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 induces superconducting properties to the material. [4] 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 [1,2] to allow for analysis of ptychography data and to add 3D visualization capabilities for further understanding of the RP domain distribution.

Introduction

RP domains can be measured with high resolution and 3D information using ptychography, a technique based in Scanning Transmission Electron Microscopy (STEM) [Fig 1].

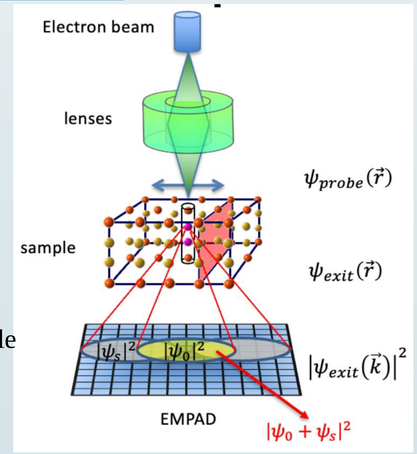
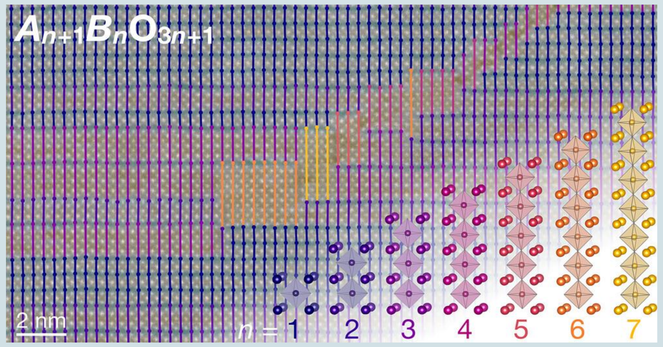


Figure 1 [3]: example ptychography set up.

A RP is defined by a specific type of atomic pattern. An RP domain is defined by how many times the unit cell repeats before there is a half unit cell jump [Fig 2]. By deliberately introducing consistent RP domain boundaries into the material, we can induce properties that nominally would not be present.



Methodology

Analysis begins with focusing on a single slice in the stack of ptychography data. This first layer is analyzed by hand, then the software analyzes the remaining layers in the sample. The software that performed analysis on the single layer was developed in previous publications.[1, 2]

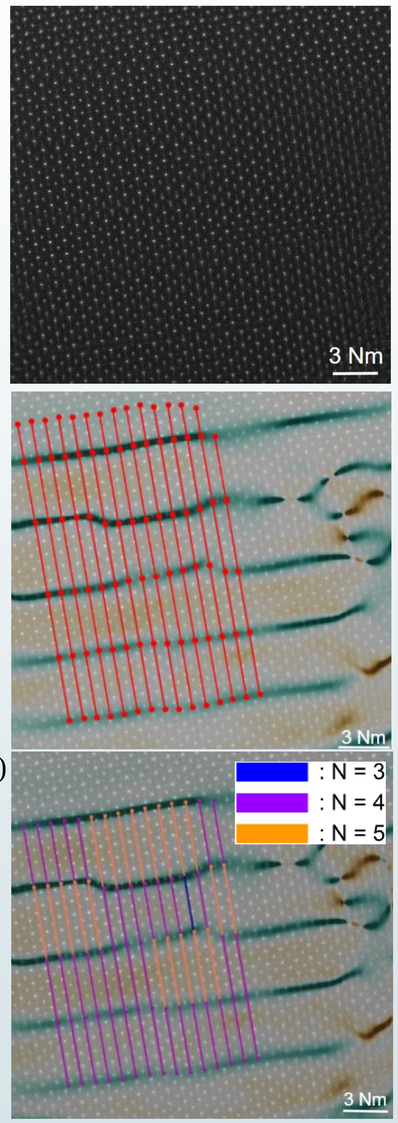
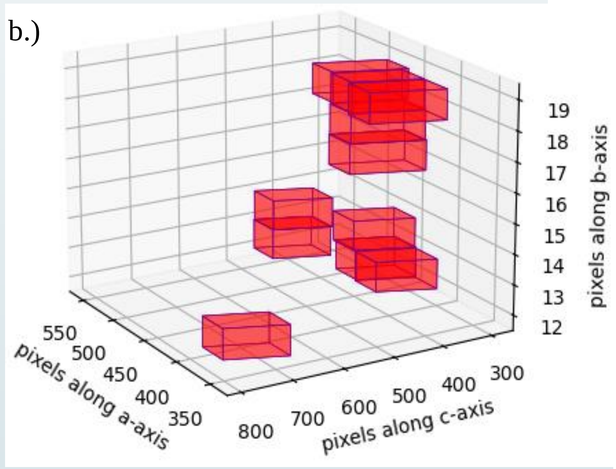


