit produce most of the figures in this paper MacLaren, Lipsett and Fraser - The structural effects of (111) growth of La2CoMnO6 on SrTiO3 and LSAT – new insights from 3D crystallographic characterisation with 4D-STEM and Digital Dark Field imaging

All these sheets run using py4DSTEM 0.14.18, to run with 0.14.19 would require changes to the disc detection steps

## Figure 2

The simulations shown in Figure 2 are generated by:

LCMO diffraction pattern sims v2.ipynb

## Figures 3, 5 and 7

The raw 4DSTEM data for the film on LSAT is found in:

IM101.hdf5

This is read in the file:

DDF LCMO LSAT 101 disk detection.ipynb

After detecting the disks in the diffraction patterns (and there are a few adaptations away from standard techniques in py4DSTEM to get the really weak ones), centering the data, rotation to take out the rotation of the diffraction data with respect to the scan image, the following files are written:

IM101\_bp\_arrayrot.npy (peaks array for Digital Dark Field Imaging)

IM101\_ADF.h5 (ADF image calculated from the original 4DSTEM data)

IM101\_bp\_lattice\_3centre.h5

IM101\_bp\_lattice\_3cut.h5

The last three are then read in, together with the real space pixel size from the raw data by:

DDF LCMO LSAT 101 strain.ipynb

This uses the strain tools in py4DSTEM to find suitable g-vectors to represent the perovskite lattice and saves these as:

IM101\_g1.p

and

IM101\_g2.p

It also then generates Figure 7 and does some theoretical strain calculations.

The sheet:

DDF LCMO LSAT 101 DDF v2.ipynb

then opens IM101\_bp\_arrayrot.npy and uses the g vectors to calculate the digital dark field images for different sets of reflections. All these are then saved in a dictionary of labelled data that is stored in:

IM101\_DDFpickle.p

This sheet also uses:

Bull2016LCMO\_010.png

Bull2016LCMO\_11-1\_b\_in\_plane\_L.png

Bull2016LCMO\_11-1\_b\_in\_plane\_R.png

in the construction of Figure 5.

The contents of IM101\_DDFpickle.p are plotted into Figure 3 in:

DDF LCMO LSAT 101 plotter v2.ipynb

## Figures 4, 6 and 8

The raw 4DSTEM data for the film on STO is found in:

IM103in.hdf5

This is read in the file:

DDF LCMO LSAT 103 disk detection.ipynb

After detecting the disks in the diffraction patterns (and there are a few adaptations away from standard techniques in py4DSTEM to get the really weak ones), centering the data, rotation to take out the rotation of the diffraction data with respect to the scan image, the following files are written:

IM103in\_bp\_arrayrot.npy (peaks array for Digital Dark Field Imaging)

IM103in\_ADF.h5 (ADF image calculated from the original 4DSTEM data)

IM103in\_bp\_lattice\_3centre.h5

IM103in\_bp\_lattice\_3cut.h5

IM103\_bp\_arrayrot.npy

The last three are then read in, together with the real space pixel size from the raw data by:

DDF LCMO LSAT 103 strain.ipynb

This uses the strain tools in py4DSTEM to find suitable g-vectors to represent the perovskite lattice and saves these as:

IM103in\_g1.p

and

IM103in\_g2.p

It also then generates Figure 8 and does some theoretical strain calculations.

The sheet:

DDF LCMO STO 103 DDF.ipynb

then opens IM103\_bp\_arrayrot.npy and uses the g vectors to calculate the digital dark field images for different sets of reflections. All these are then saved in a dictionary of labelled data that is stored in:

IM103in\_DDFpickle.p

This sheet also uses:

Bull2016LCMO\_100.png

Bull2016LCMO\_11-1\_b\_in\_plane\_R.png

Bull2016LCMO\_111\_a\_in\_plane.png

in the construction of Figure 6.

The contents of IM103in\_DDFpickle.p are plotted into Figure 4 in:

DDF LCMO STO 103 plotter v2.ipynb

This also uses an additional data dictionary from our previous work in <https://doi.org/10.1093/mam/ozae104> for one image made from the Zero Order Laue Zone:

LCMOSTO\_001\_DDF\_001\_pickle.p