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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

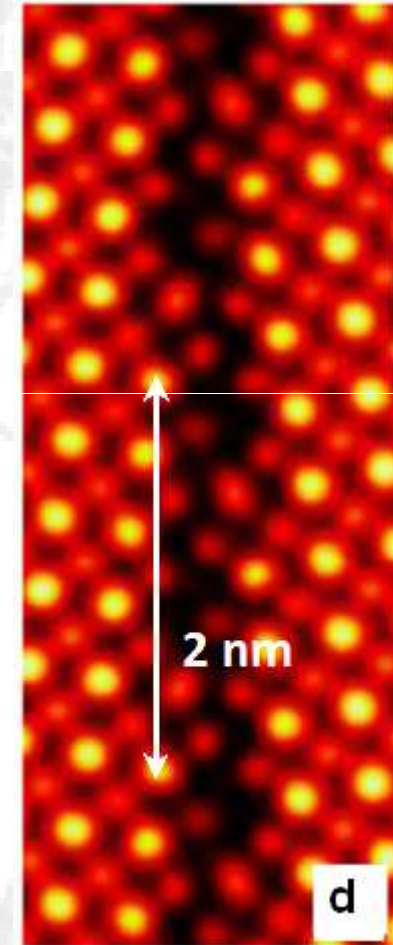
By Andrew Maas

Portland State University

Nano-Crystallography Research Group

What is Bicrystallography?

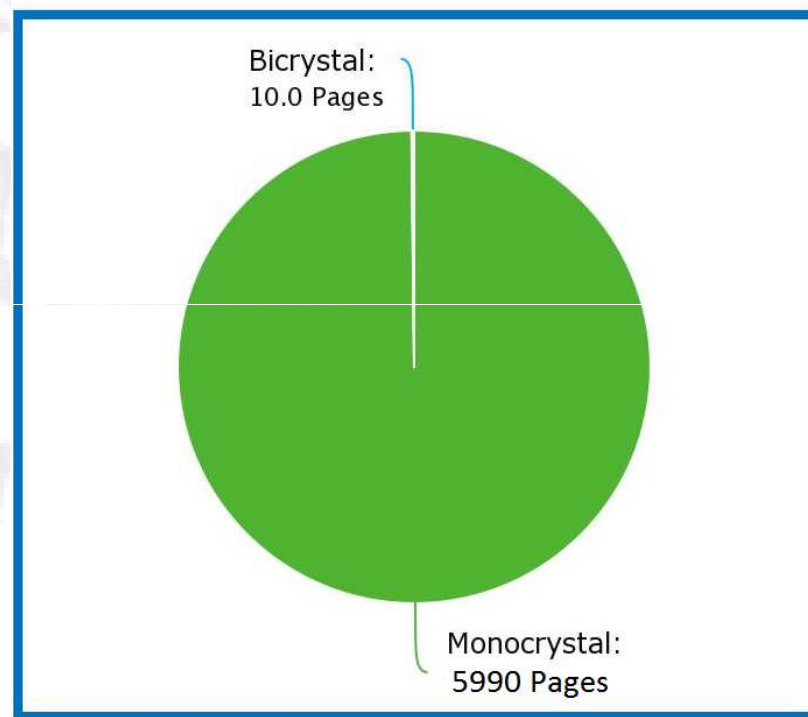
- Describe Ideal Bicrystals
- Atomic Level Description
- Like crystallography, but studying bicrystals, rather than monocrystals.
- Correlate physical properties to internal structure (Shubnikov-Curie principle)
- Ideal 3D bicrystals related to real ones by free energy minimization



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?

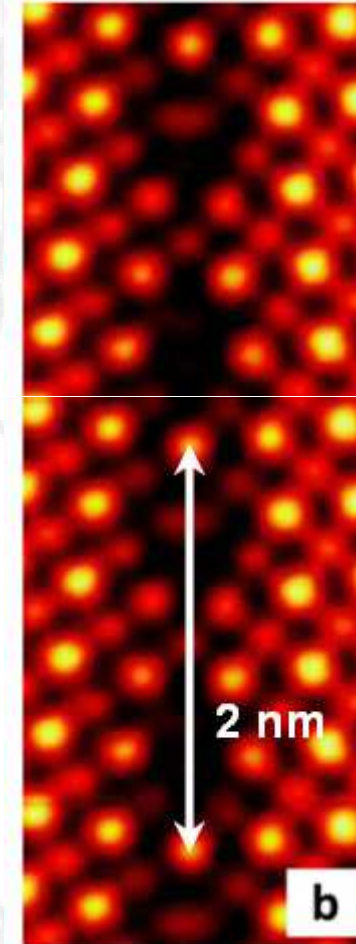
Breakdown of International Tables of Crystallography



■ Monocrystal ■ Bicrystal

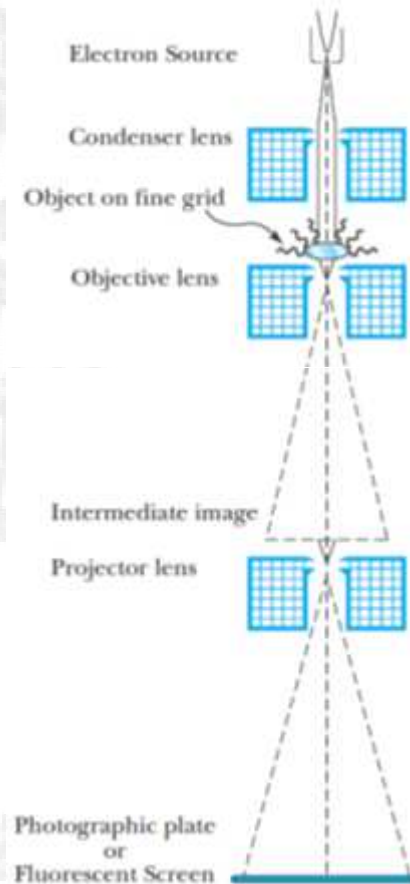
Objective

- 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



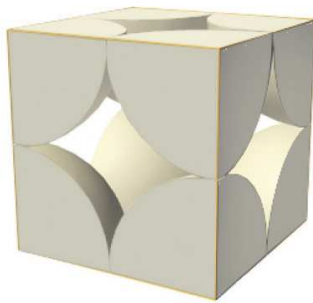
Why 2D Bicrystallography?

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

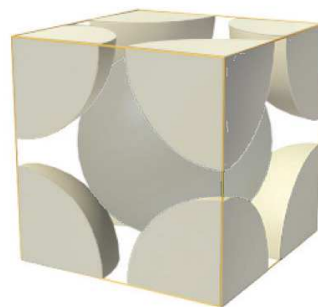


Terms and Abbreviations

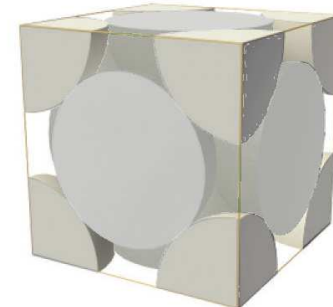
- Simple (SC), Body Centered (BCC), and Face Centered Cubic (FCC), refers to a crystal lattice that has a cube shaped unit cell:



