Visualizing 3-Dimensional Ptychography Data

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Abstract

Ruddlesden-Popper Phases (RP) are a method of growing materials to induce specific properties in the material. In nickelates, the proper RP domain gives superconducting properties to the material. Unfortunately, measuring the distribution of RP domains in a sample in a statistically significant area is tedious and time consuming. To aid in this endeavor, we modified a previously created RP-domain tracking code[2, 3] to allow for analysis of ptychography data and to add 3-dimensional visualization capabilities.

Introduction

Scanning Transmission Electron Microscopy (STEM) is an atomic imaging technique that utilizes the small wavelengths of electrons to view the material at the atomic level. It works by aiming a beam of electrons at the sample and recording the subsequent electron scattering. This process repeats across the entire sample. There are two STEM techniques that are similar to ptychography: High Angle Annular Dark Field (HAADF) and Annular Bright Field (ABF). In HAADF, as the beam moves across the sample, only the high angle electron scattering is recorded. This technique creates an image with z-contrast. An issue with HAADF is that lighter atoms, like oxygen, are not measured. In ABF, only the low angle electron scattering is recorded. The images created by ABF have contrast in both heavier and lighter atoms, but the images are difficult to interpret.

An alternative to ABF and HAADF is ptychography. Ptychography is a technique based in STEM that allows for deep sub-angstrom resolution and robust contrast in both light and heavy atoms. The setup is similar to HAADF and ABF. The main difference lies in the type of detector. Instead of using a detector in the shape of a ring, ptychography uses a pixelated detector called the Electron Microscope Pixel Array Detector or the EMPAD. Ptychography records the entire electron scattering pattern instead of a specific angle range. A ptychography data set is a 4-D STEM data set. We use phase information from overlapping diffraction disks to reconstruct the potential of the sample. Ptychography gives us 3-dimensional information and a quantitative way of measuring light atoms. This opens up the door to studying more kinds of materials, including RPs as RP domains are easily measured using ptychography.

A RP is defined by a specific type of atomic pattern. By deliberately introducing consistent RP domain boundaries into the material, we can induce properties that nominally would not be present. An RP domain is defined by how many times the unit cell repeats before there is a half unit cell jump in the sample. For example, in nickelates, a RP domain of five causes the nickelate to have superconducting properties.[6] RP domains and boundaries are difficult to see and analyze in the raw data returned by ptychography. This paper explains the process behind the program built to aid in analysis and visualization.

Method

Analysis begins with focusing on a single layer in the stack of ptychography data. This first layer is analyzed by hand to pick the optimal parameters, then the software analyzes the remaining layers in the sample. The software that performed analysis on the single layer was developed in previous publications.[2, 3]

On each layer in the stack, we use a fourier transform to convert the data into reciprocal space [fig 1, b]. Next we perform a phase lock-in method on the bragg-peak of interest to obtain the strain map as described in [2,3] [fig 1, c & fig 2, a]. The higher strain regions in the map highlight the RP boundaries within the sample. The user now sets the minimum strain threshold that will count as an RP boundary. Using this threshold, the locations of the local maximum in the strain map along the atomic columns are recorded in the software [fig 2, b] . Now, the software will determine the RP domains present between the chosen boundaries.

Each RP domain is mapped and color coded [fig 3, a] and then RP domains are automatically counted and visualized as a bar graph [fig 3,b]. These figures created by the software provide an easy way to visualize how much of this layer in the sample grew as expected. The map gives us a way to visualize what domains grew in the sample, while the bar graph allows us to see the ratio of the domains. Now that we have the basic analysis of a single layer, the software runs the same analysis on each layer in the stack using the parameters set previously by the user. After this analysis, a 3-Dimensional representation of all RP domains within the sample is created [fig 4].

This program allows the user to customize the visualization as needed. The colors and opacities of each domain can be adjusted. Another capability of this software is filtering the visible RP domains [fig 5].

Results and Discussion

Ptychography is a STEM technique that can achieve sub-atomic resolution on both heavy and light atoms. The data gained from ptychography is 3-Dimensional, making it difficult to visualize. This software creates a visualization of the RP domains in a given sample [fig 4]. We offer a way to easily see where in the sample the material grew unexpected domains as well as allowing the viewer to see if the issue is throughout the entire sample or merely on a single layer. By creating a 3-Dimensional visualization of the RP domains within a sample, researchers will be able to determine the RP domains within the material at a glance.

References

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a.) b.) c.)

