

T7: Registration and Atomic Column Position Identification

In this 2-part activity, we will go over how to register atomic resolution STEM images, where quickly acquired frames are aligned and averaged to yield a high signal to noise image, and then identify the positions of atomic columns in a STEM image and use them to visualize domains in ferroelectric PbTiO_3 .

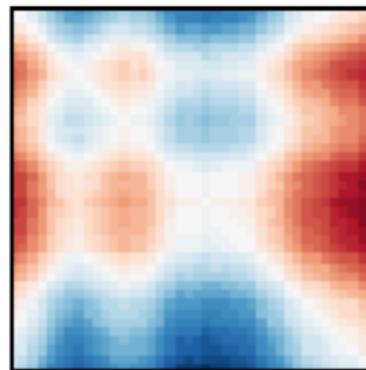
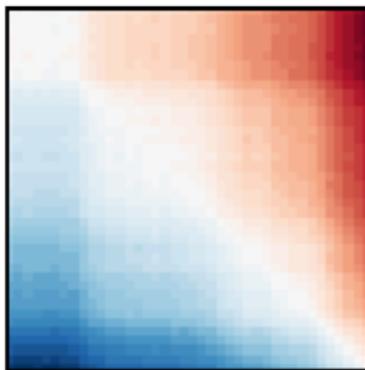
1. Registration

To register images we will be using the rigidregistration python package. For more detail on the technique, see "Image registration of low signal-to-noise cryo-STEM data", Ultramicroscopy (2018), DOI: 10.1016/j.ultramic.2018.04.008.

The T7_registration.ipynb notebook on the Azure VM has instructions for registering datasets. To begin, copy the T7 folder from the shared drive to your home folder, launch jupyter notebook with the Anaconda Prompt, open T7_registration.ipynb in the Notebooks folder, and load the dataset:

```
../Data/BSCMO_0047 3.7 Mx_0.tif
```

Follow the instructions in the notebook to register it – note that you will have to change the parameters such as the mask size, outlier detection threshold, etc. A report for a good registration for this dataset is shown below:



Note that because the cross correlation parameters were set well, no outliers needed to be masked and corrected. However, even with this fairly easy to register dataset, this rigid registration technique is able to do a better job identifying correct shifts and avoiding image artifacts than other techniques. On the following page is a comparison between a registration with Nion Swift, in the left column, and this rigid registration, in the right column.

