Estimating Accuracy of X-Ray Diffraction Peak Separation

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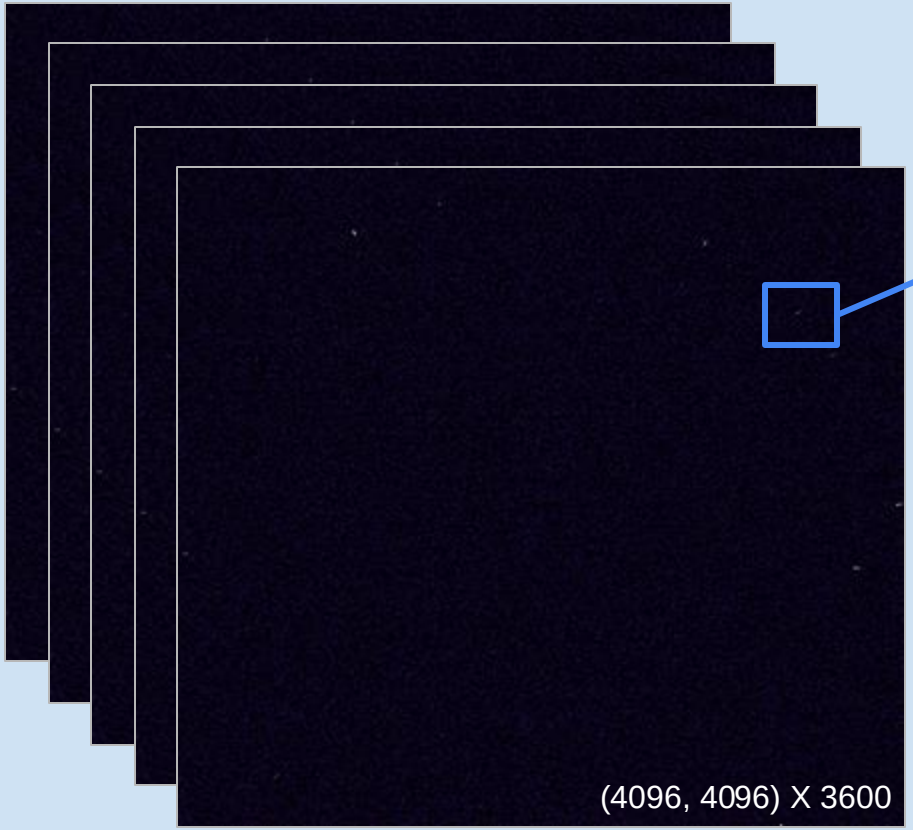
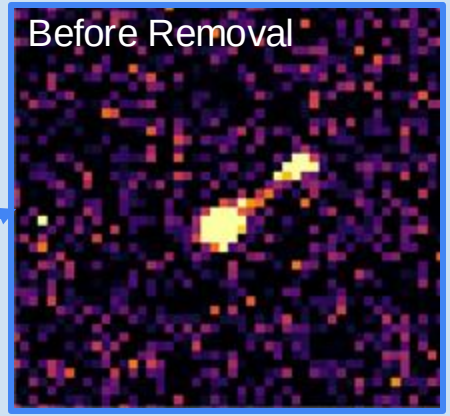
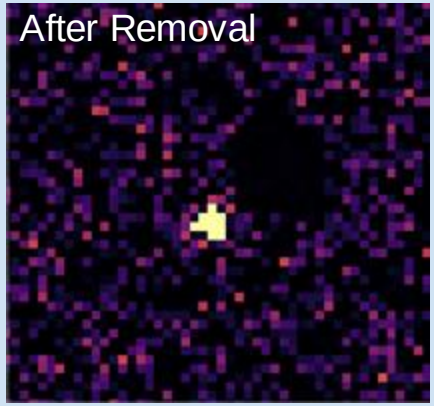
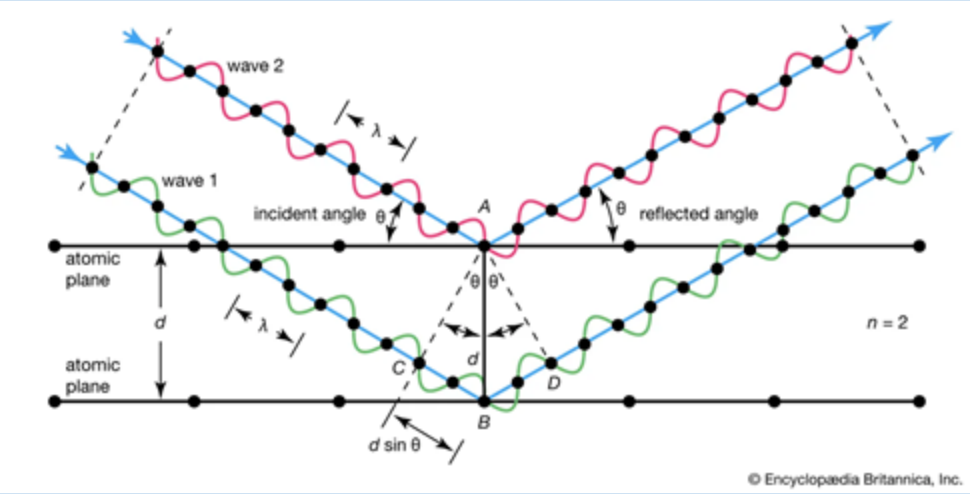
Objective: Test Secondary Peak Removal