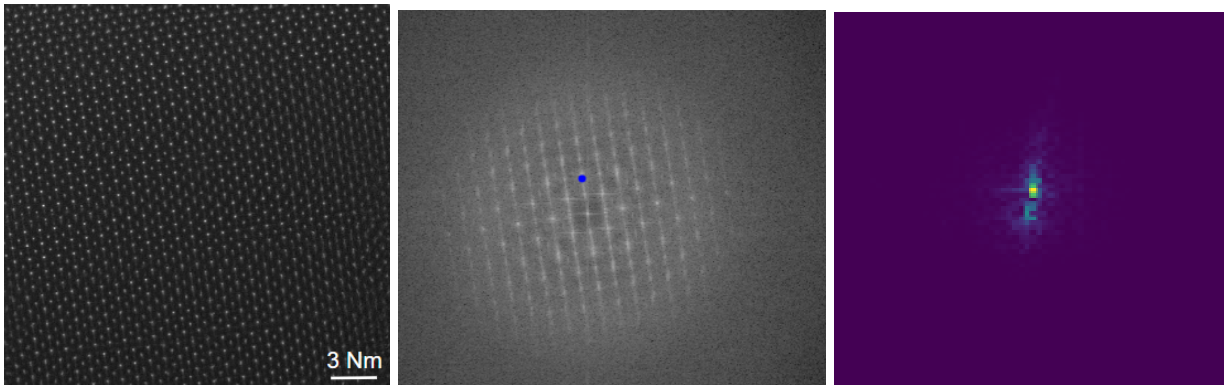


Figure 1:
a.) a slice of a stack of a N5N4Ox nickelate sample. b.) the fourier transform performed on the slice given in (a). c.) the 002 filtered peak

a.) b.)

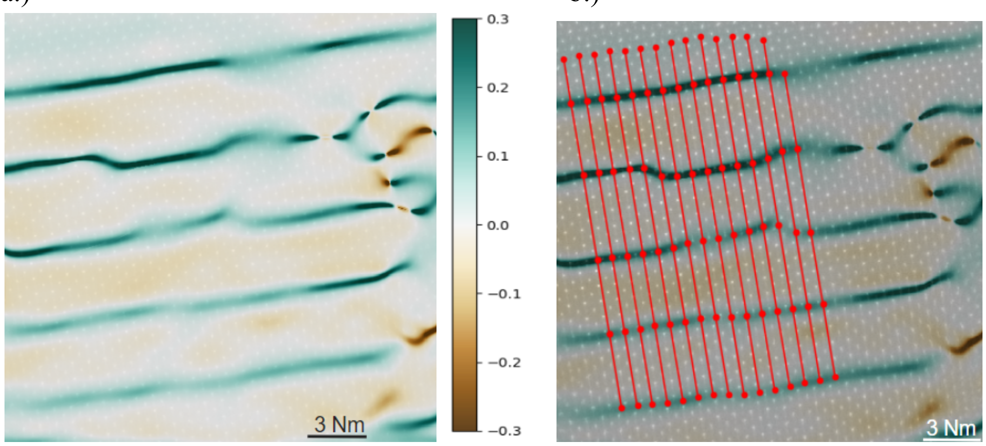


Figure 2:
a.) the strain map associated with the 002 peak of the sample shown in (fig 1,a). The higher strain regions in the map are the RP boundaries detected by the software. b.) detected RP boundaries. The software marks a point along each atomic column.

a.) b.)

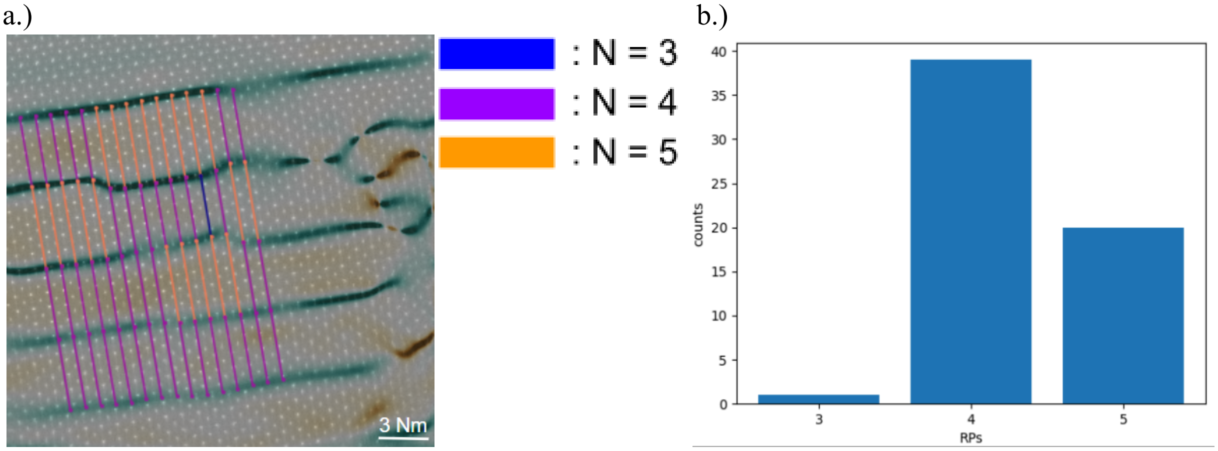


Figure 3:
a.) the colored map created on the initial analysis slice of the N5N4Ox sample. b.) the resulting bar graph for this layer. The x-axis has the RP domains in question. The y-axis is the number of times the software detected the RP domains.

