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Bicrystallography in two dimensions: A graphical procedure and comparison of its results to experiments

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Bicrystallography in two dimensions: A graphical procedure

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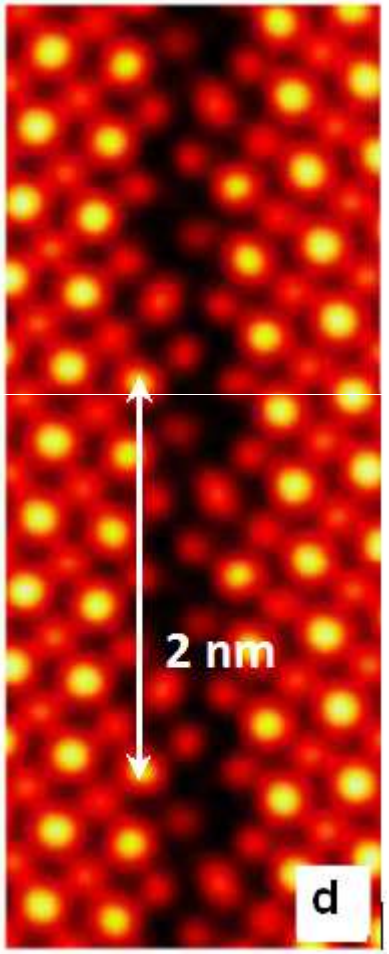
What is Bicrystallography?

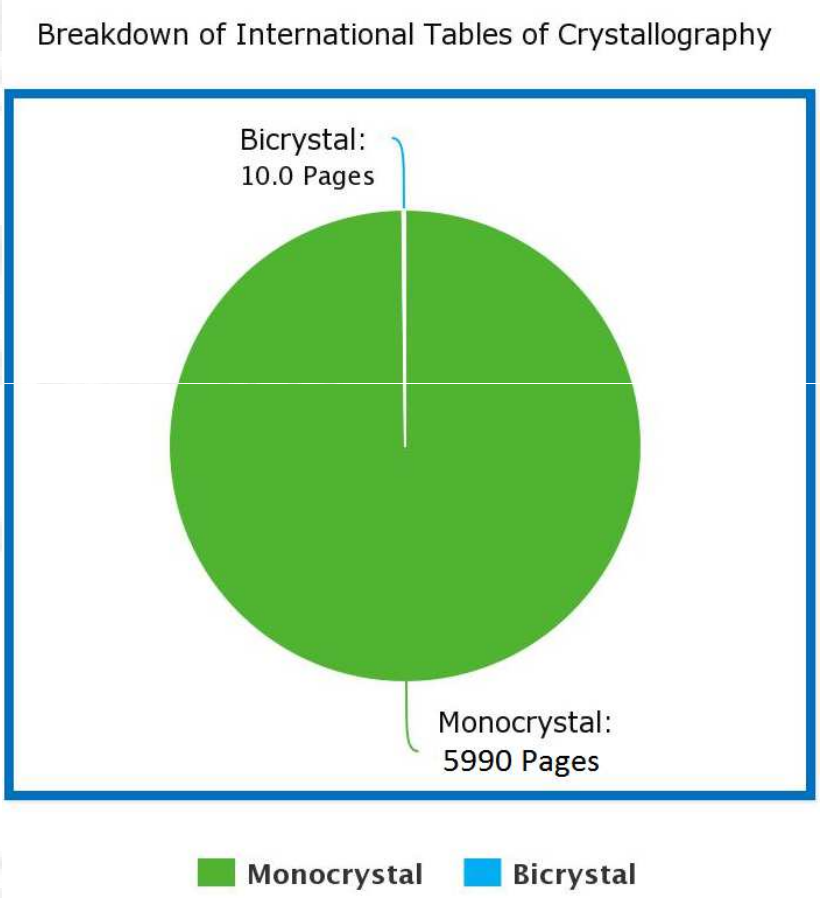
- Describe Ideal Bicrystals
- Atomic Level Description
- Like crystallography, but studying bicrystals, rather than monocrystals.
- Correlate physical properties to internal structure (Shubnikov-Curie principle)
- Ideal 3D bicrystals related to real ones by free energy minimization



State of the Field

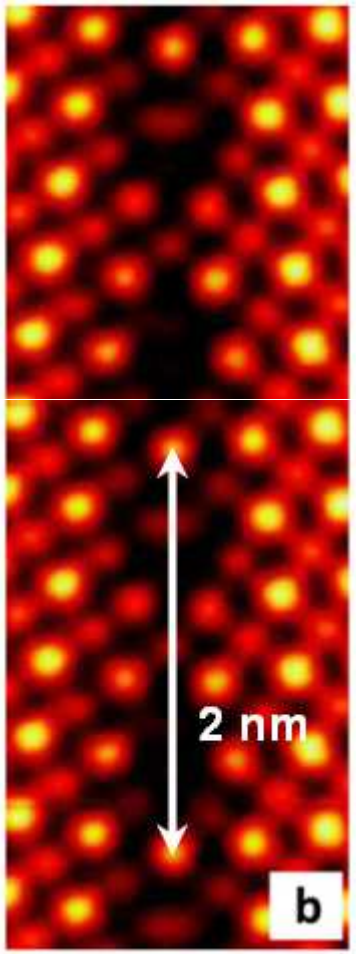
- ~6000 pages of structures in the International Tables of Crystallography
- Less than 10 pages of the 6000 dedicated to domain and grain boundaries

- Can we make useful Bicrystallographic predictions in such a way as to encourage the community to discover more bicrystal structures?



Objective

- We want to see more discovery of bicrystal structures
- High quality sub angstrom resolution images available for the first time
- Create straightforward method to make predictions for, and to help interpret, these new images



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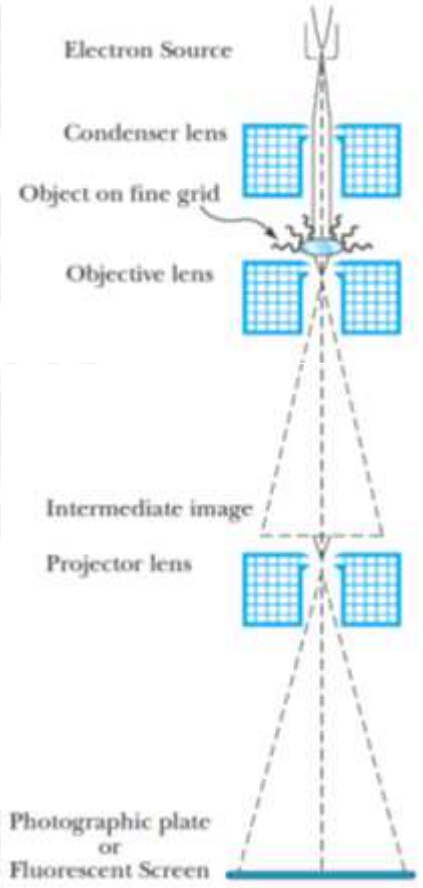
Why 2D Bicrystallography?

- Growing availability of quality aberration corrected STEM images
- Projection technique, 2D output
- Make predictions of what will be seen in experiment
- Interpret STEM images



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Terms and Abbreviations

- Simple (SC), Body Centered (BCC), and Face Centered Cubic (FCC), refers to a crystal lattice that has a cube shaped unit cell:

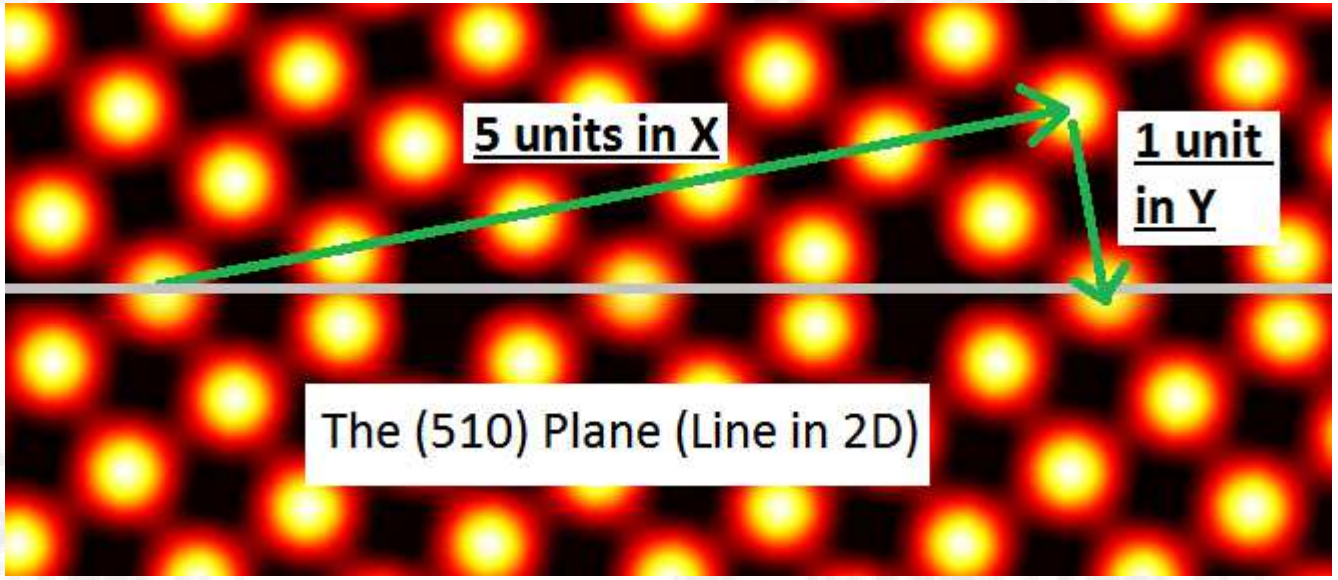
(a) Simple cubic

(b) Body-centered cubic

(c) Face-centered cubic

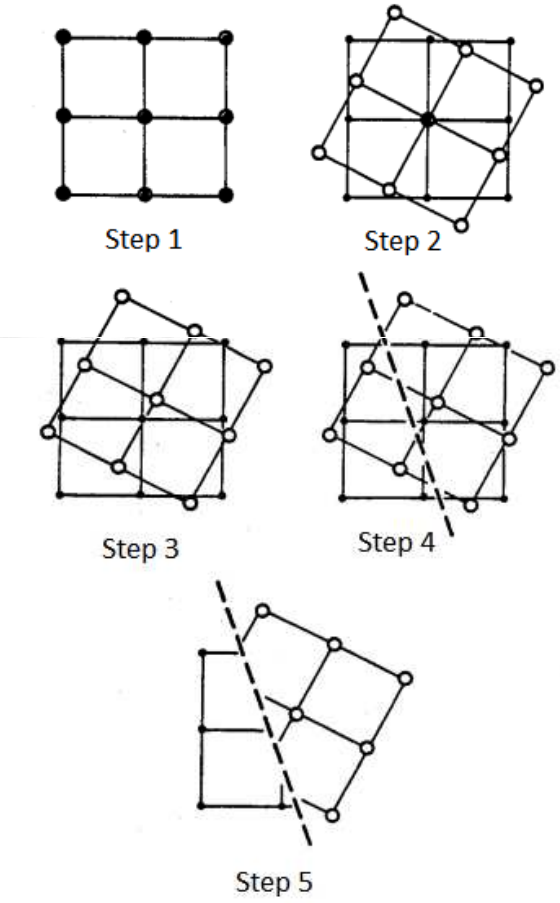
Terms and Abbreviations

- (510), (310), etc. refers to a plane drawn through a crystal. (510) is the plane passing through (5,1,0) in the coordinate system of the crystal. The sectioning line (gray) follows this plane in 2D projection.



Modeling a Bicrystal

- A method shown in “A Roadmap For The Use of Interfacial Symmetry Groups” by G. Kalonji.
- Published in 1985, did not account for boundary migration and expansions
- Our method is based upon these steps, and carried out in the drawing program GIMP (www.gimp.org)



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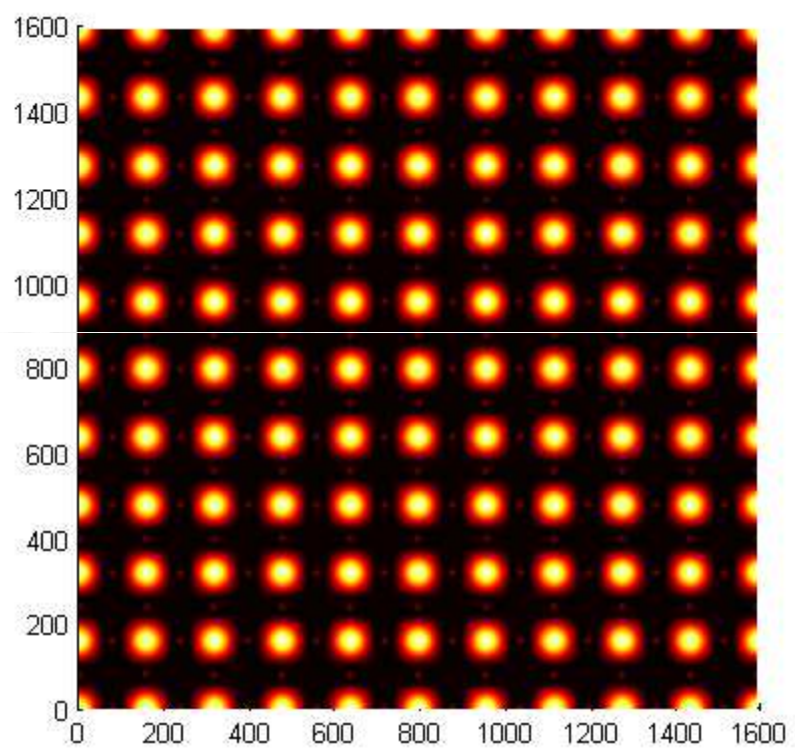
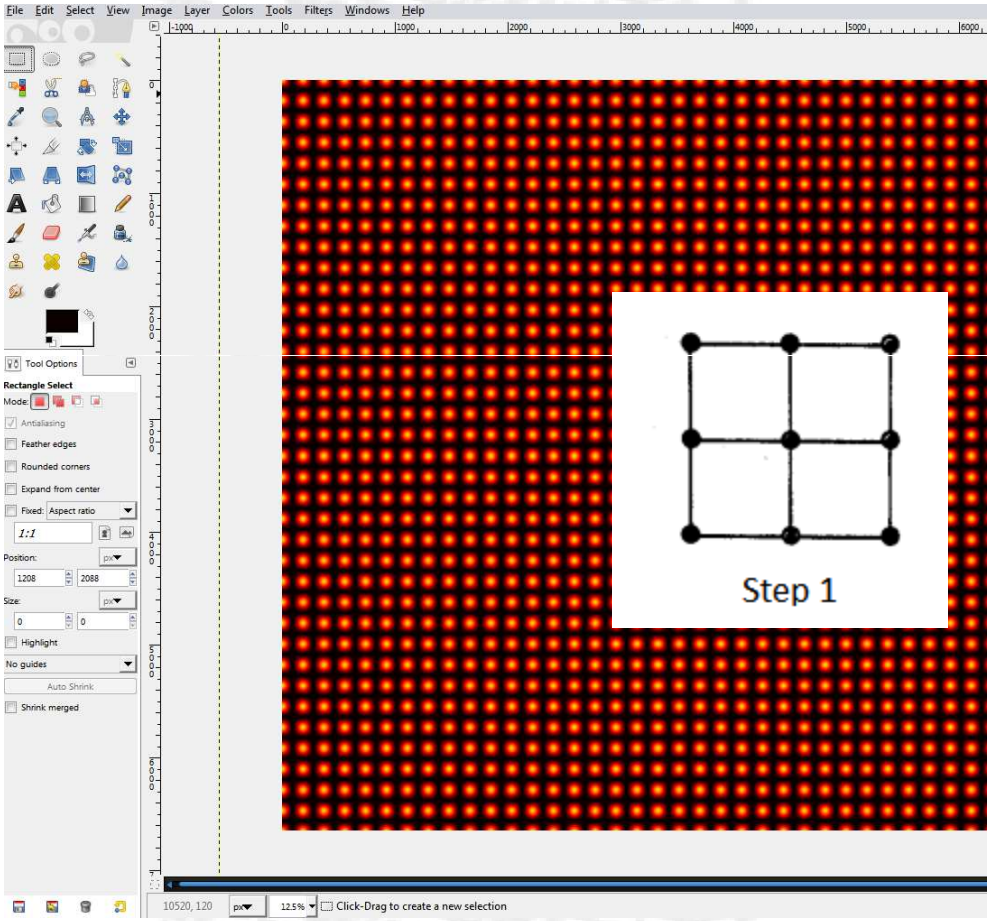
MatLab to Create Simulated Images

- MatLab code outputs:
- Crop, copy, and expand to desired lattice size
- Code outputs (001) projections of Simple, Body Centered, and Face Centered Cubic lattices