(a) Simple cubic



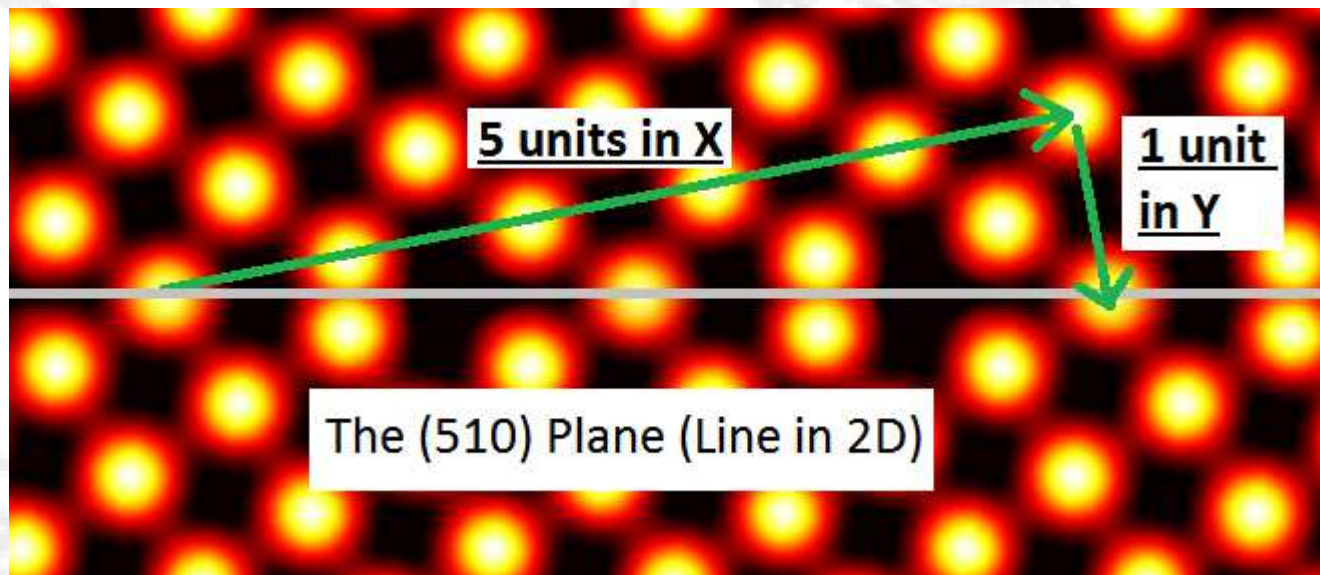
(b) Body-centered cubic



(c) Face-centered cubic

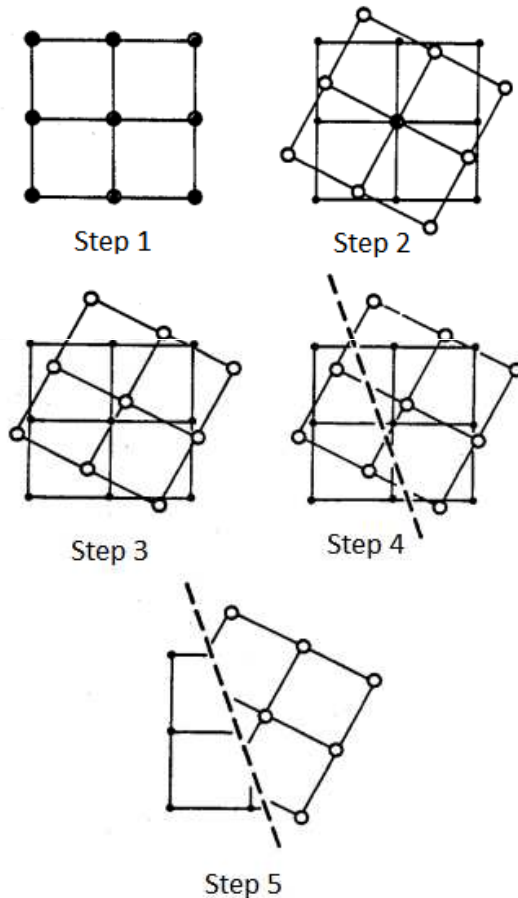
Terms and Abbreviations

- (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.



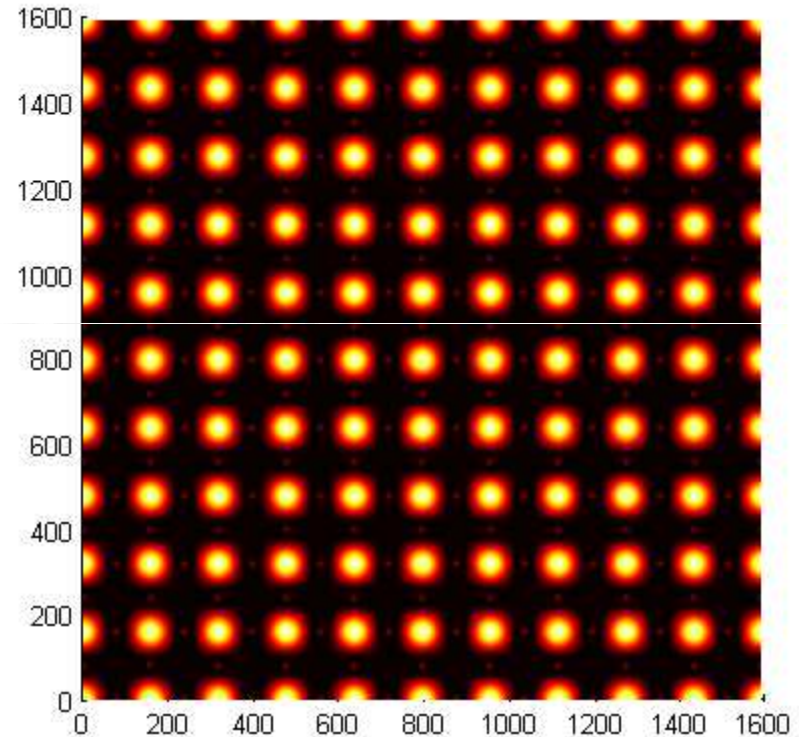
Modeling a Bicrystal

- 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)