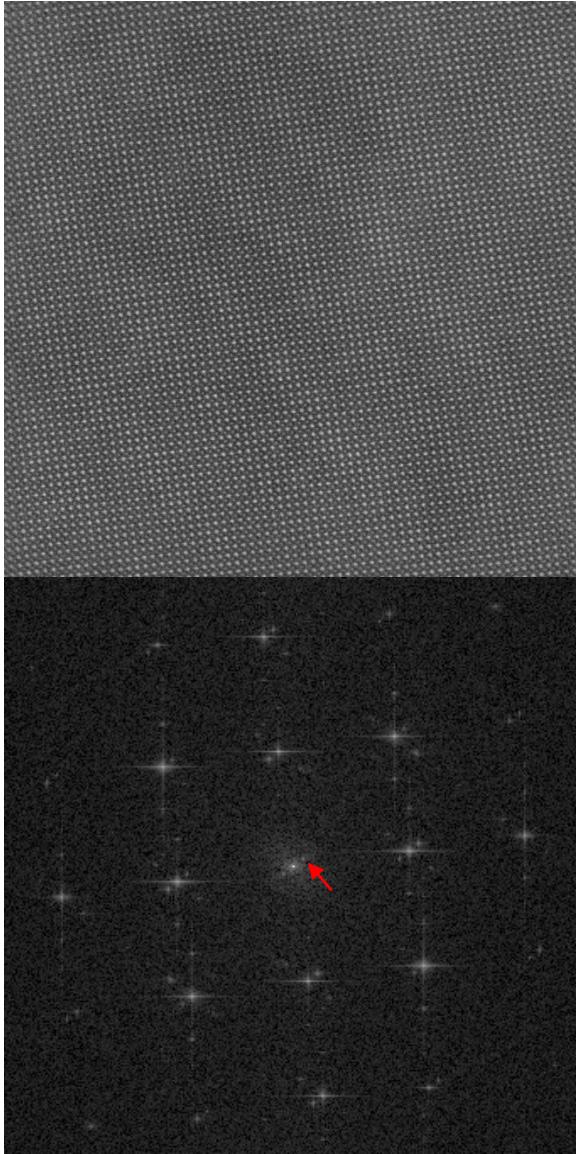


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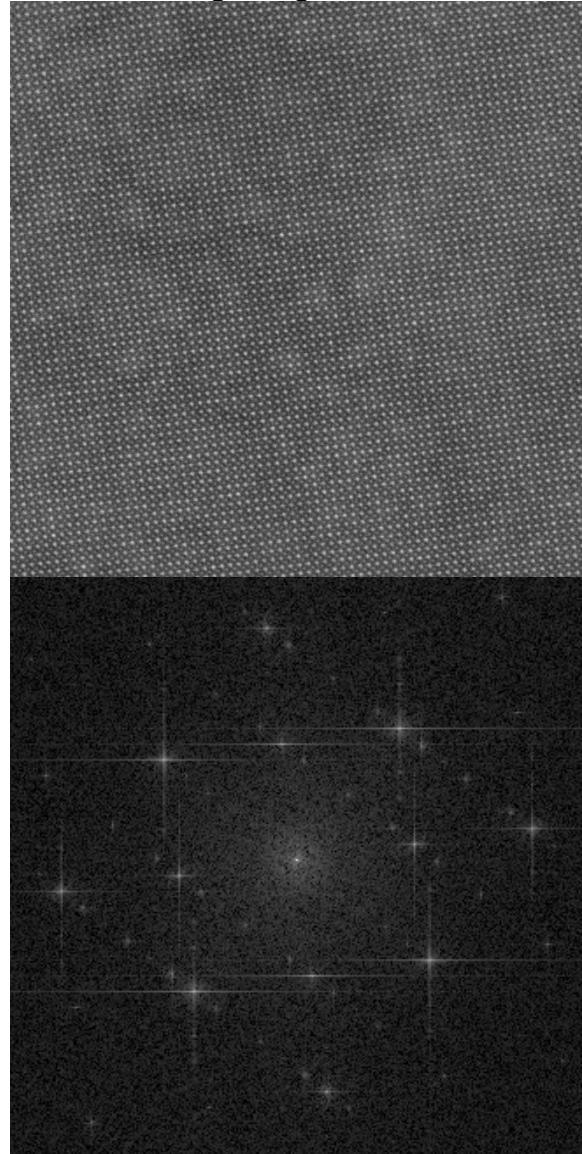


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Nion Swift



rigidRegistration



At first glance, both real space registrations look very good – we have good signal to noise and sharp atomic columns. However, notice the peaks that appear in the swift registration but not the python one, marked with the red arrow in the FFT. These are not physical, but an artifact introduced by incorrect registration.

Looking closely at the real space images, it's also possible to see that in the swift registration the amorphous surface layers (diffuse white splotches) appear blurred out compared to the rigid registration, and the random cation doping (varying intensity of the A site columns) is averaged out. Because you generally will not know exactly what the real and reciprocal space pictures of your material should look like, it's important to use



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robust image registration techniques such as the rigidRegistration package to pre-process images before further analysis to avoid tricky artifacts like these.

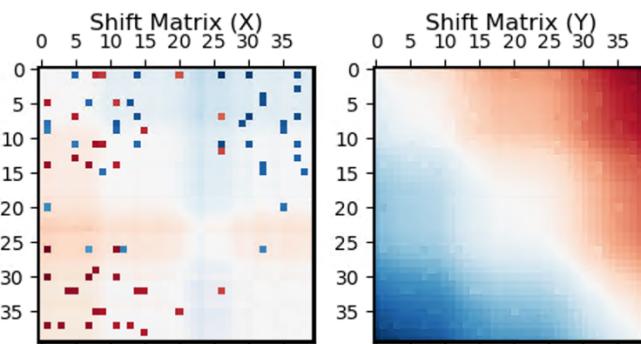
If there is more than an hour left in the tutorial, proceed below with registering another dataset. Otherwise, if there's less than an hour left proceed to section 2, atomic column position identification.

Next try registering a dataset collected on Bismuth strontium calcium copper oxide (BSCCO) at cryogenic temperature (liquid nitrogen, ~93 K):

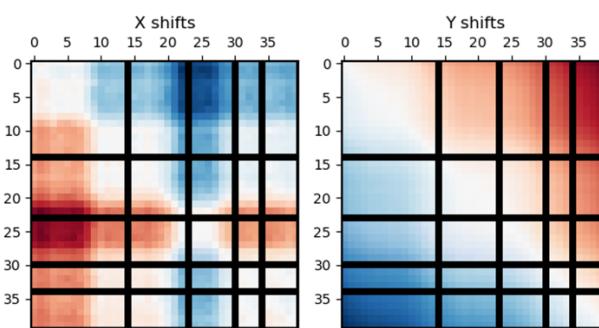
Data/BSCCO_56_3p6mx_1024px_0p3us_s40_1.tif

This dataset may be a bit trickier to get a good registration for – it was acquired at cryo, so drift and instability from the cryogen such as bubbling will lead to more significant shifts and outliers in your shift matrices, and the lattice vectors have very different lengths, so using an elliptical gaussian mask may be necessary.

Your uncorrected shift matrices may look something like the below for a good parameter selection:



Your corrected shift matrices may look something like the following for a very strict masking of the shift matrices:





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If you want more practice, more datasets are included in the data folders. A really tricky one is:

`CsBiNb207_06_3 . 6Mx_50x0 . 25us_1024px_130mmCL_mono50_15pA_70umC2_1 . tif`

And an easier one is:

`29_LSCO_cryo_50x0 . 5us_1024px_5 . 1Mx_1 . tif`

2. Atomic column position identification

Follow the instructions in the `T7_atom_finding.ipynb` notebook for a quick demonstration of atomic column position identification, and visualization of domains in PbTiO_3 . Note that this just a rough demonstration of position identification and domain visualization – pay attention to how error propagates through the procedure, and note that great care must be taken for this type of analysis to be trustworthy.