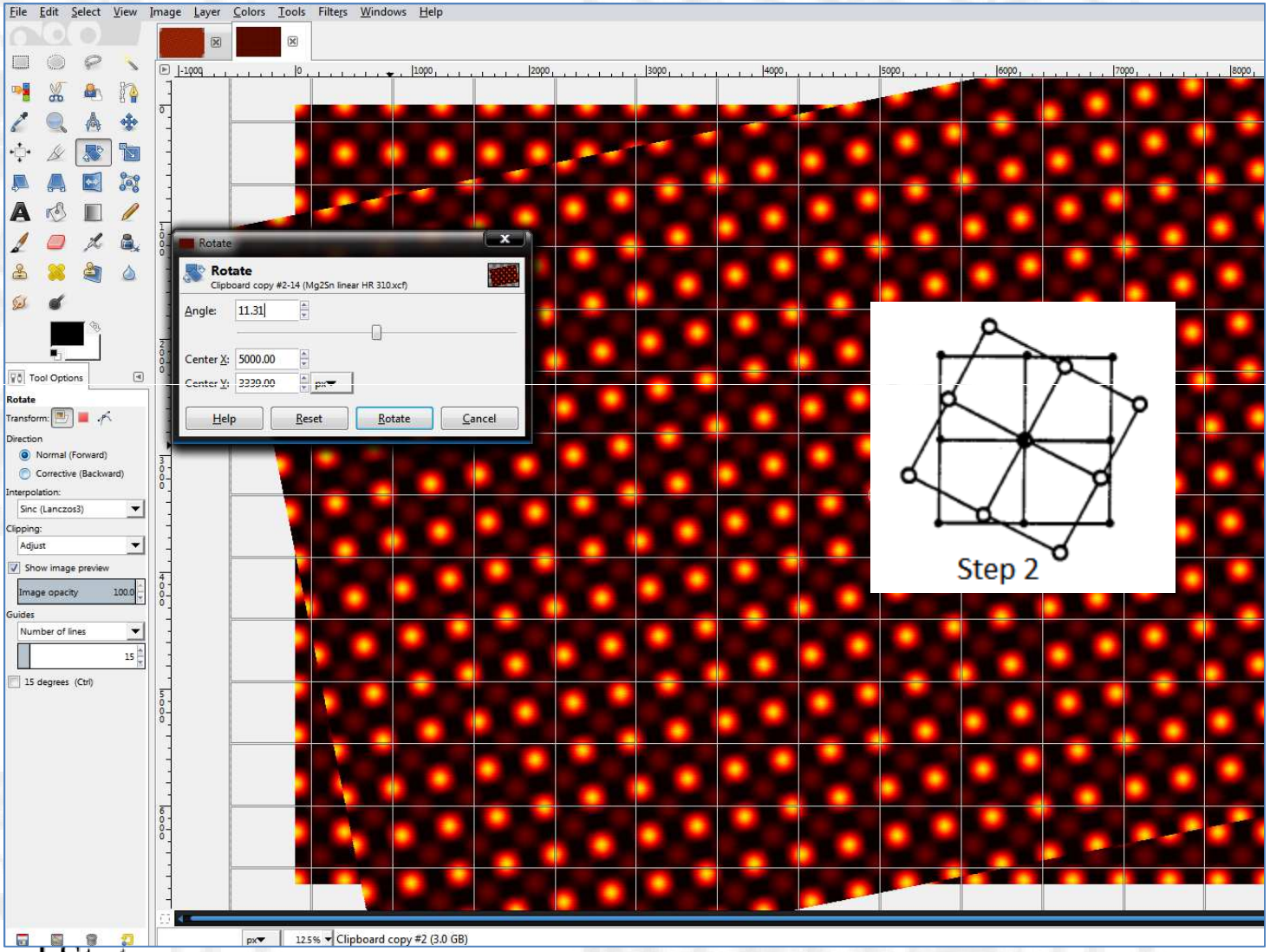


Create the Two Lattices

- After expanding the monocrystal lattice, create a copy of it in GIMP
- These are to be the two interpenetrated crystals

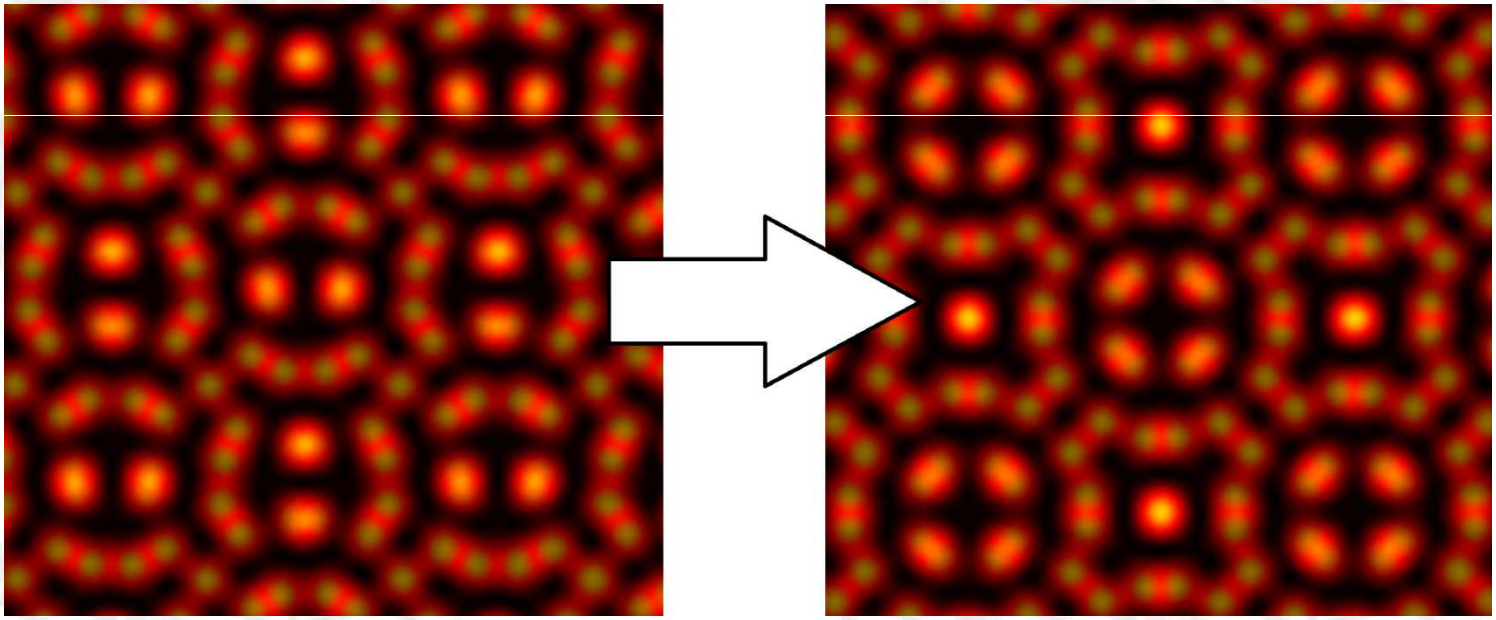


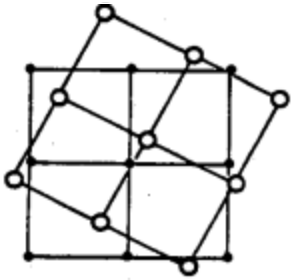
Apply Rotation



Apply Translation

- For our images, we align the Coincident Site Lattice (CSL) points.

