Multimodal Modeling of DPC-STEM To Improve Electrostatic Sensitivity

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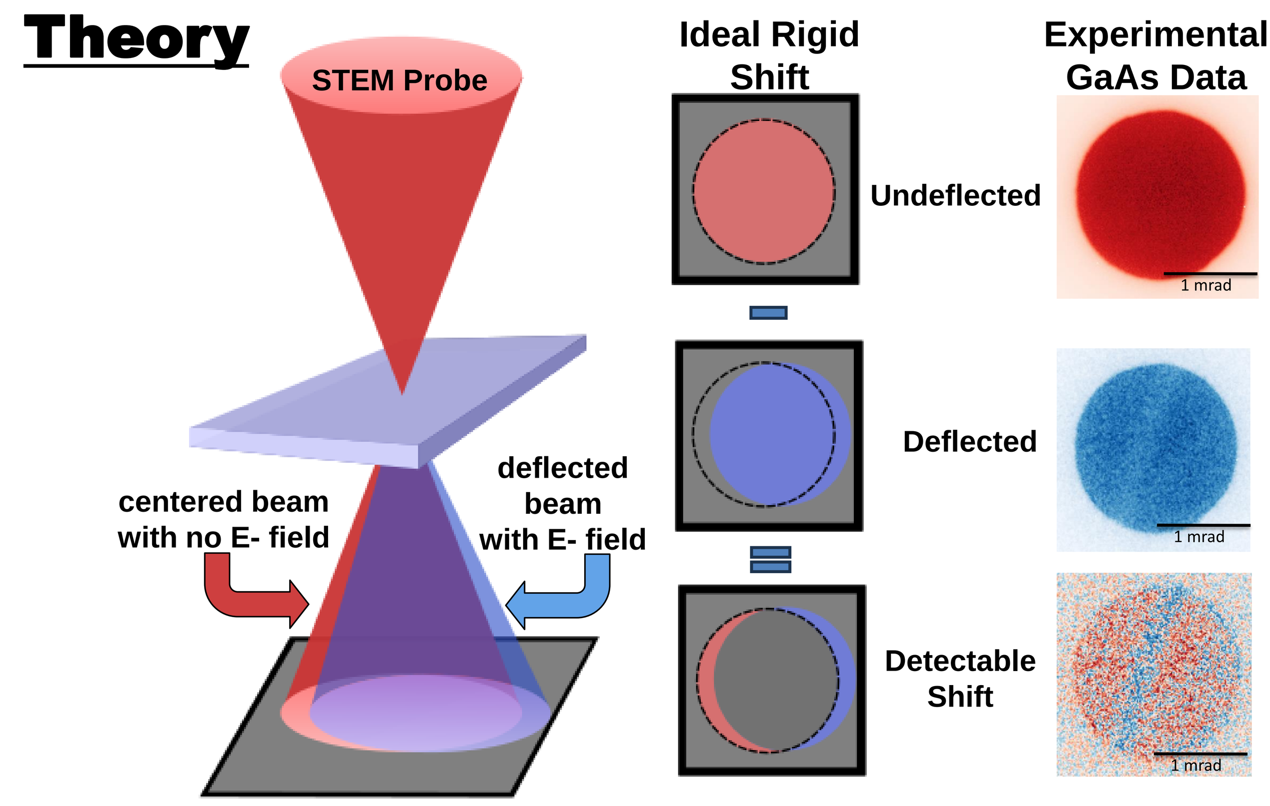
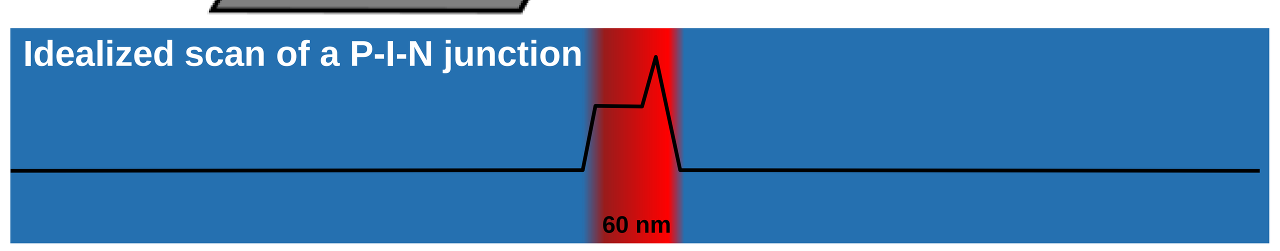
BACKGROUND