Britannica, The Editors of Encyclopaedia. "Bragg law". Encyclopedia Britannica, 9 Aug. 2024, https://www.britannica.com/science/Bragg-law. Accessed 20 August 2024.

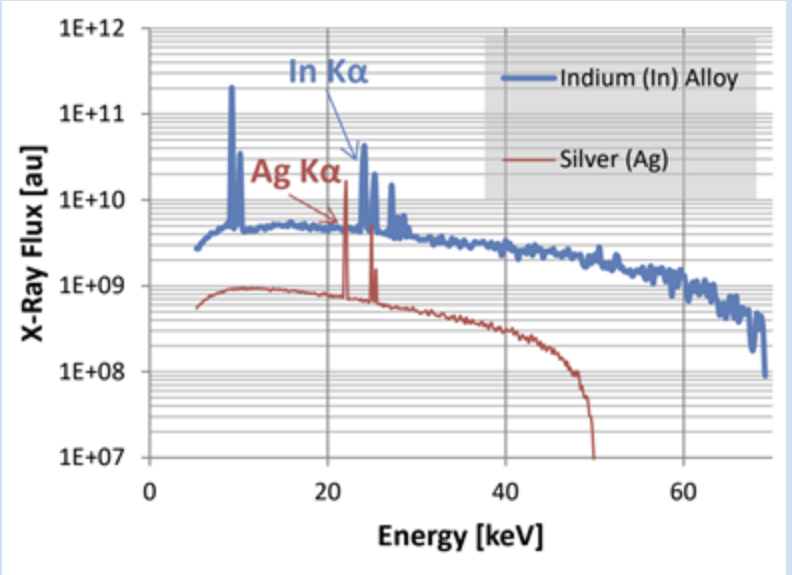
Bragg's Law

$$n\lambda = 2d\ sin\theta$$

Wavelength

Interplanar Spacing

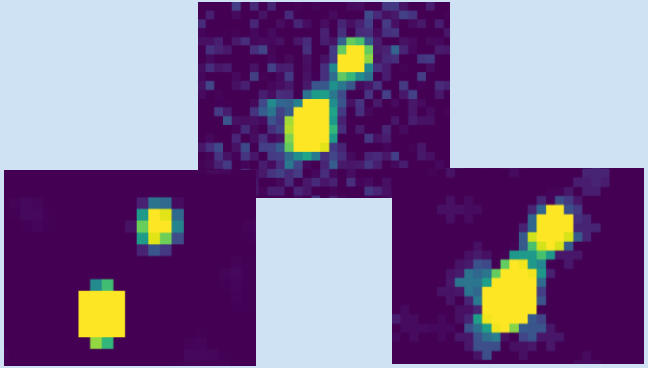
Incident Angle



Two wavelength values **λ** → Two separate scattering angles ***θ*** → Two separate peaks

Methodology

Create synthetic data to model lab dataset



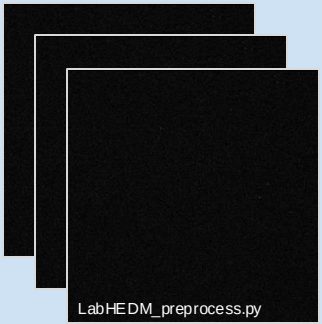
Identify method to segment peaks

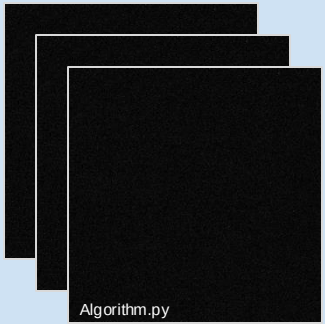
```python
def find_peaks_2d(img, method, method_kwargs):
    if method == 'label':
        # labeling mask
        structureNDI_label = ndimage.generate_binary_structure(2, 1)

        # First apply filter if specified
        filter_fwhm = method_kwargs['filter_radius']
        if filter_fwhm:
            filt_stdev = fwhm_to_sigma * filter_fwhm
            img = -ndimage.filters.gaussian_laplace(
                img, filt_stdev
            )

        labels_t, numSpots_t = ndimage.label(
            img > method_kwargs['threshold']
```