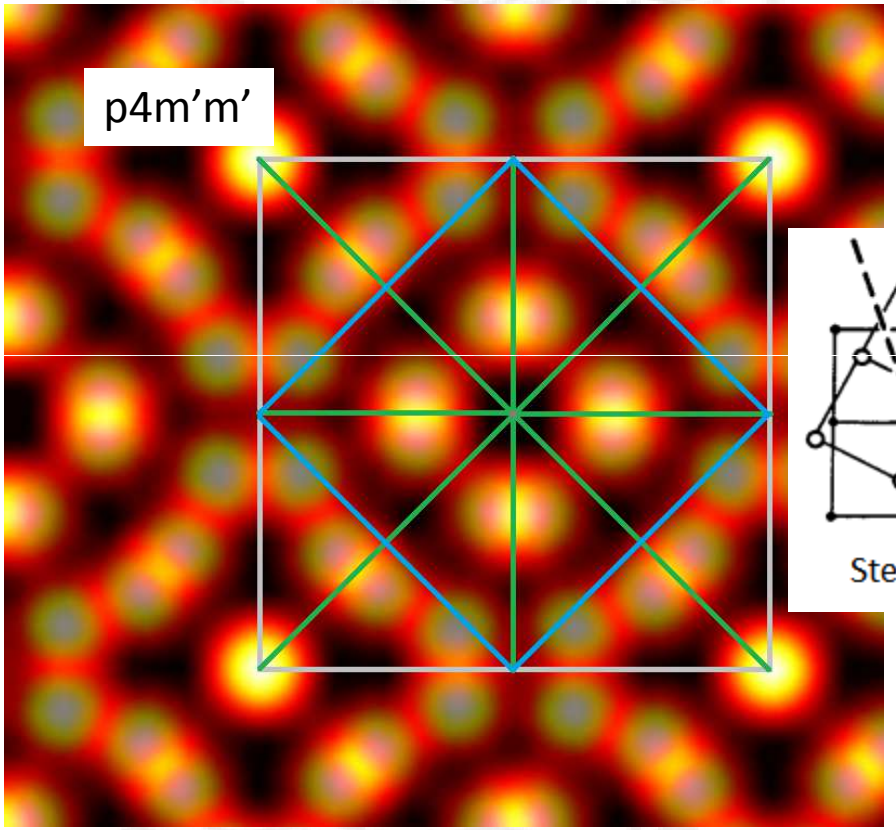


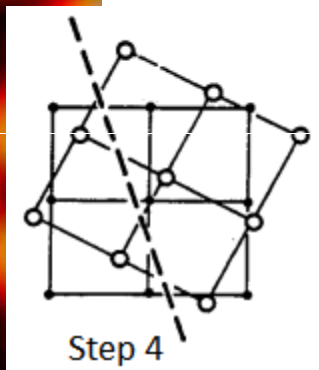


Step 3

Apply Black – White Symmetry

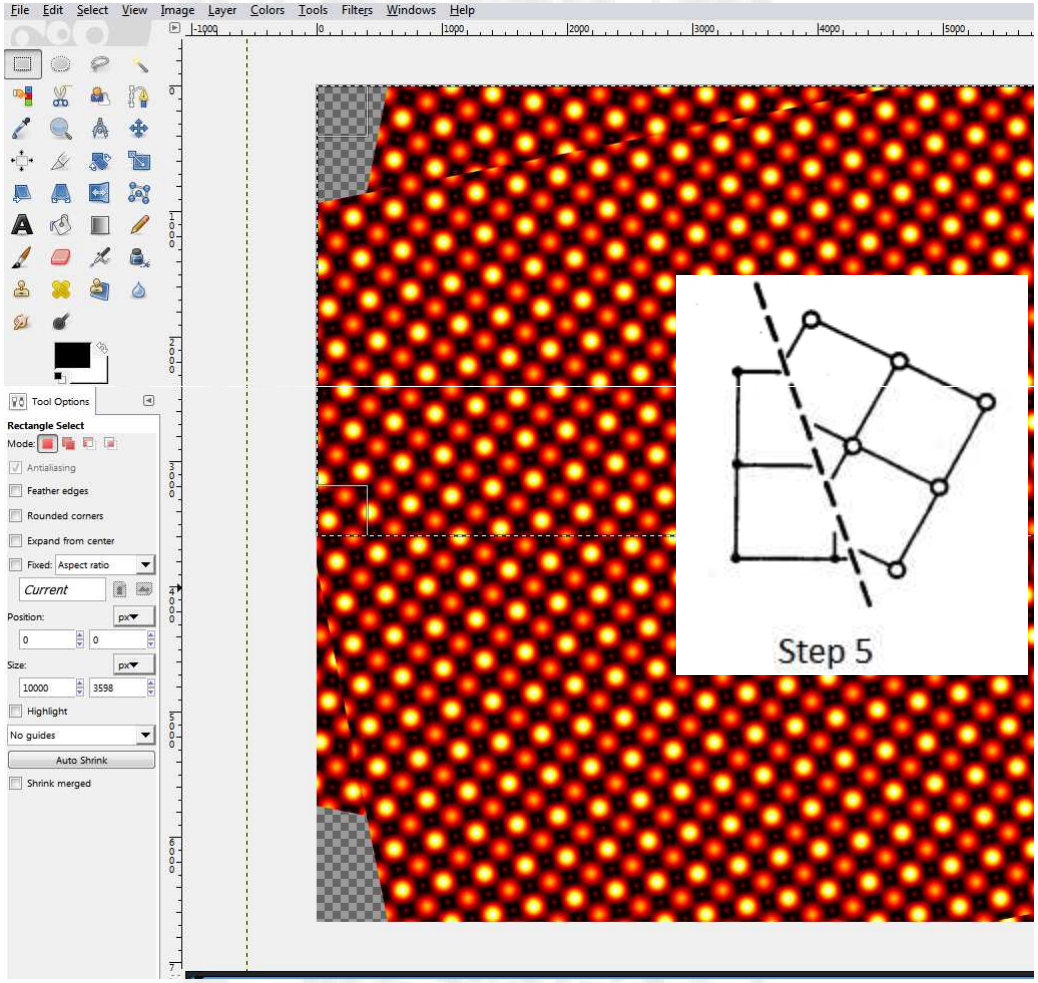
- Select a mirror line (Green) to create an *p*11m' boundary.
- Select a glide line (Blue) to create an *p*11g' boundary.
- Section with a line not shown to create an *p*1' boundary.
- The gray box outlines the CSL unit cell.



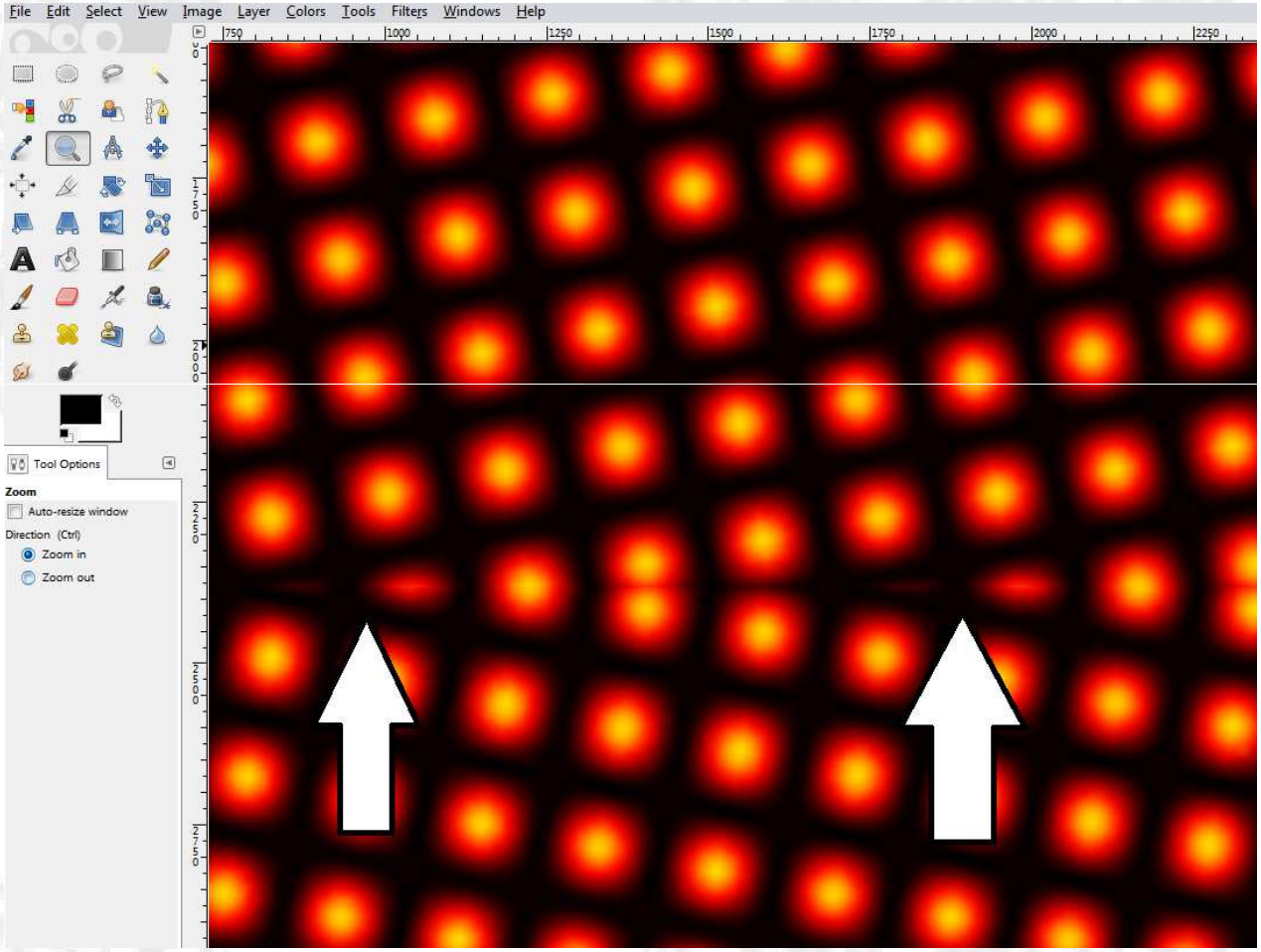


Sectioning the Monocrystals

- The lower extreme of the selected area acts as a sectioning line.
- Remove from the lower crystal the selected area.
- Invert Selection and remove from the upper crystal.