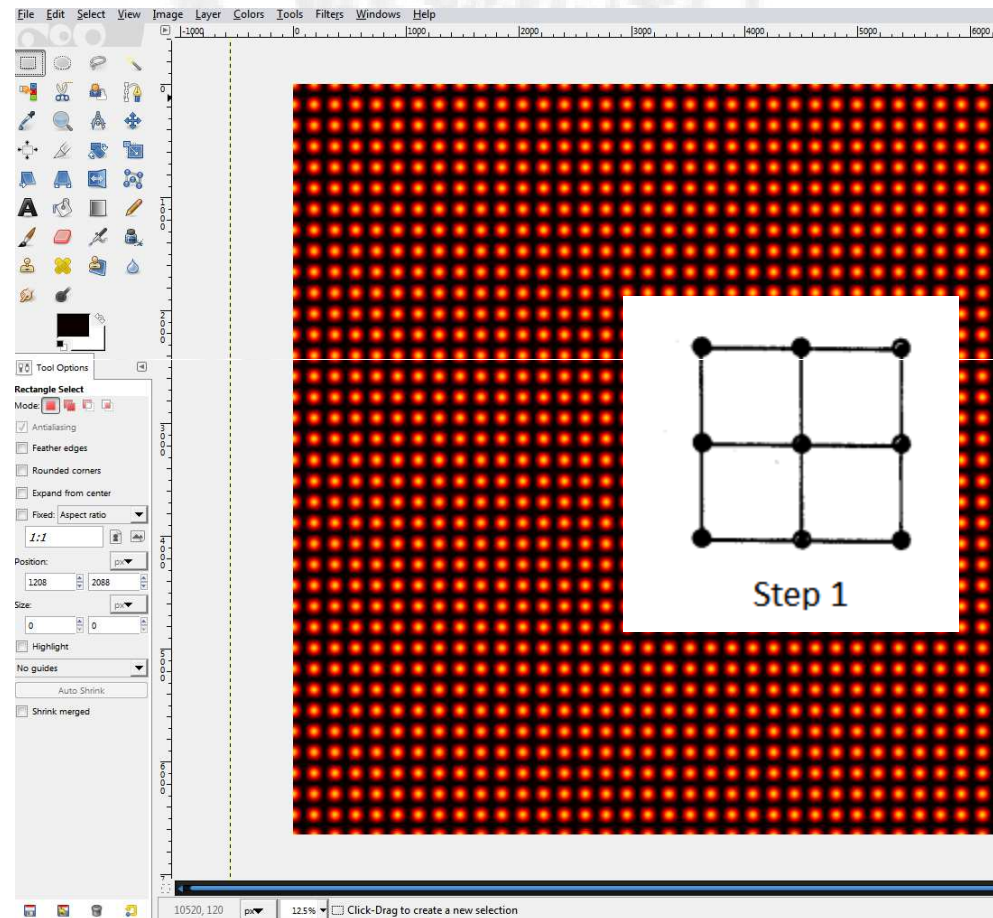
MatLab to Create Simulated Images

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

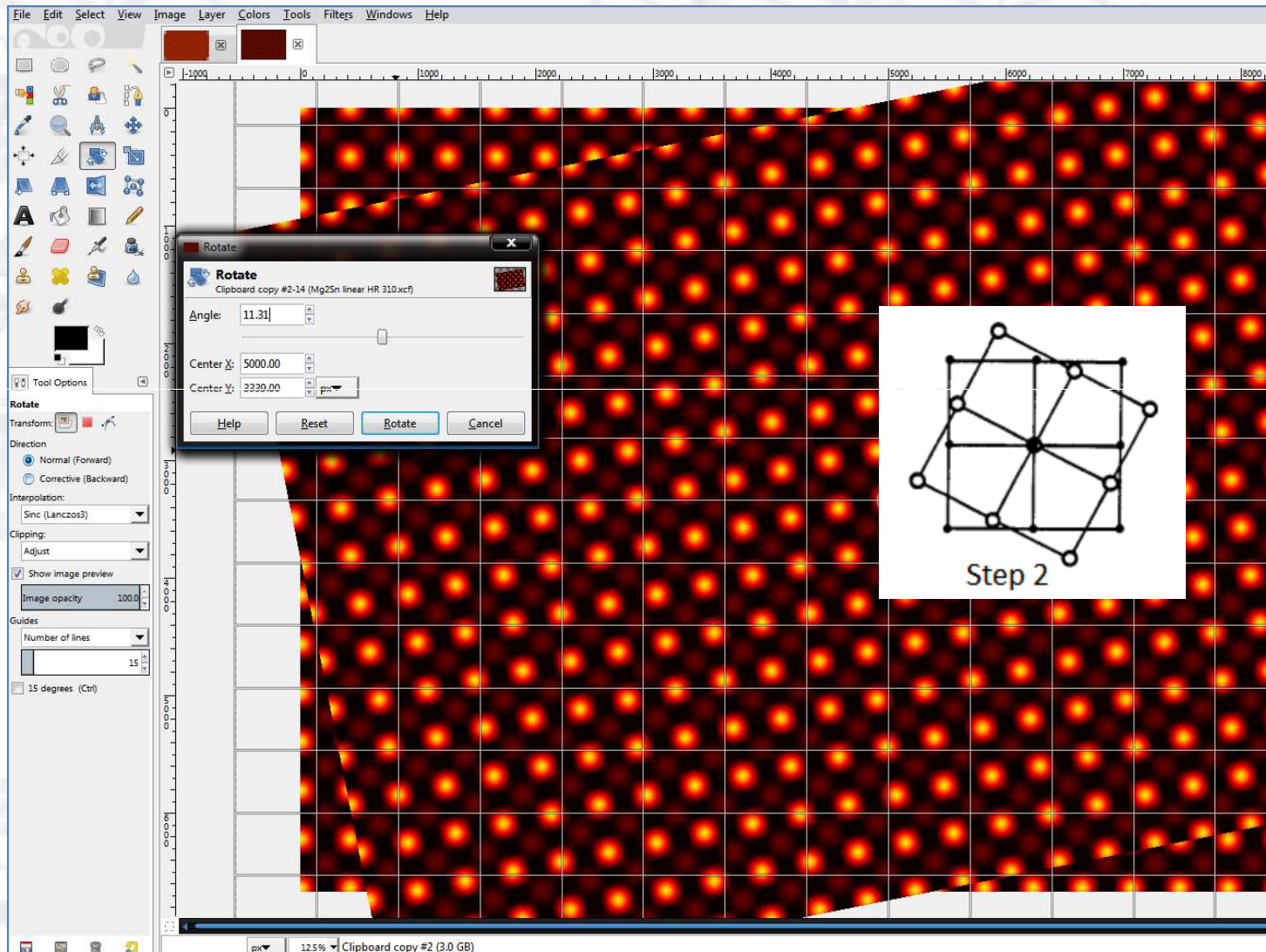


Create the Two Lattices

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

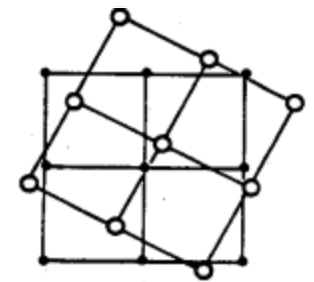
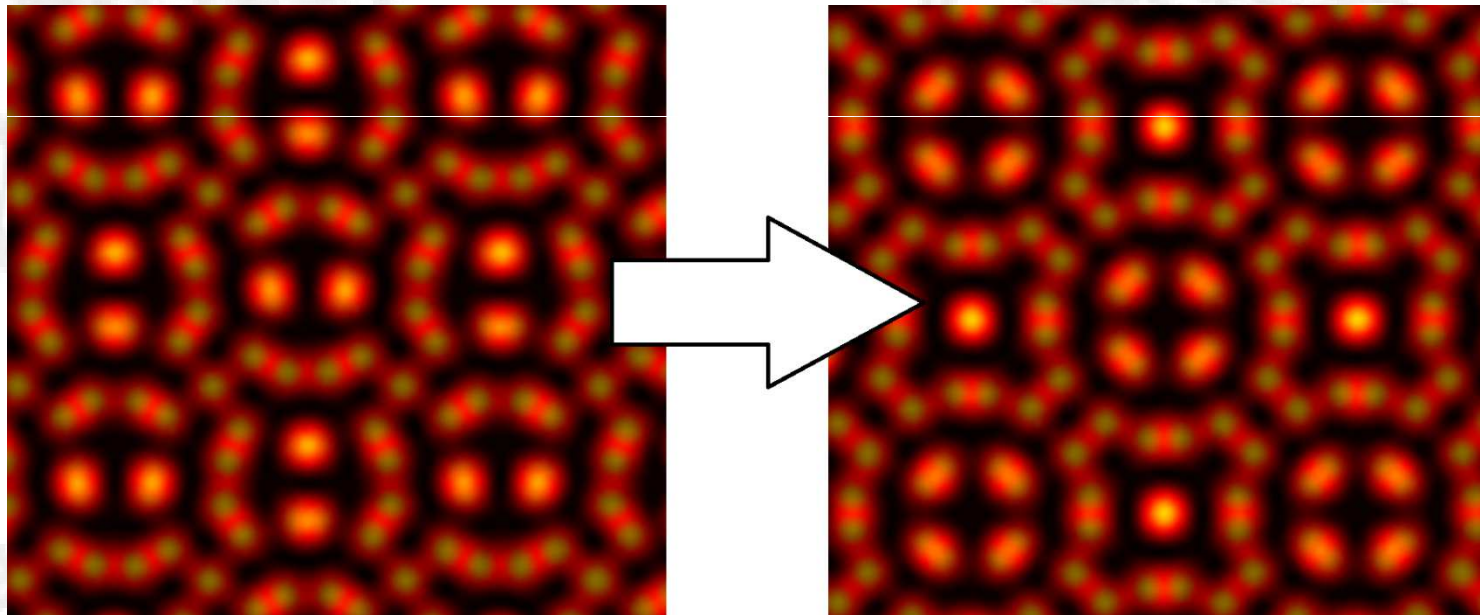


Apply Rotation



Apply Translation

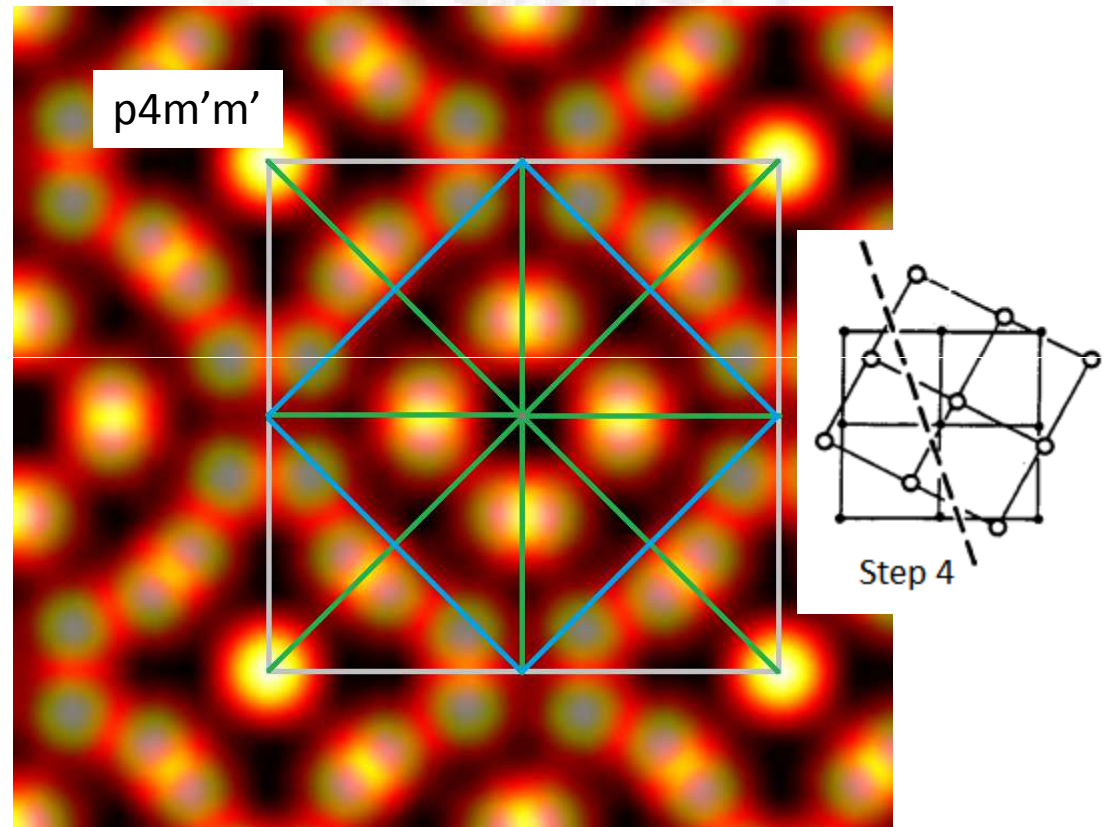
- For our images, we align the Coincident Site Lattice (CSL) points.