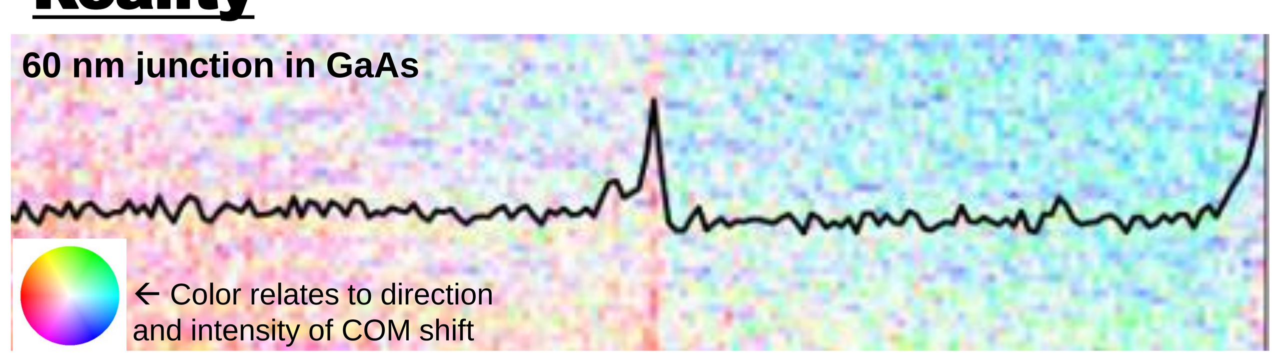
Differential Phase Contrast Scanning Transmission Electron Microscopy (DPC-STEM) is a method by which electrostatic forces can be spatially resolved around atomic-scale defects and junctions.

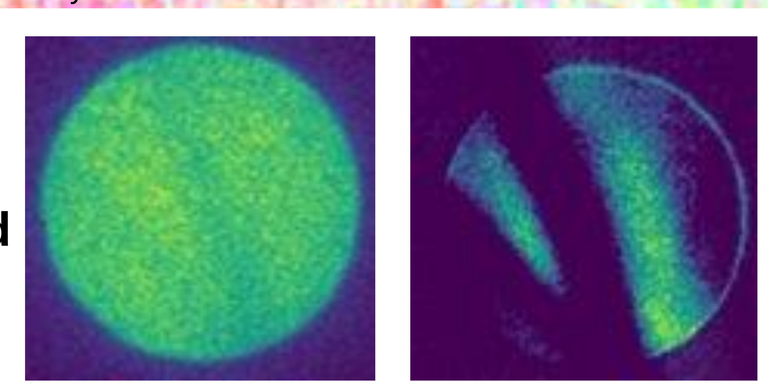
Theory





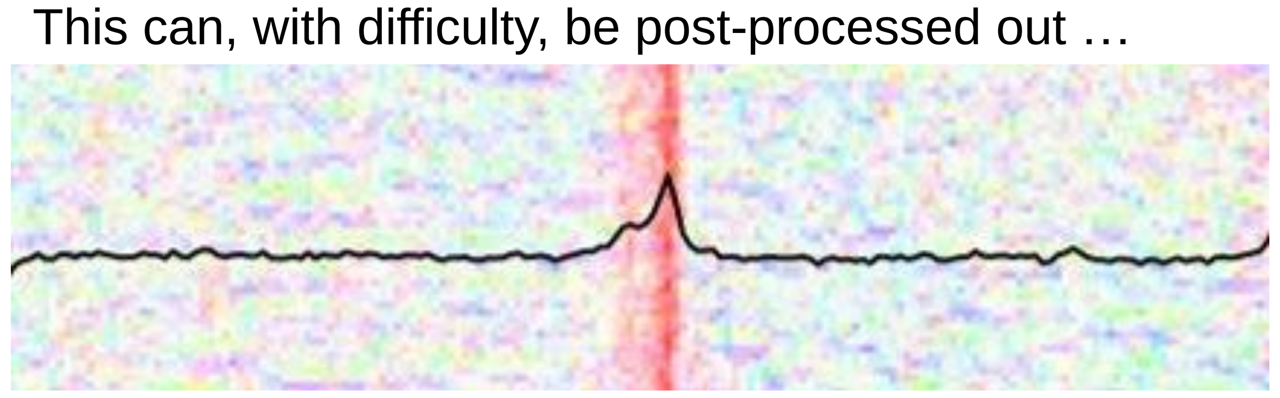
Reality





Inherent diffraction events like Kikuchi and HOLZ lines affect the probe, altering the **Center-of-Mass** (COM) calculation and obscuring the electric field data.