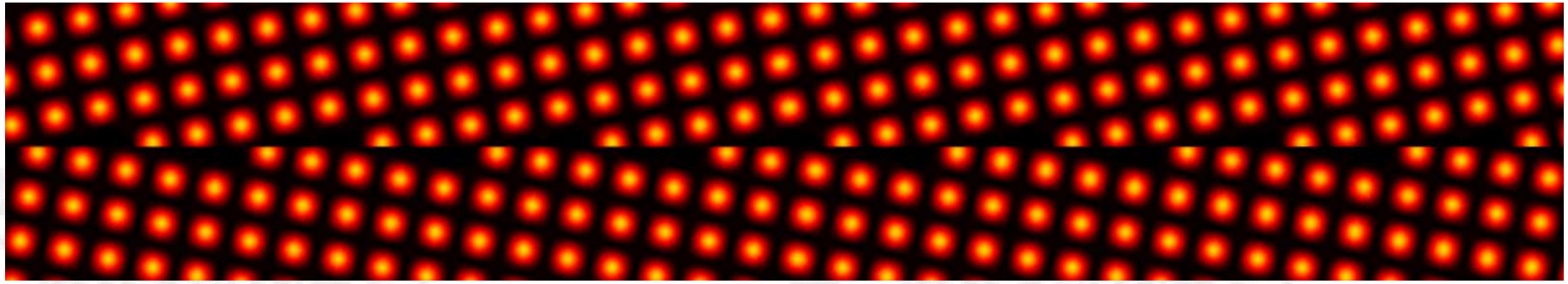
Remove partially resolved columns



Remove partially resolved columns

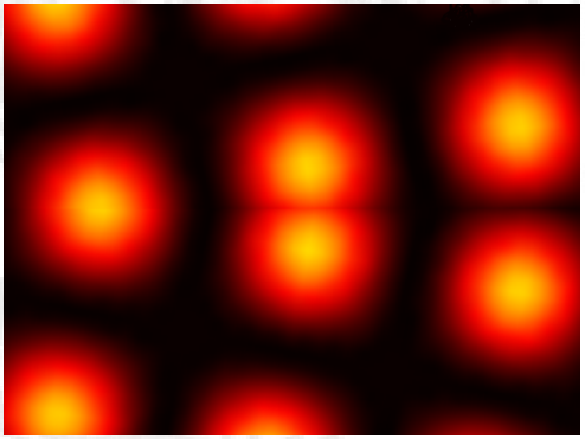
- Exclude partial columns if their corresponding lattice point is not on that side of the section line.

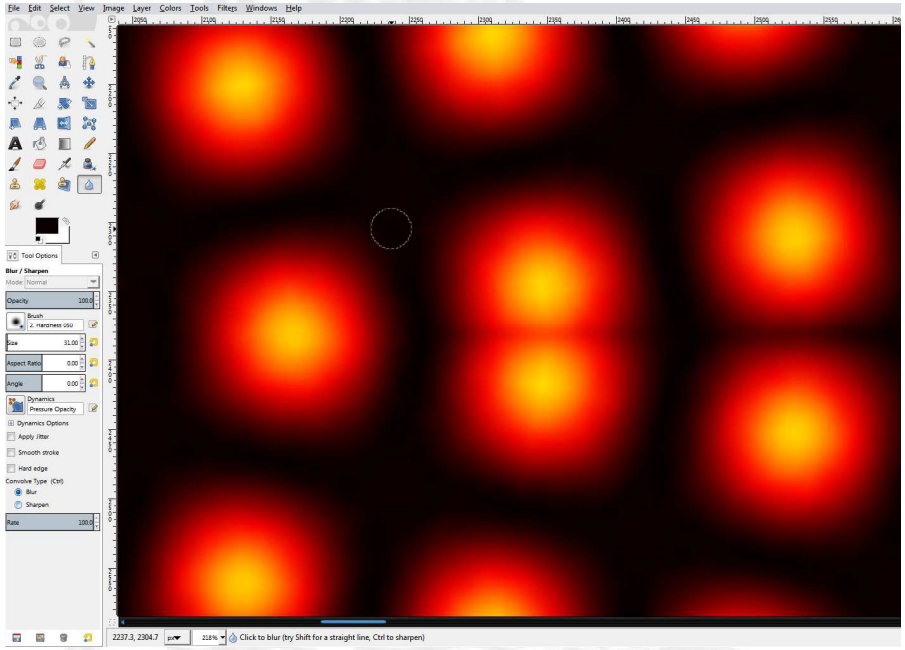
- The white points represent a mathematical lattice after sectioning.



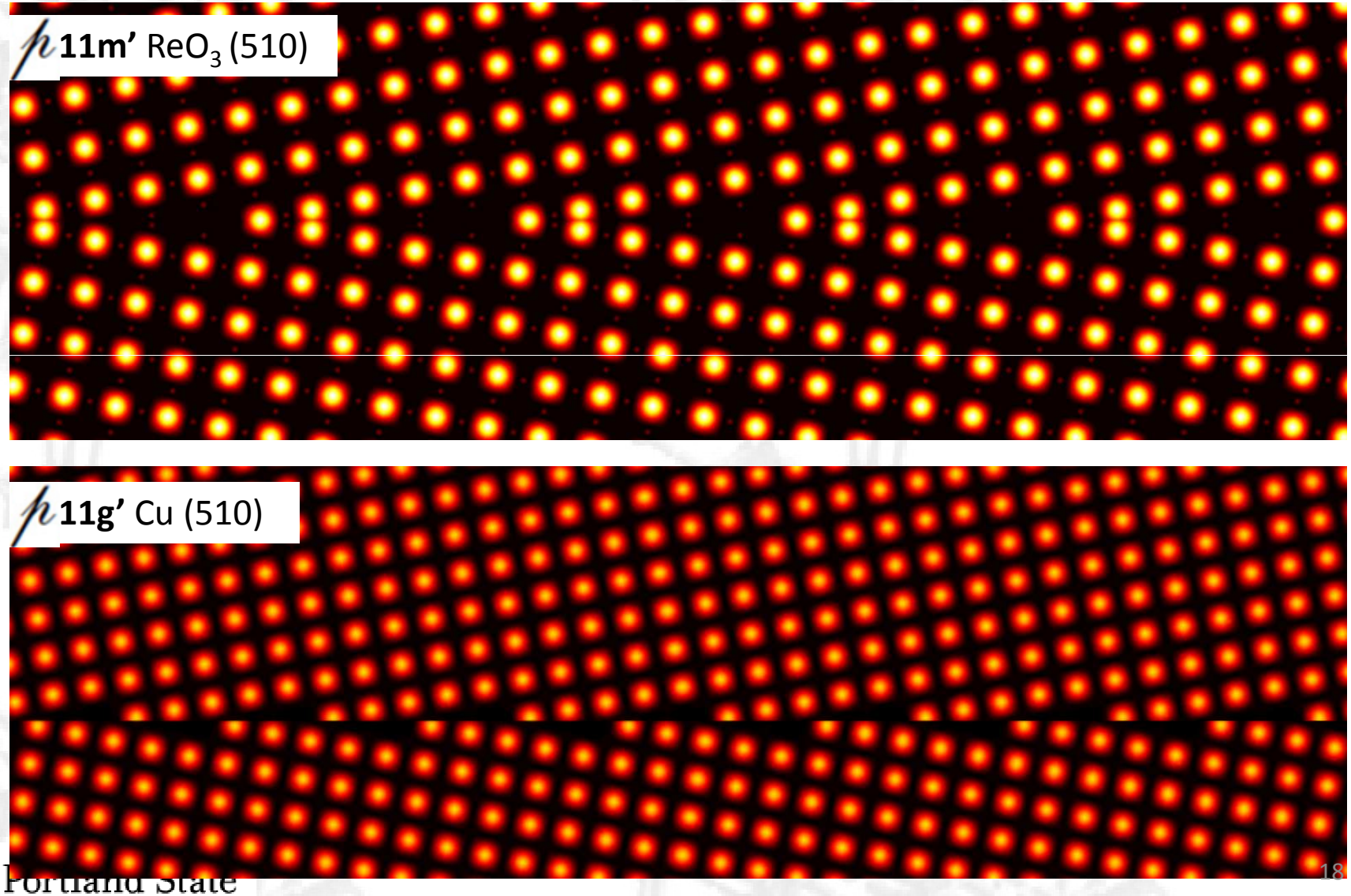
Smooth and Polish

- Blur tool to smooth hard edges
- General touch up to make things look more natural
- Some materials need very little of this