Step 3

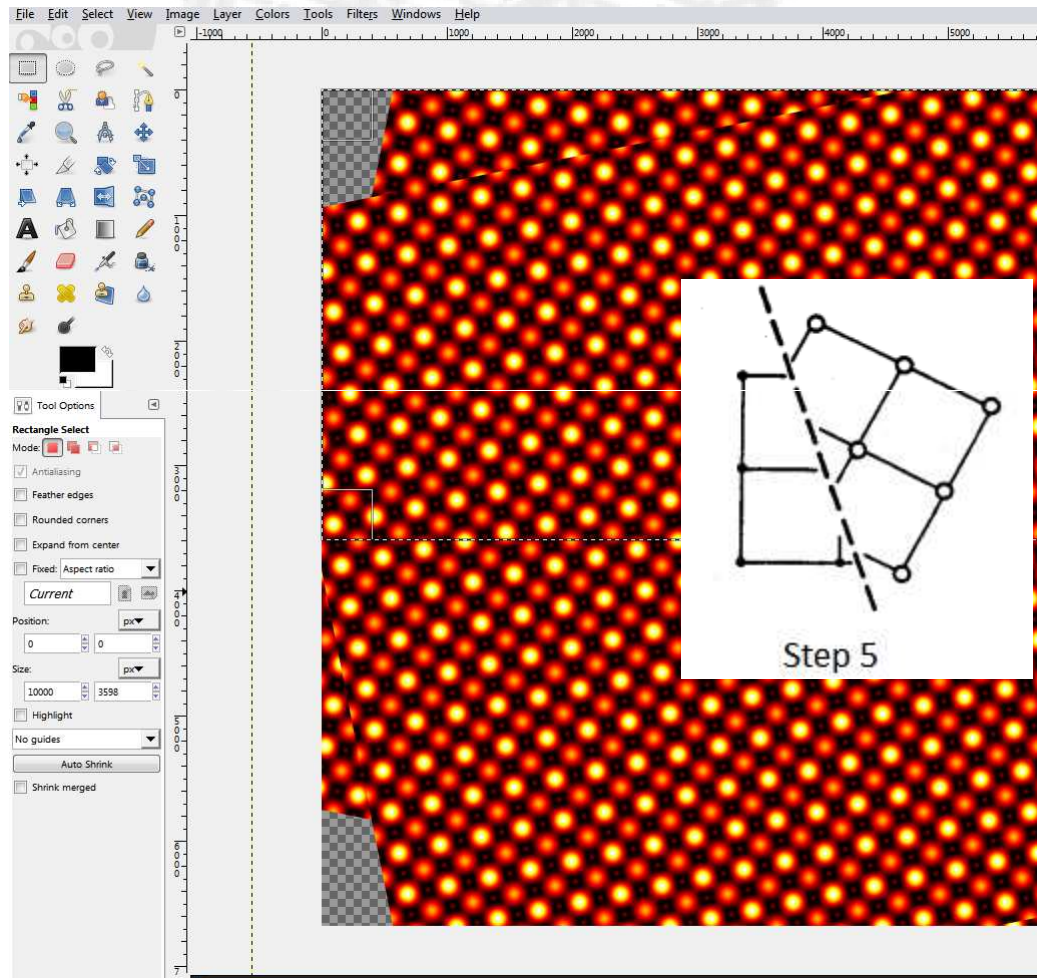
Apply Black – White Symmetry

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

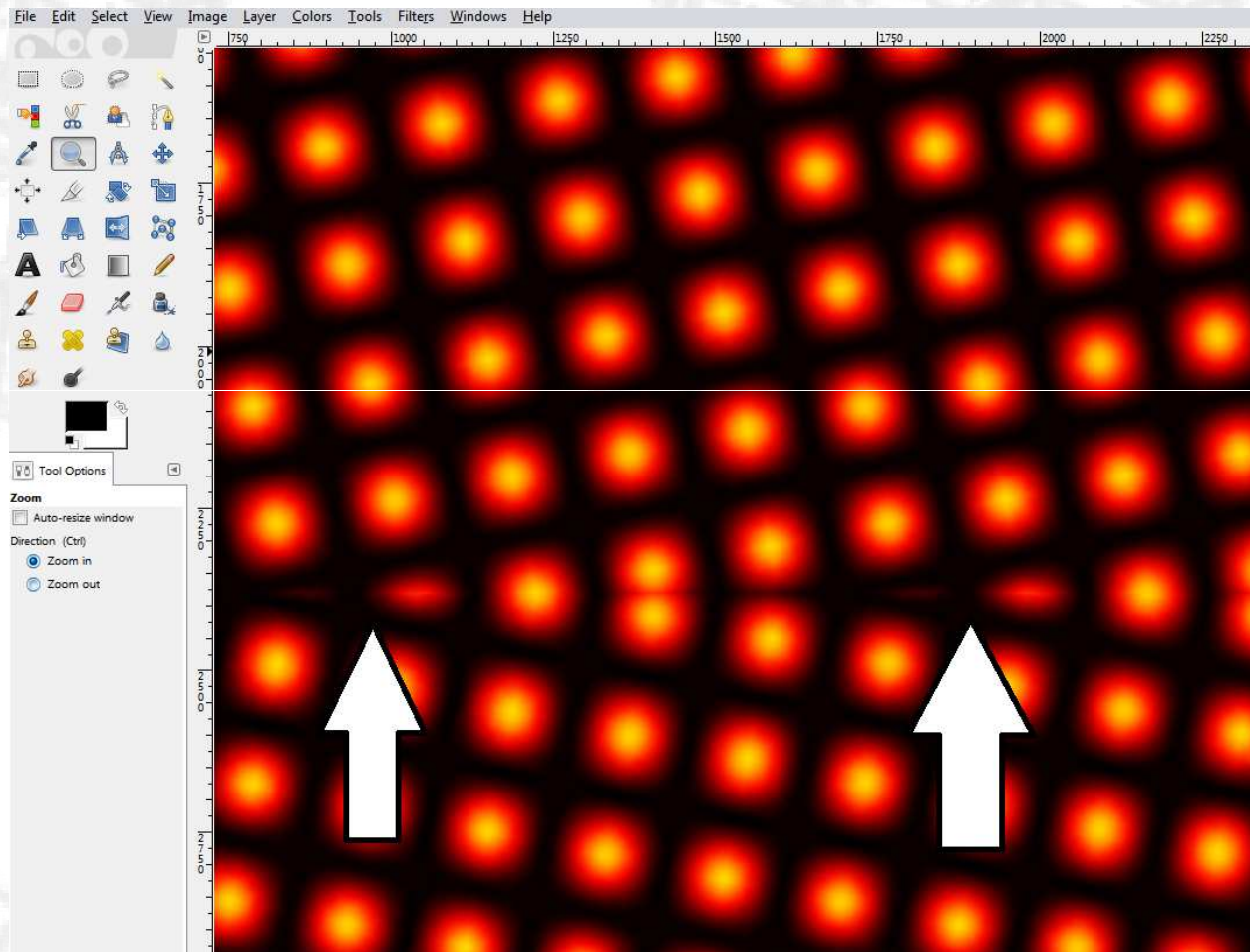


Sectioning the Monocrystals

- 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

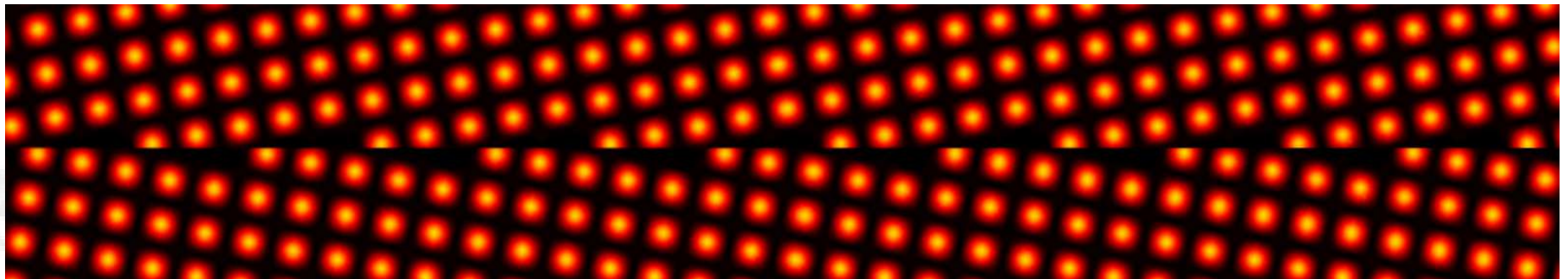


Remove partially resolved columns

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