This can, with difficulty, be post-processed out …



Motivation: **What if instead, the diffraction events could be modeled *a-priori* and thus avoided altogether?**

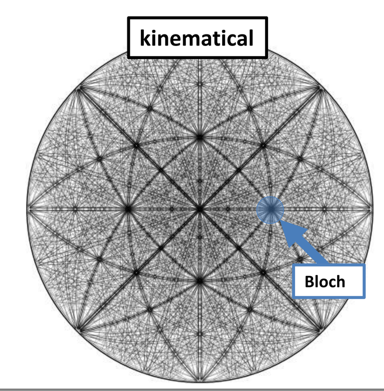
GOAL

Can we quickly predict which specimen orientations will minimize diffraction interference for DPC-STEM?

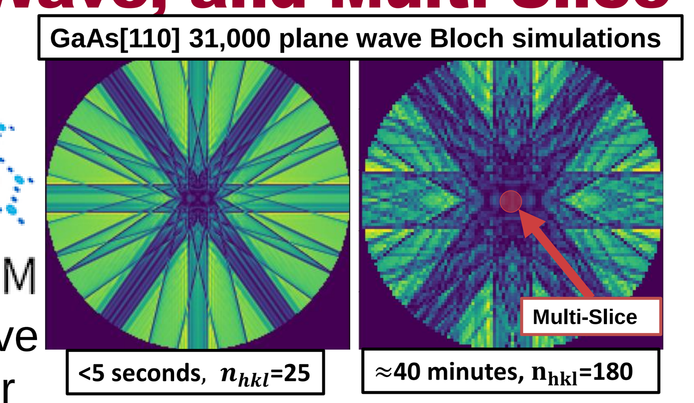
Modeling options: Kinematical, Bloch Wave, and Multi-Slice

kikuchipy

≈ Million simulations/second
No interactions between diffracted beams.
Ideal for building "road map"



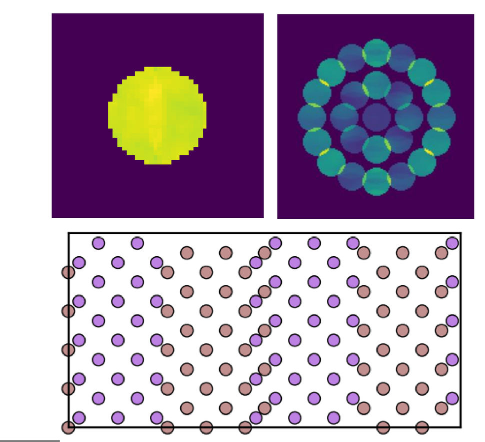
py4DSTEM
Bloch wave simulator



Between 10 and 100,000 simulations/second.
Assumes dynamical diffraction in a homogenous material, Scales $\approx (n^2)\log(n)$ with the number of [hkl] reflections considered.

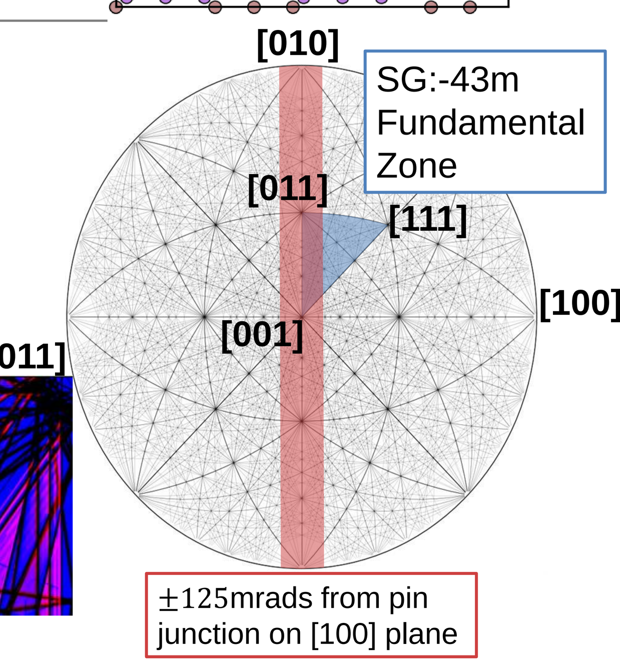
abTEM

Between 1-1000 simulations /hour. The most accurate and most customizable. Can model the whole junction instead of only an ideal crystal.