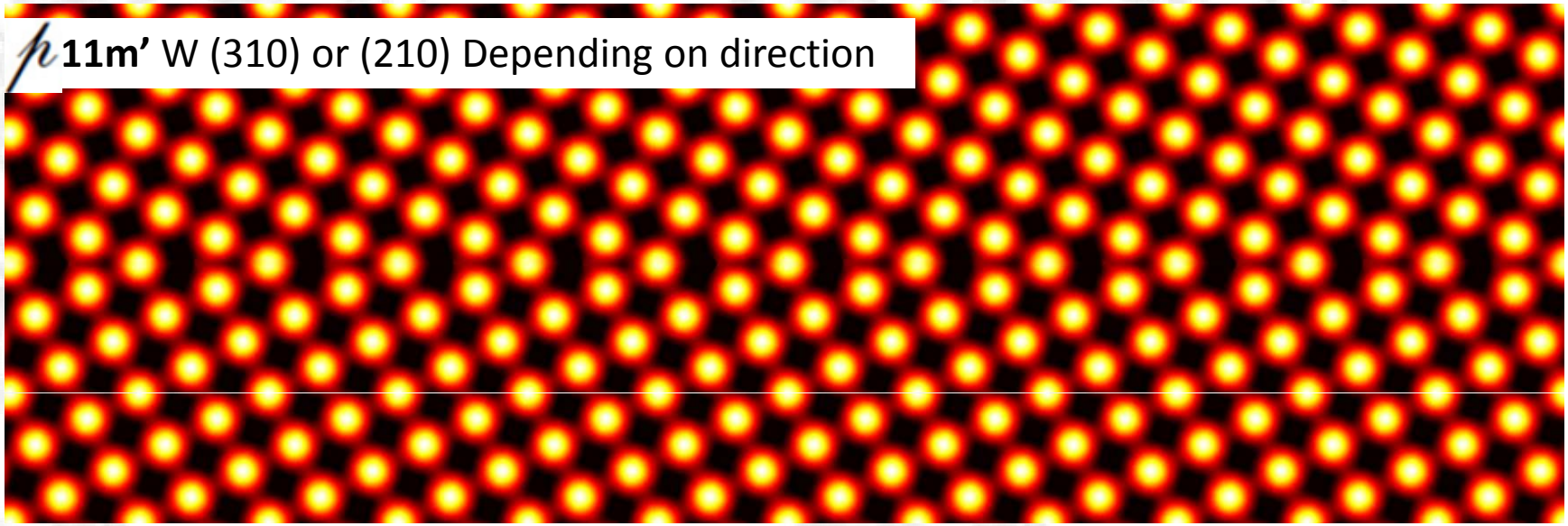


Results

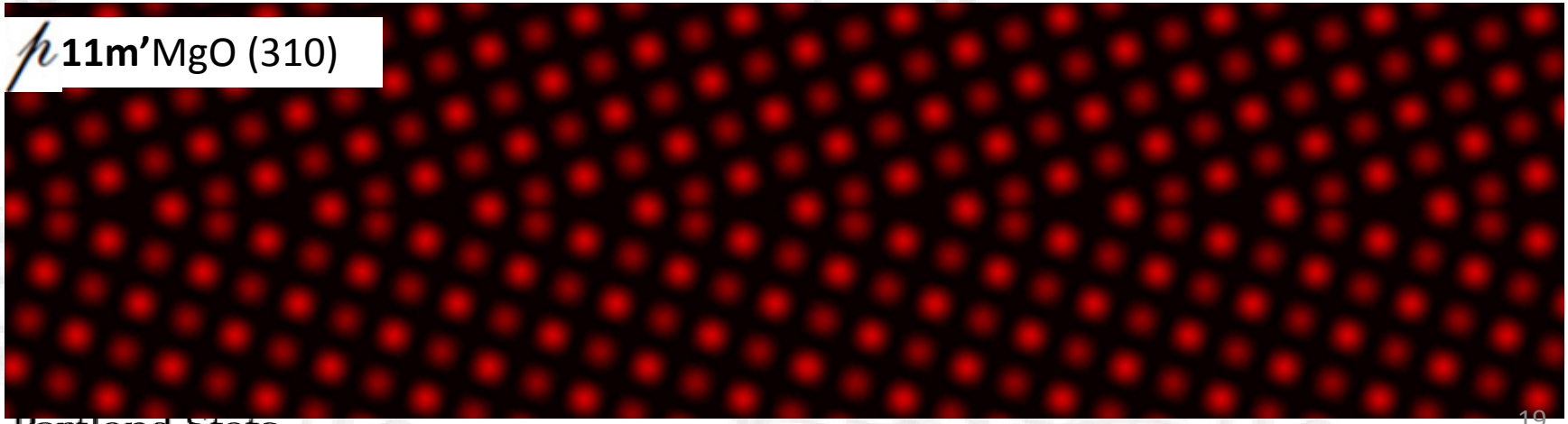


Results

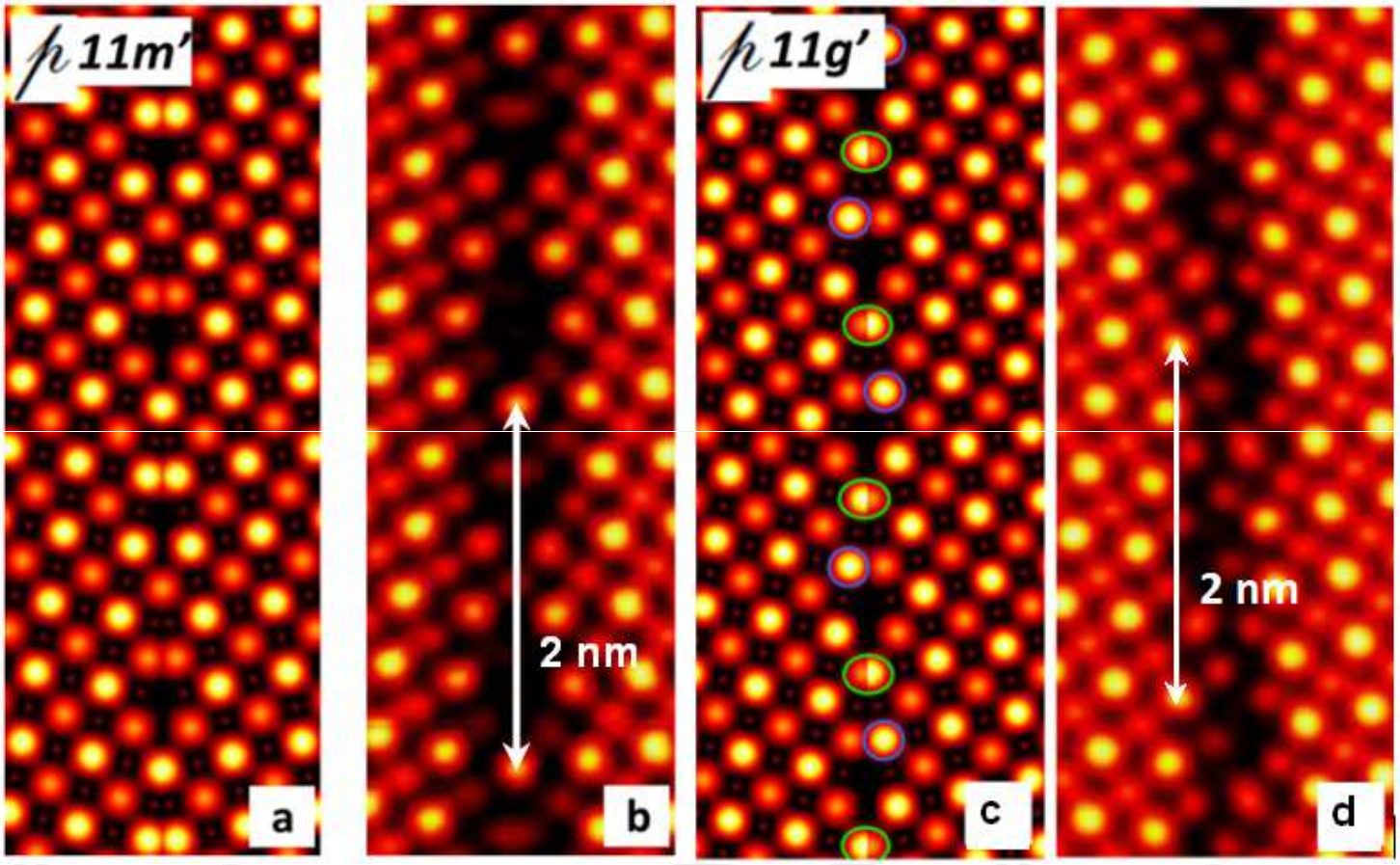
11m' W (310) or (210) Depending on direction