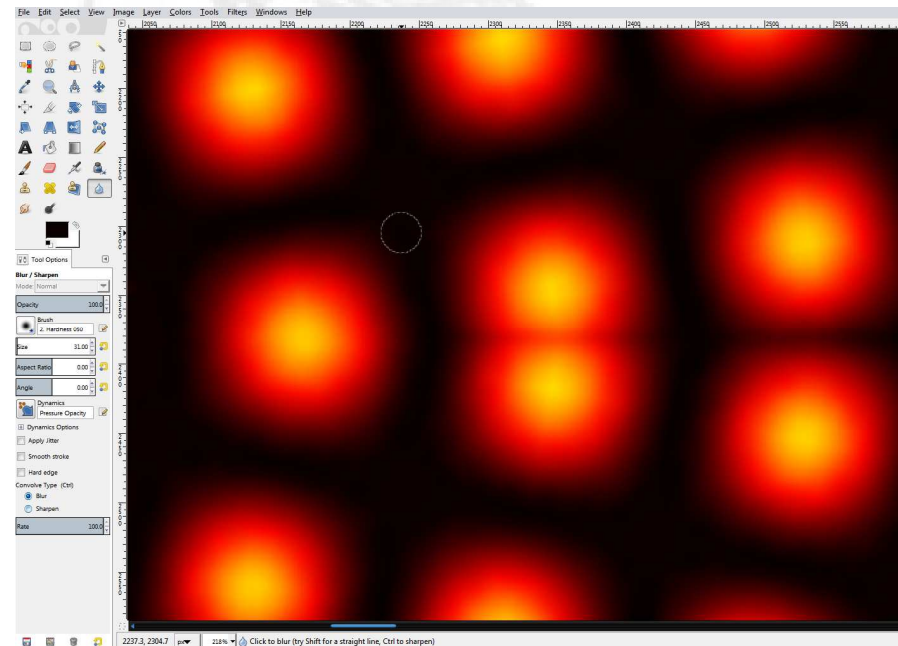
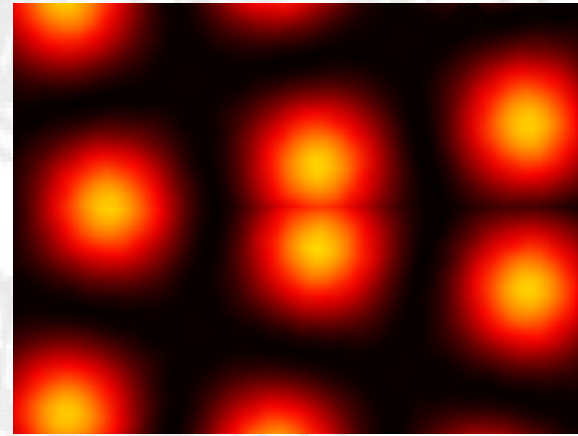


- The white points represent a mathematical lattice after sectioning.



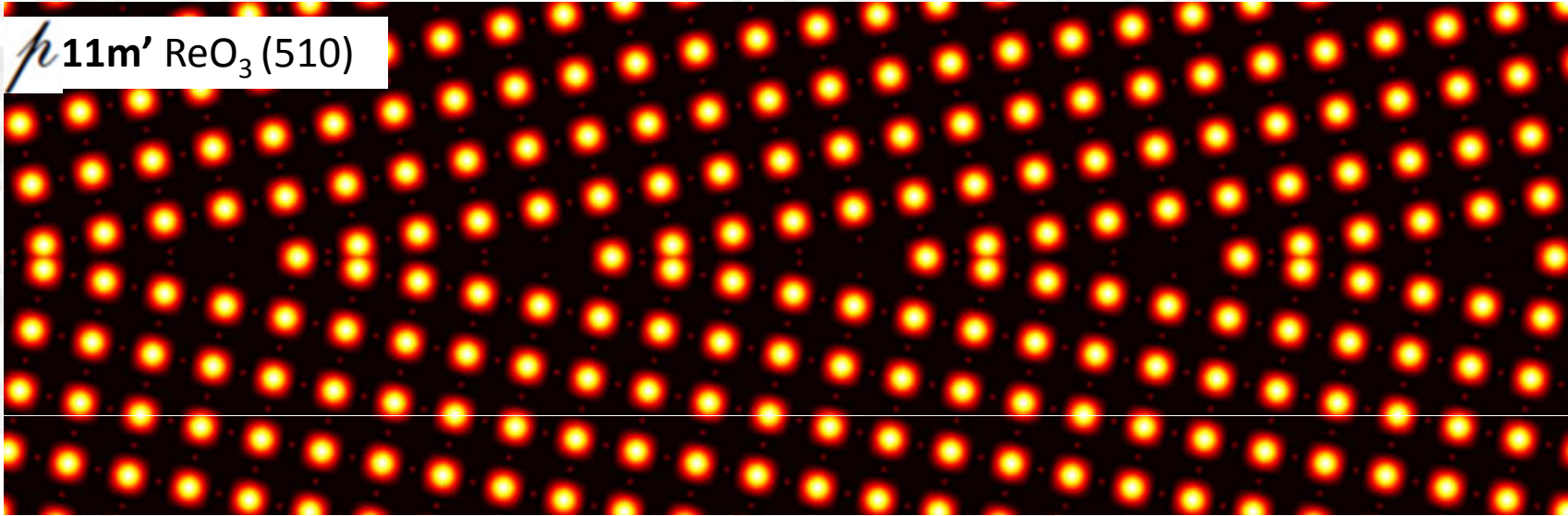
Smooth and Polish

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

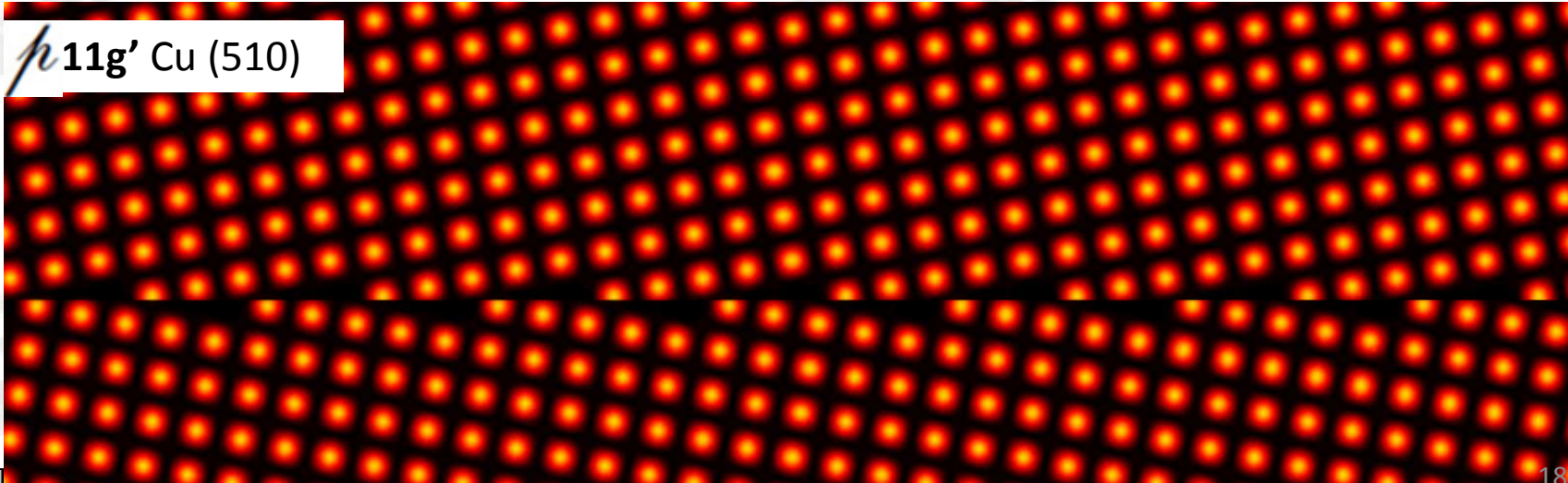


Results

μ 11m' ReO₃ (510)