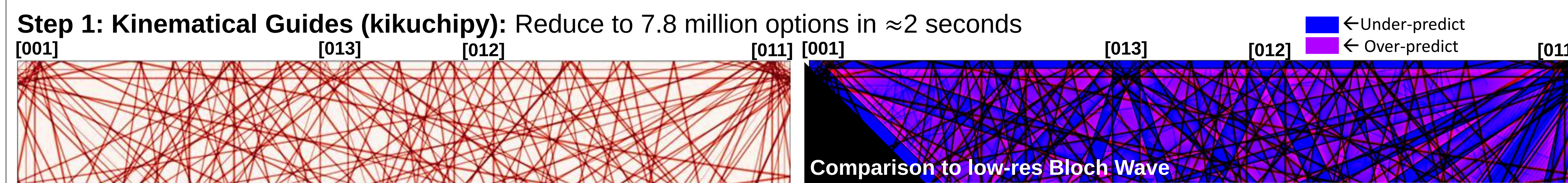


Sequential Search models of increasing fidelity

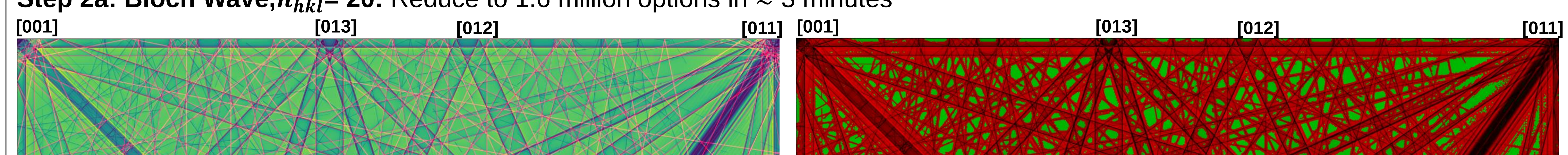
- At a 100 μ-rad mesh, ≈**1 billion** unique probes. Symmetry and experimental constraints reduces this to ≈**9.8 million.**
- This is still too many to fully model, but many options can be eliminated by fast, lower-fidelity checks.



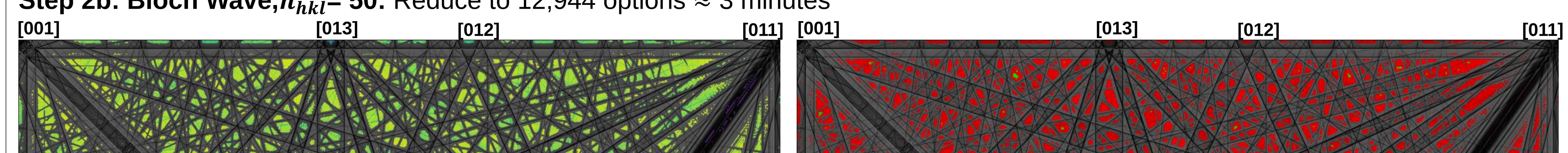
Step 1: Kinematical Guides (kikuchipy): Reduce to 7.8 million options in ≈2 seconds



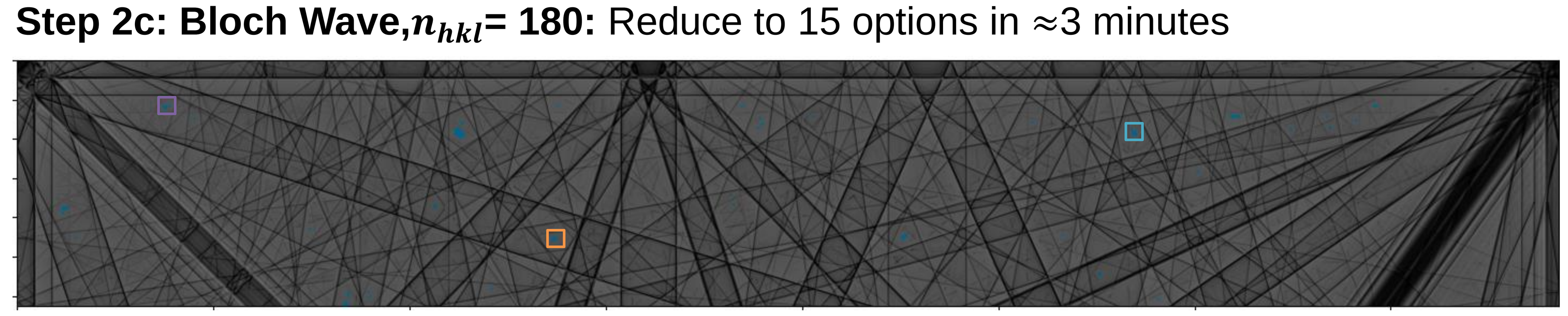
Step 2a: Bloch Wave, n_{hkl}= 20: Reduce to 1.6 million options in ≈ 3 minutes

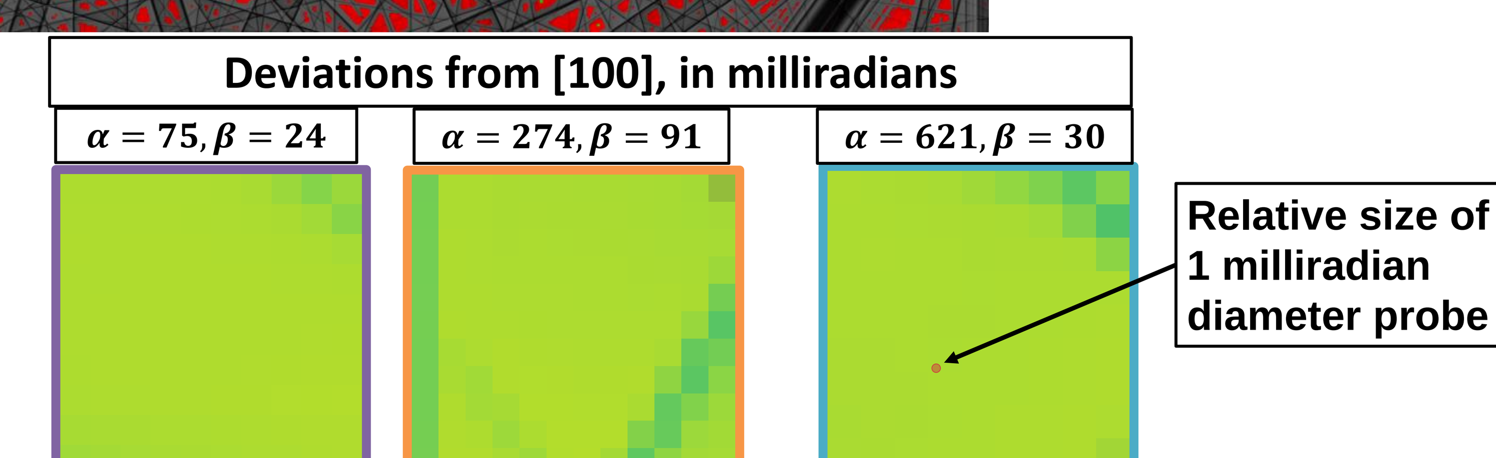


Step 2b: Bloch Wave, n_{hkl}= 50: Reduce to 12,944 options ≈ 3 minutes



Step 2c: Bloch Wave, n_{hkl}= 180: Reduce to 15 options in ≈3 minutes





Next Steps

- **Computational verification via Multi-Slice**
  - Ab-TEM is capable of capturing crucial additional physics (lattice strain at the junction, thermal effects, lens aberrations, etc), and is an ideal final verification step.
- **Experimental verification**
  - Scheduled for mid-August 2025
- **Additional modeling for a radially processed probe**
  - Akin to searching a "donut" of minimal change. Procession is an additional technique for reducing unwanted background signal.
- **Allow real time feedback from microscope to the model, aka "Digital Twin"**

SCAN ME

Link to poster, references, and more on GitHub!