11m'MgO (310)



Comparison to Experiment



Figures a, c are predicted structures
Figures b, d are Z-Contrast STEM images
Material is $SrTiO_3$

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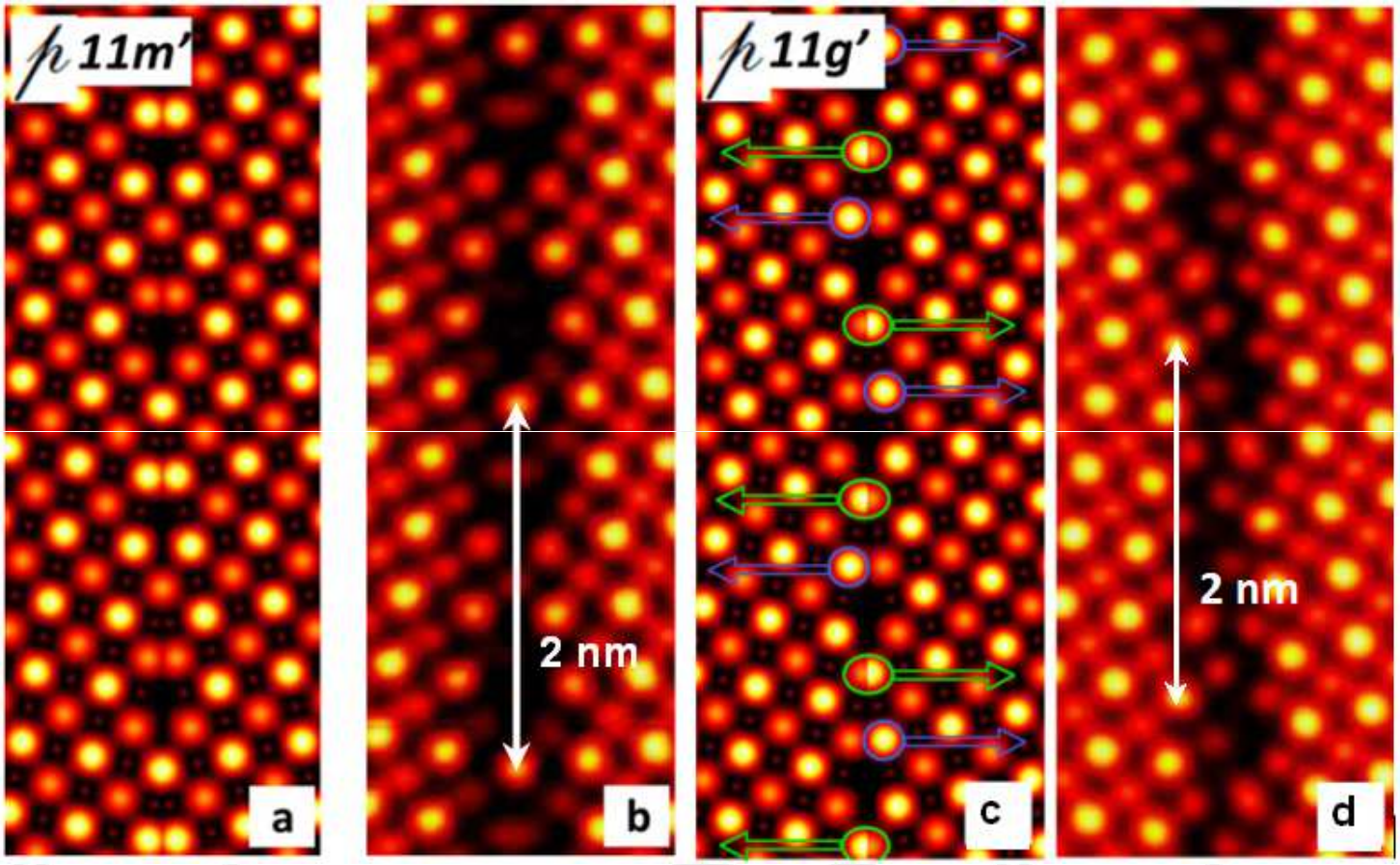
Comparison to Experiment



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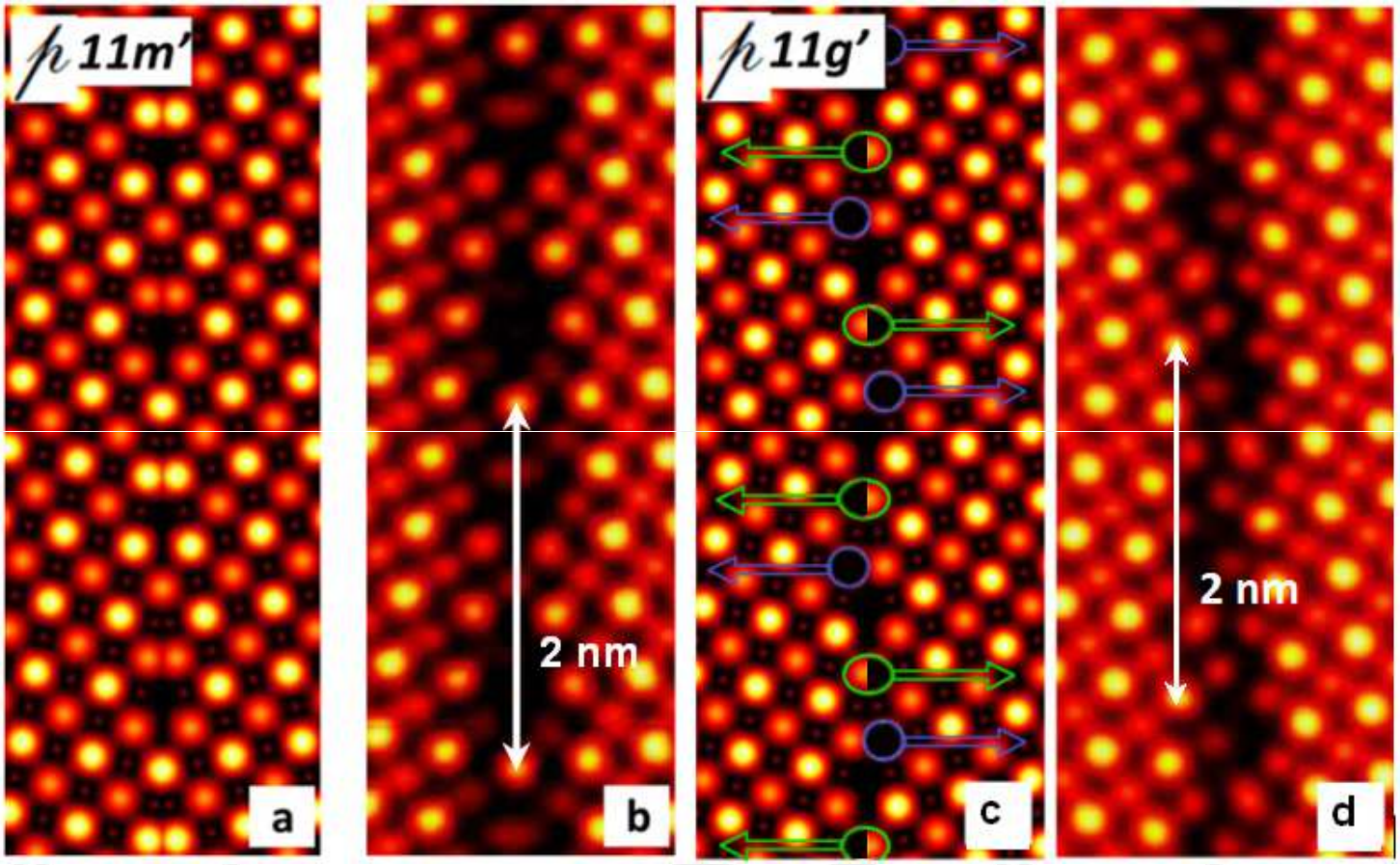