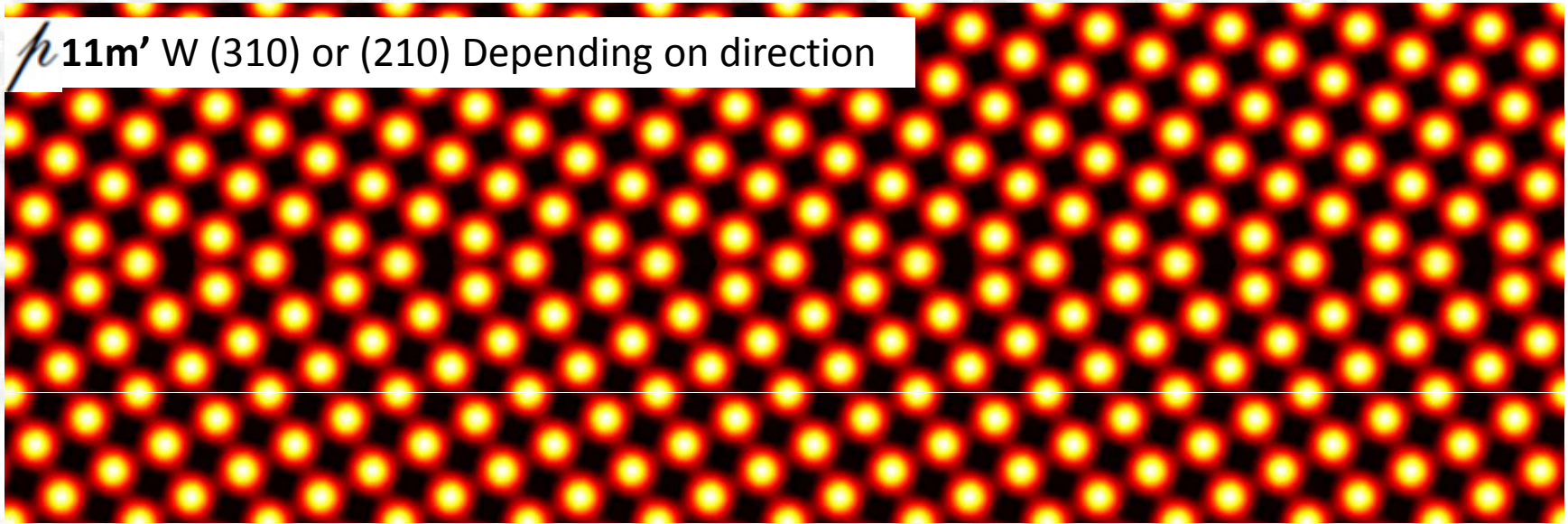


μ 11g' Cu (510)

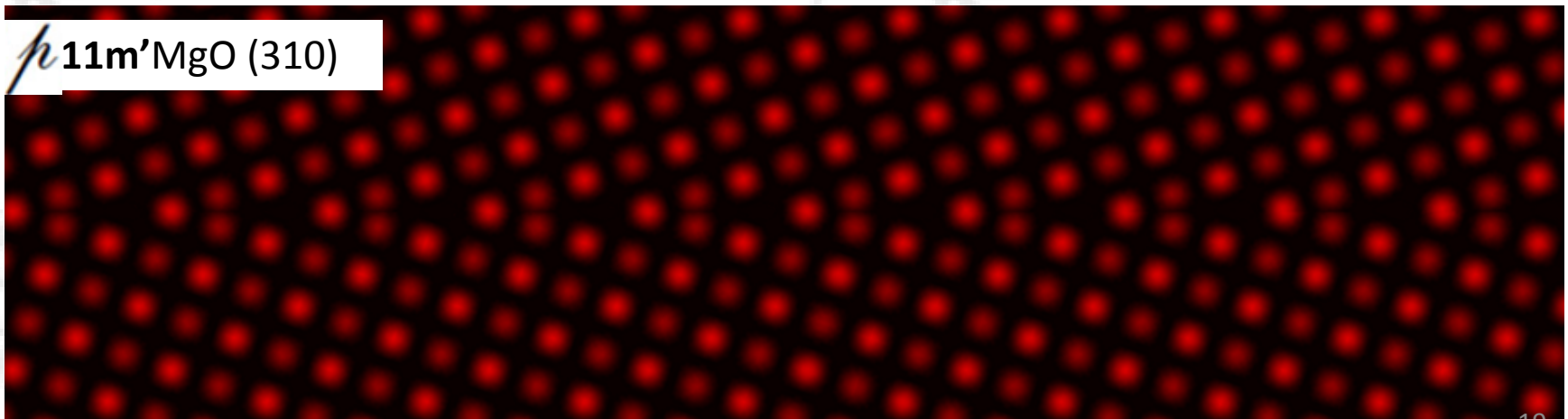


Results

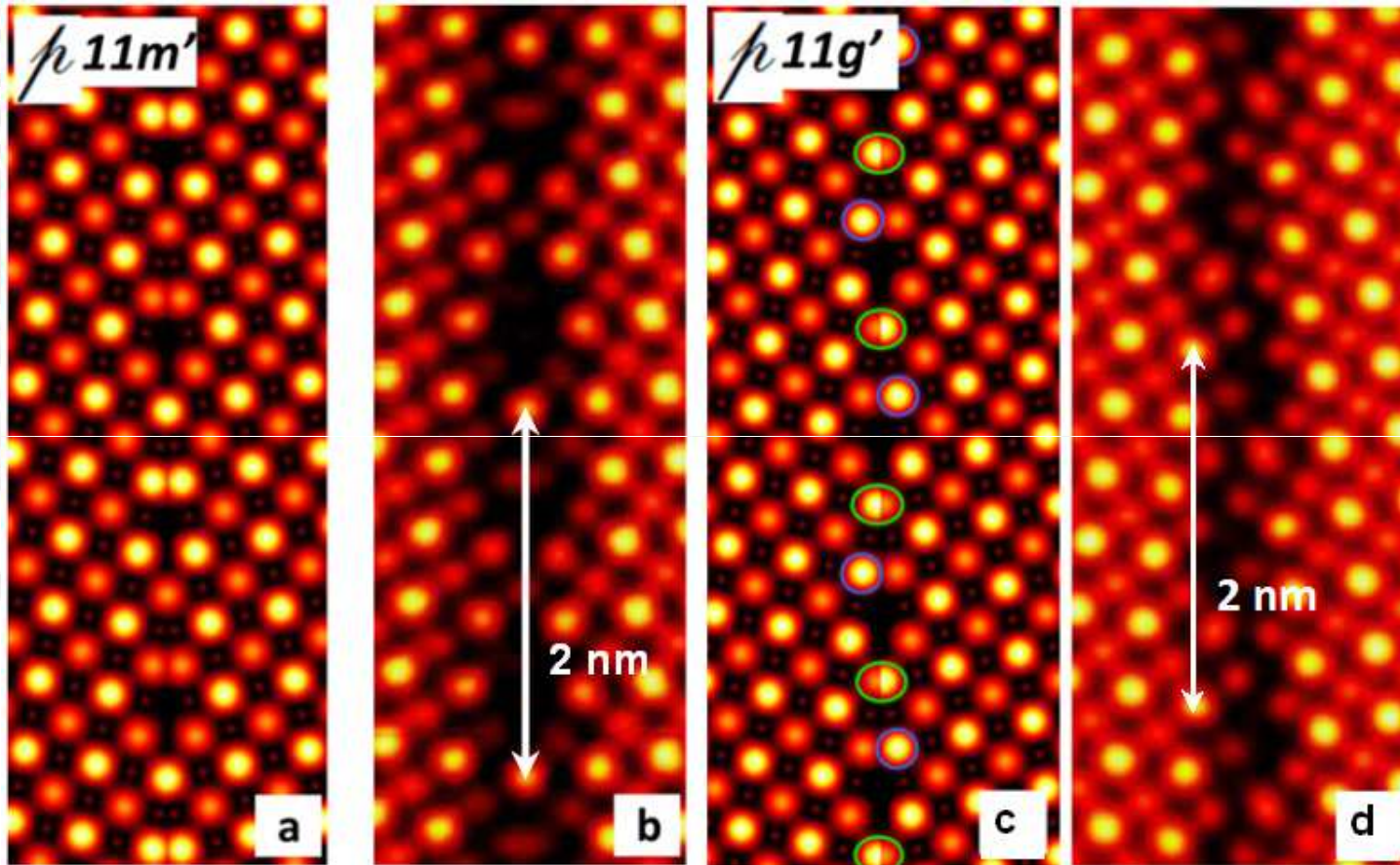
μ 11m' W (310) or (210) Depending on direction