Figure 3: a.) slice of a stack of a N5N4Ox nickelate sample b.) detected RP boundaries. The software marks a point along each atomic column. b.) detected RP boundaries c.) colored map of RP domains on the initial analysis slice of the N5N4Ox sample.

Figure 2 [1,2]: Example RP domains.

Results

This software creates a 3D visualization of the RP domains in a sample. This allows researchers 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 sample or merely on a single layer. By creating a 3D visualization of the RPs domains within a sample, researchers will be able to instantly determine the RP domains within the material.



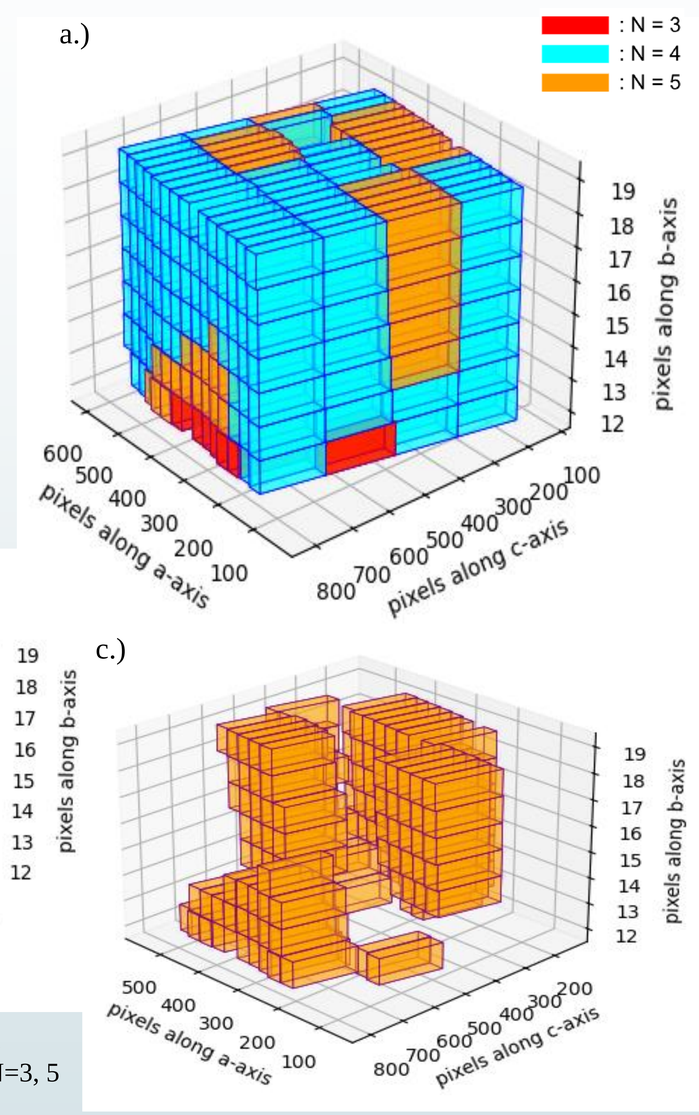


Figure 4: a.) 3-dimensional representation of a N5N4Ox sample. b, c respectively.) Individual N=3, 5 RP domains visualization

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References

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