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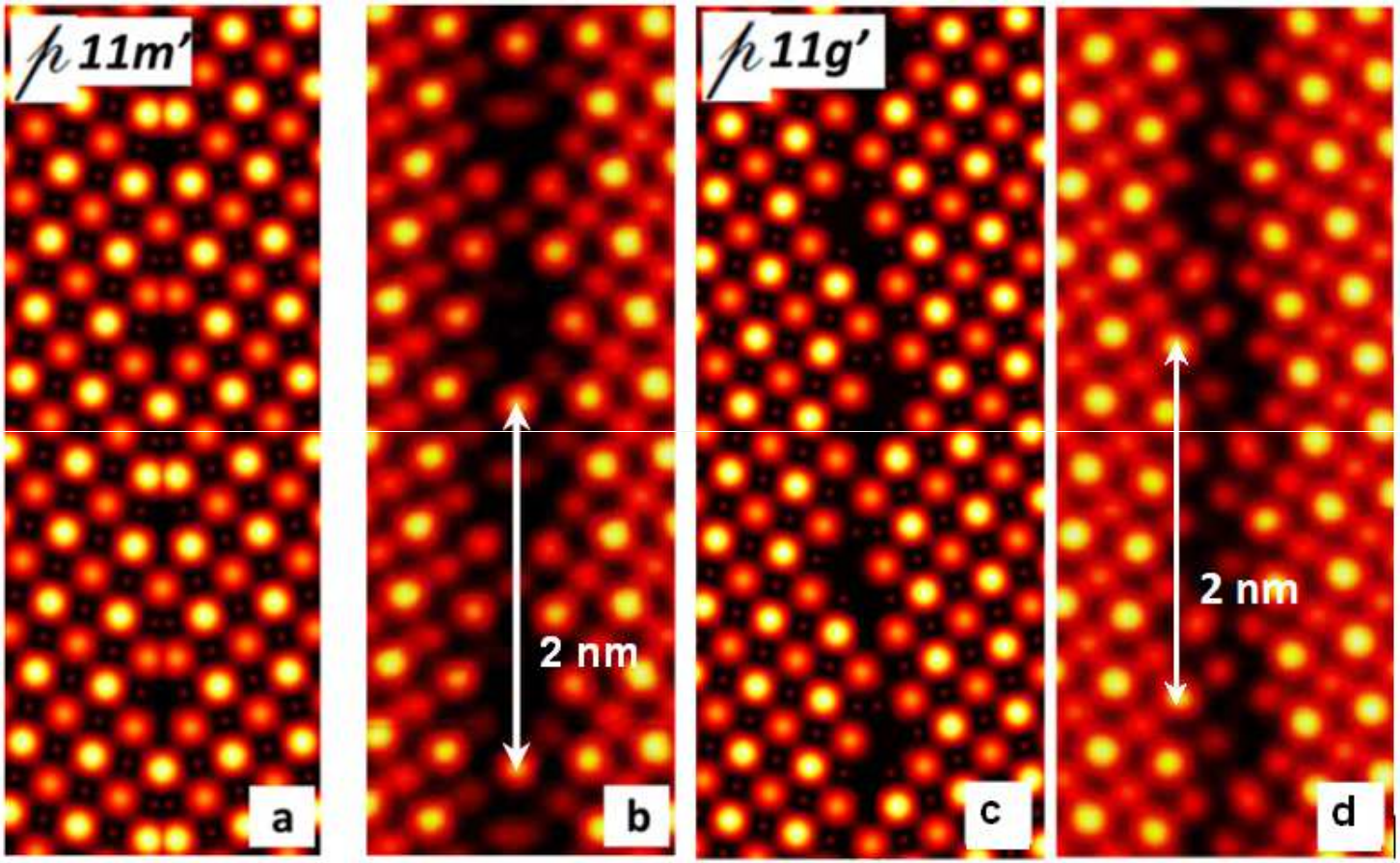

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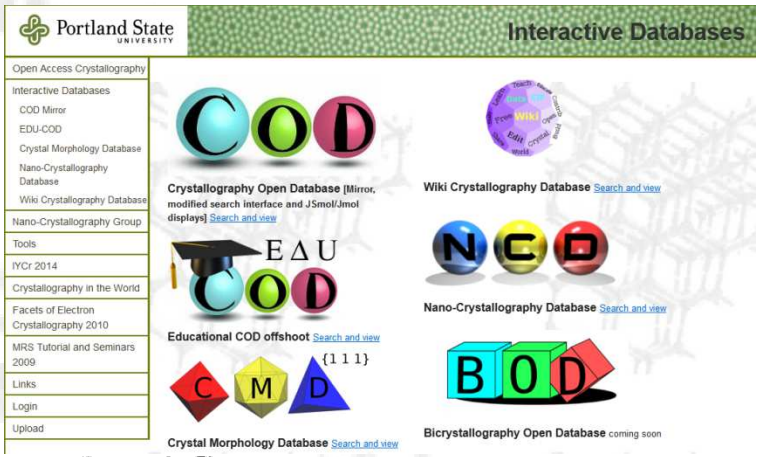
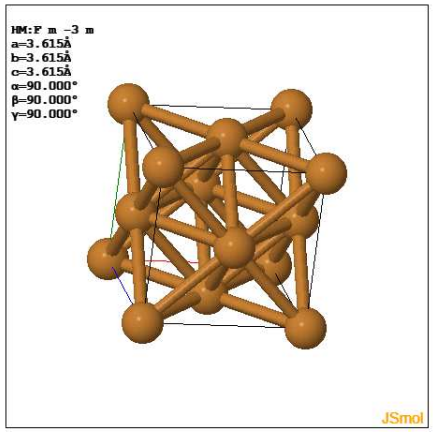
The Future of the Project

- MatLab code improvements
- ρ1’ boundaries
- Integration into Open Access Crystallography (resources available at nanocrystallography.research.pdx.edu)





Formula: Cu
3D Model Controls:
Display options
Unit cell Spin Label element(s)
Atomic: Radii
Wireframe: bonds off
Axes: UVW
Show: Conventional unitcell
Stereo: Stereo Mode Off
Background: Grey
Rotate X axis 45° | Rotate Y axis 45° | Rotate Z axis 45°
Reset | Console
Zoom 150% | Zoom 100% | Zoom 50%

Draw Planes
None

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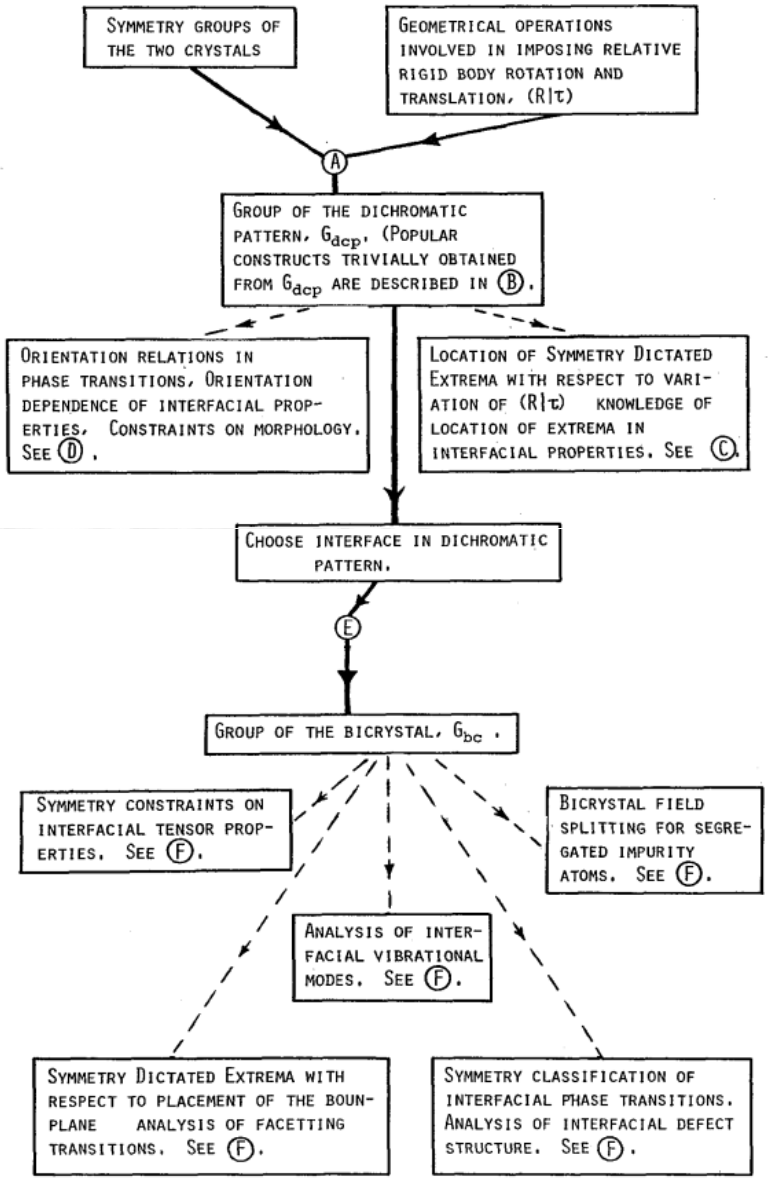
Thank you for listening!



Shubnikov-Curie Principal:

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