μ 11m' MgO (310)

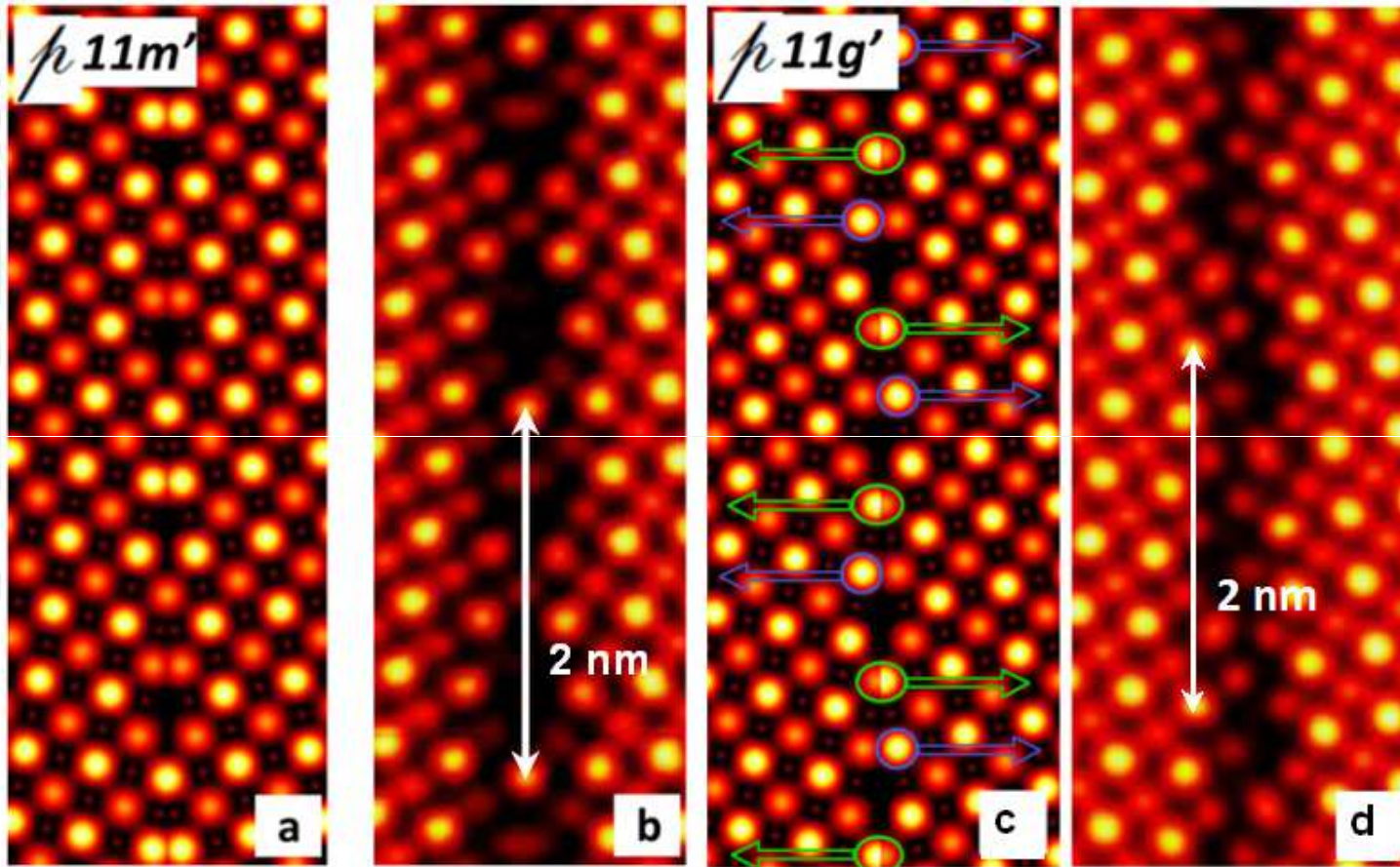


Comparison to Experiment



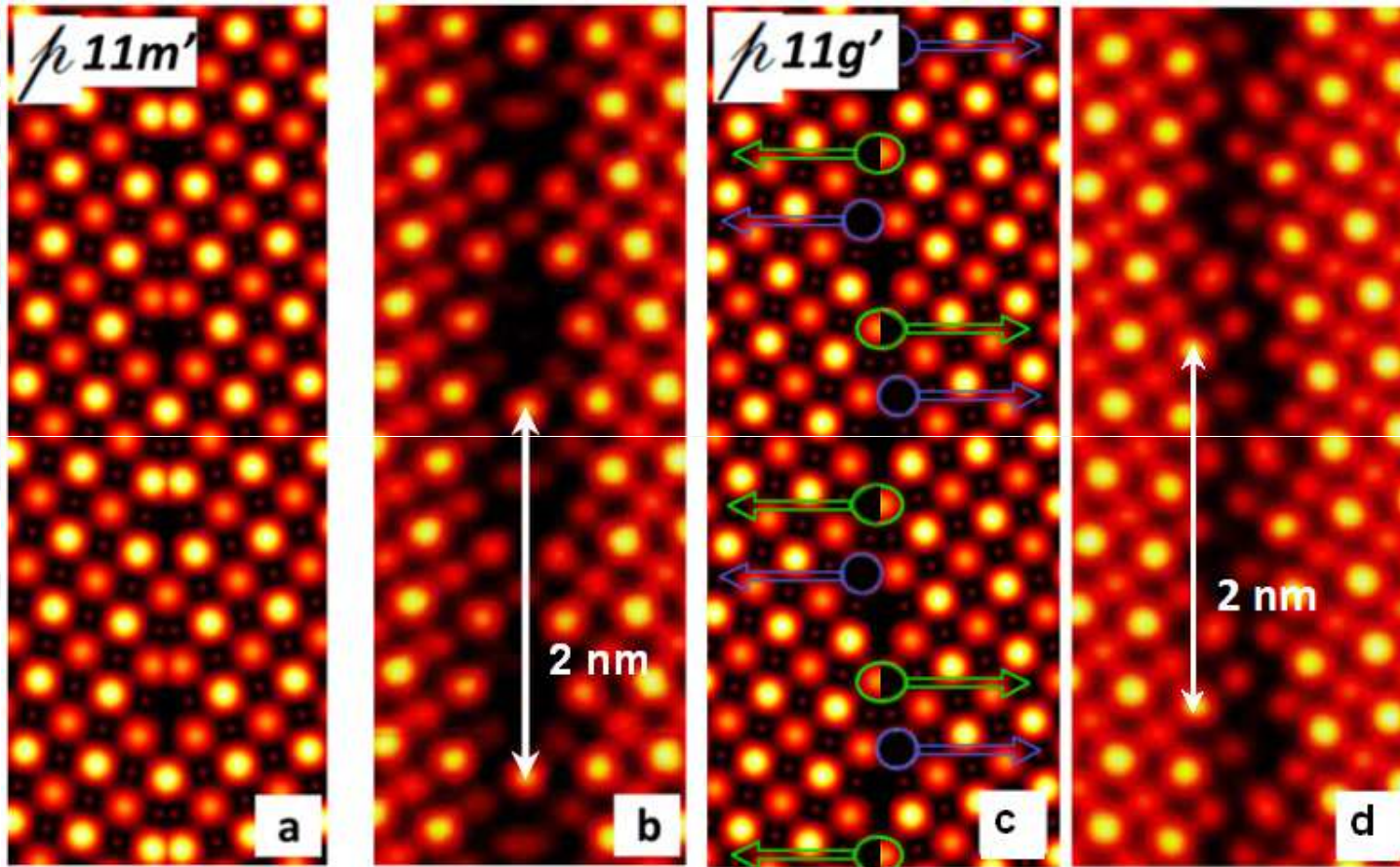
Figures a, c are predicted structures
Figures b, d are Z-Contrast STEM images
Material is SrTiO_3