Create algorithm to test secondary peak removal

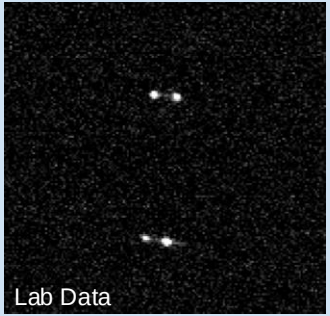


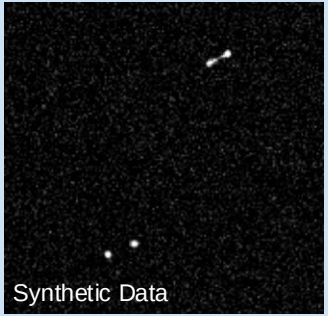


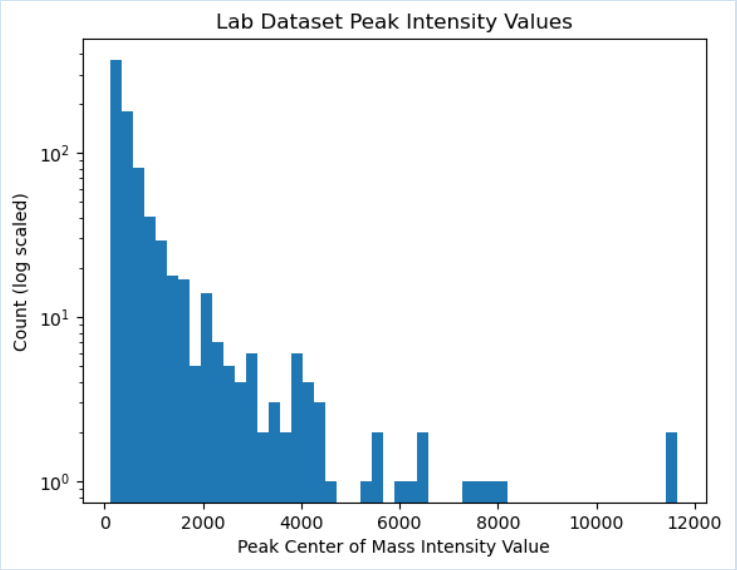
Compare algorithm to preprocessed dataset

Synthetic Data

- **Goal:** Better understand the lab dataset by creating synthetic images that imitate it
- Use synthetic data to simulate edge cases
- Test hexrd's find_peaks_2d() on known peaks
- Find way to accurately simulate background noise





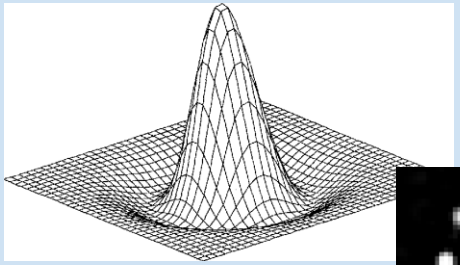



```python
def main():
    num_images = 10 # number of synthetic diffraction images to be generated
    peaks_per_level = 4 # peaks per radius level
    p_second = 1 # probability of secondary peaks being generated for each primary peak
    p_tail = 0.5 # probaility of a pair of peaks having additional "tail" noise
    size_mult = 1 # size multiplier. higher value (ex. 1.3) results in a higher chance of generating large peaks
    generate_images(num_images, peaks_per_level, p_second, p_tail, size_mult)
```

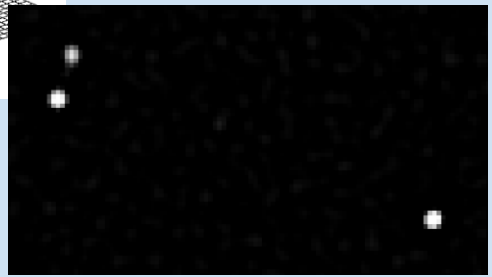
Comparing Filtering Methods

Laplacian of Gaussian

- Second-derivative values after gaussian filter is applied
- Fixed gaussian kernel
- Longer runtime



Sotak, George E. and Kim L. Boyer. "The laplacian-of-gaussian kernel: A formal analysis and design procedure for fast, accurate convolution and full-frame output." *Comput. Vis. Graph. Image Process.* 48 (1989): 147-189.



Opening

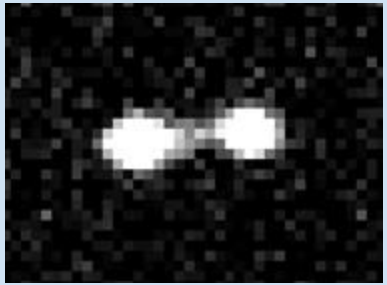
- Erosion of foreground objects followed by Dilation
- Flexibility when deciding kernel
- Inaccurately labels close-together peaks
- Shorter runtime

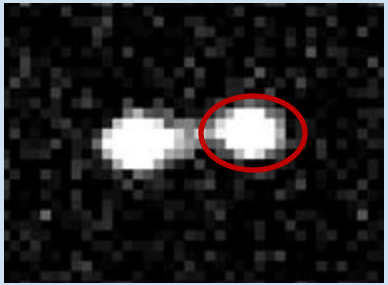
"Morphological Transformations." *OpenCV*, docs.opencv.org/4.x/d9/d61/tutorial_py_morphological_ops.html.

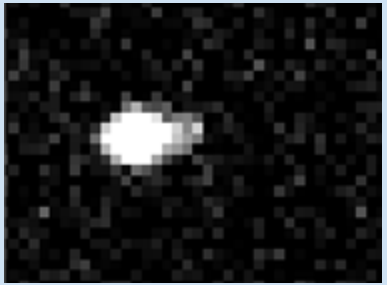
Algorithm

For all images:

1. Segment all peaks and store their locations
2. Compare with neighboring images and separate secondary peaks
3. Remove secondary peaks from image and replace with noise to match background
4. Save new preprocessed image
5. Compare peaks found by Algorithm.py with peaks removed by Lab_HEDM.py



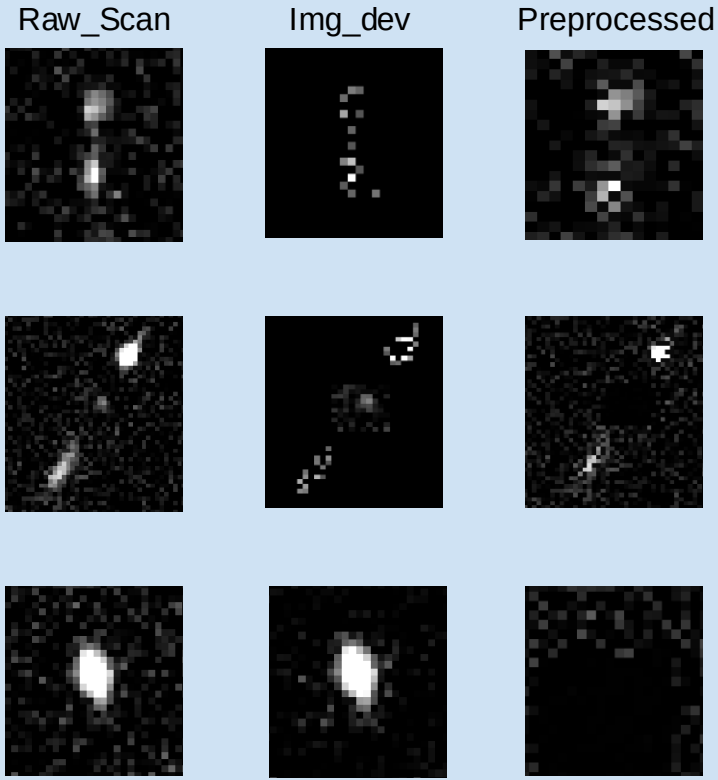




Algorithm Comparison & Results

- Algorithm.py somewhat effective at identifying peaks not completely removed by Lab_HEDM.py
- Estimated secondary peaks incorrectly removed appears to be high
- Saw good results when replacing second peaks with background noise, some debugging still needed

```
100 images tested
approximate secondary peaks identified by LabHEDM.py: 1919
estimated secondary peaks not removed: 72 (3.616273229532898%)
```



Conclusion/Future Outlook

- Saw success learning with synthetic data
  - Future goal: Further explore edge cases to refine peak classification
  - Future goal: Incorporate hardware specification to better simulate data
- Completed a rudimentary algorithm for testing success rate
  - Future goal: Optimize runtime
  - Future goal: Improve peak-finding capabilities
- Devised an effective method for simulating background noise
  - Future goal: Utilize this for to explore alternate peak segmentation methods

Works Cited

Britannica, The Editors of Encyclopaedia. "Bragg law". Encyclopedia Britannica, 9 Aug. 2024, https://www.britannica.com/science/Bragg-law. Accessed 20 August 2024.

Sotak, George E. and Kim L. Boyer. “The laplacian-of-gaussian kernel: A formal analysis and design procedure for fast, accurate convolution and full-frame output.” *Comput. Vis. Graph. Image Process.* 48 (1989): 147-189.

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