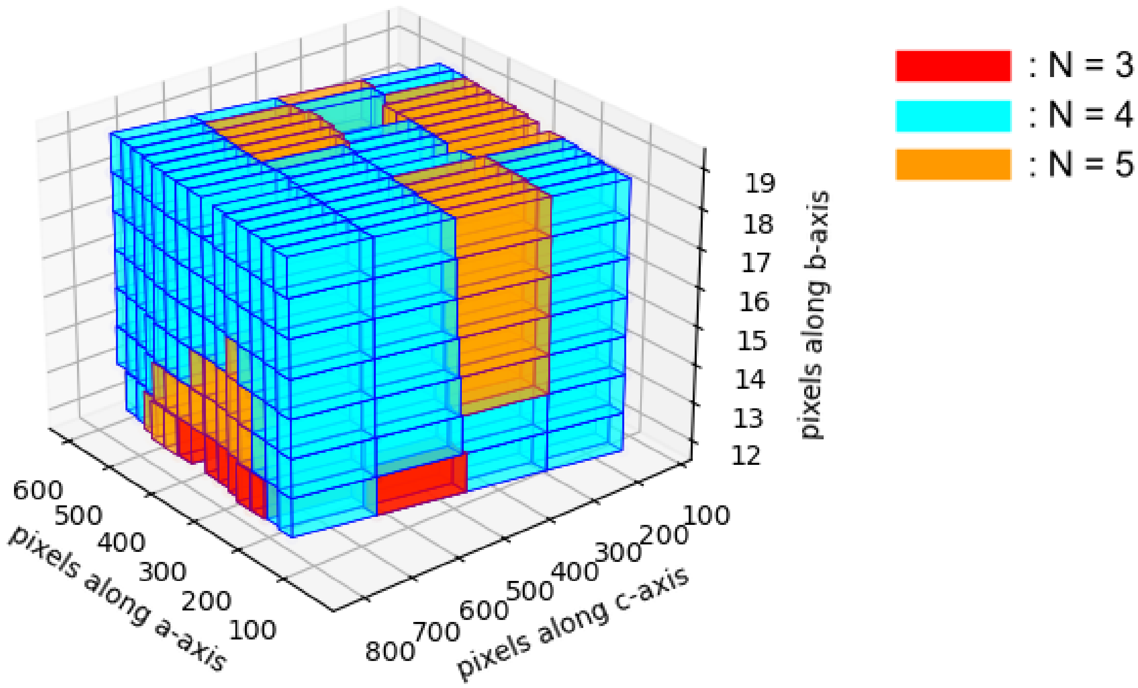
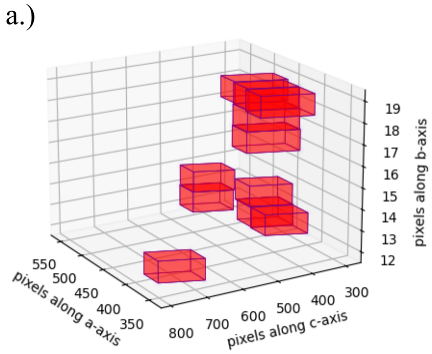
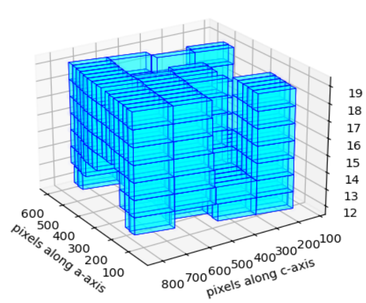


Figure 4:
RP domain representation of the N5N4Ox sample.

a.)



b.)



c.)

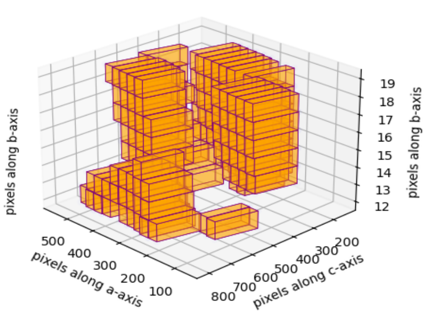


Figure 5:
Individual N=3,4,5 (a,b,c respectively) RP domains visualization