Comparison to Experiment



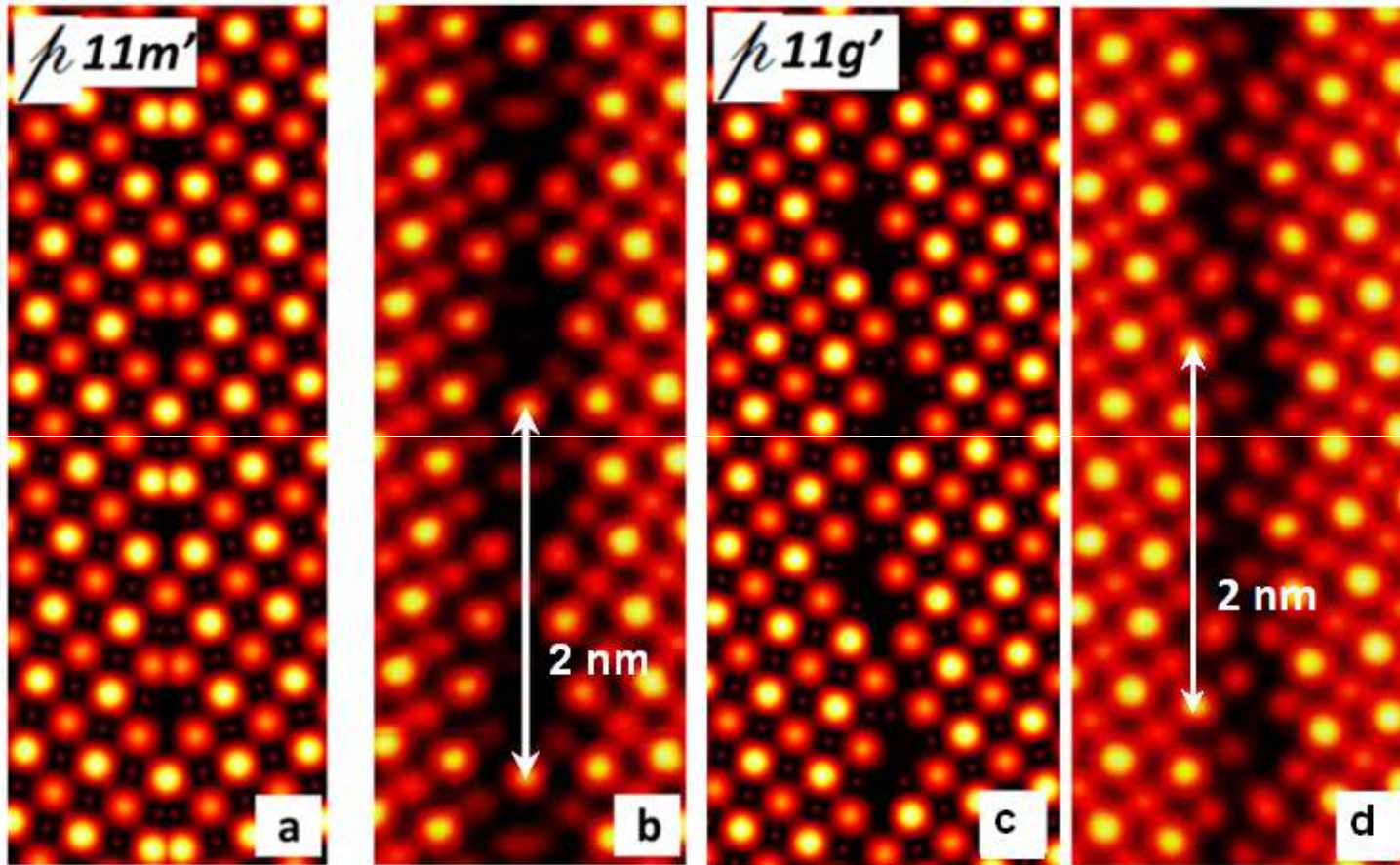
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Comparison to Experiment



Figures a, c are predicted structures
Figures b, d are Z-Contrast STEM images
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Comparison to Experiment



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

The Future of the Project

- MatLab code improvements
- μ 1' boundaries
- Integration into Open Access Crystallography (resources available at nanocrystallography.research.pdx.edu)

Portland State UNIVERSITY

Interactive Databases

Open Access Crystallography

Interactive Databases

COD Mirror

EDU-COD

Crystal Morphology Database

Nano-Crystallography Databases

Wiki Crystallography Database

Nano-Crystallography Group

Tools

YCr 2014

Crystallography in the World

Facets of Electron Crystallography 2010

MRS Tutorial and Seminars 2009

Links

Login

Upload

Crystallography Open Database [Mirror, modified search interface and JSmol/Imol displays] [Search and view](#)

Wiki Crystallography Database [Search and view](#)

EΔU

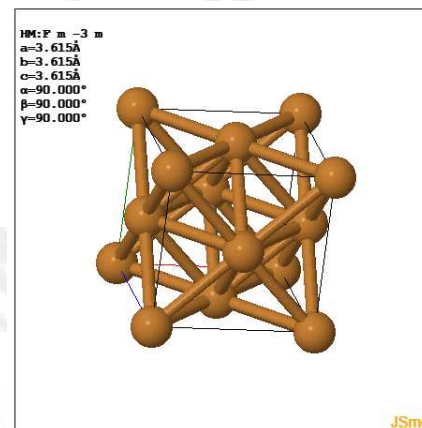
Educational COD offshoot [Search and view](#)

Nano-Crystallography Database [Search and view](#)

BOD

Bicrystallography Open Database coming soon

Crystal Morphology Database [Search and view](#)



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°

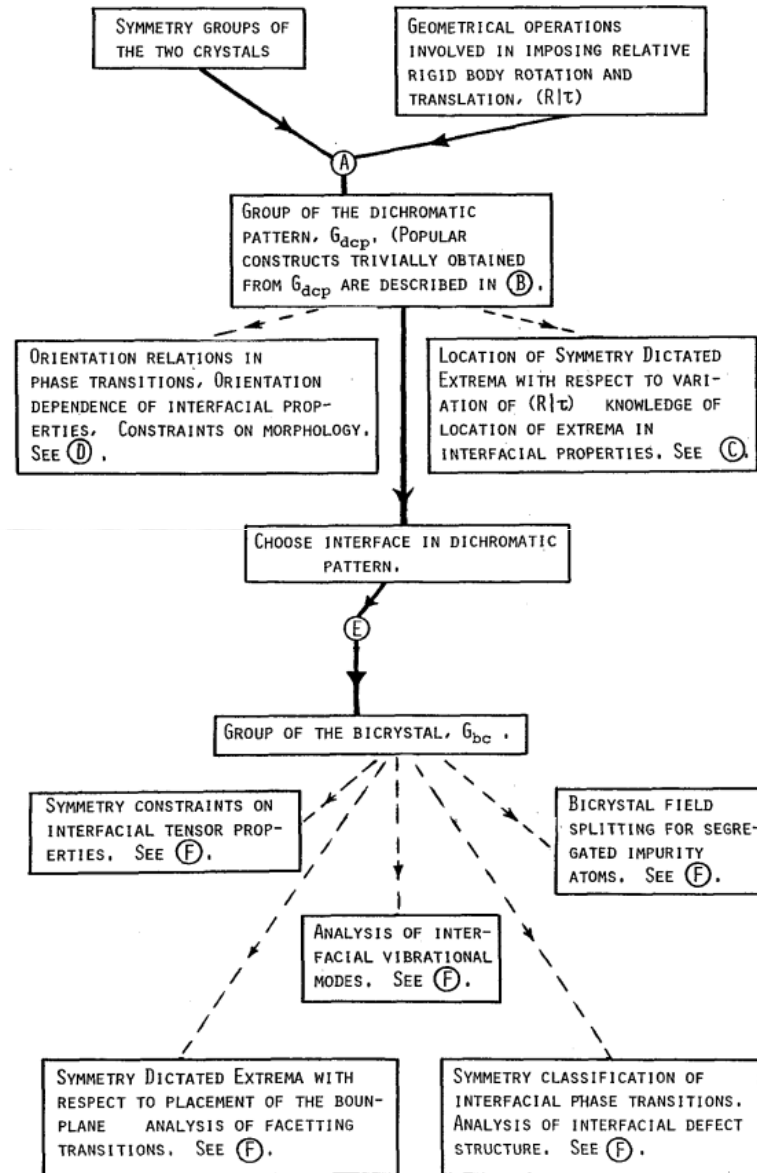
Reset Console

Zoom 150% Zoom 100% Zoom 50%

Draw Planes

None

Thank you for listening!



Shubnikov-
Curie Principal: