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Genuine Parts Award

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Automated Process to Find Facets on Nanocrystals with Stereographic Projection

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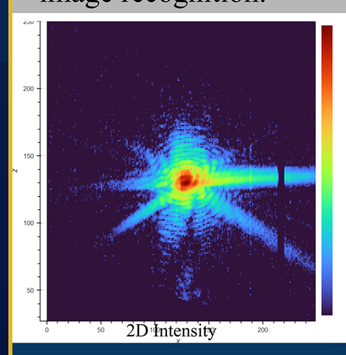
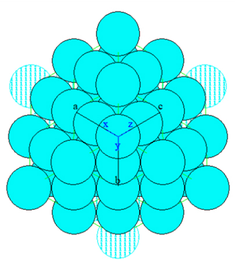
Background

- This research project aims to develop an automated method for determining the morphology and facet orientation nanocrystals.
- The evolution of sample morphology under reaction brings critical information about facet-dependent phenomena.(Embrittlement and Corrosion)
- Some techniques are stereographic projection and image recognition.

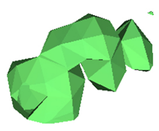




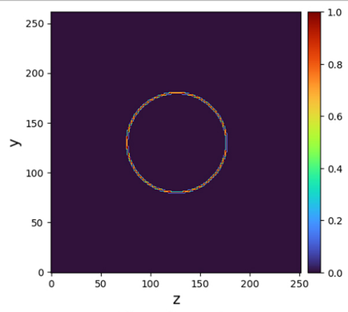
(111) Facet top view

Theory

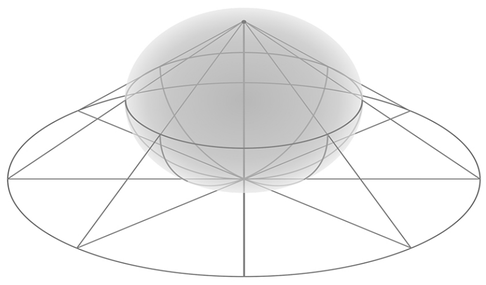
- The theory of our approach is that we can isolate a slice of the 3D intensity data and project it onto a 2D stereographic procjection.
- Then using Python we can analyze the data and assign facets to our crystal.



3D look of intensity(Harder to conceptualize)



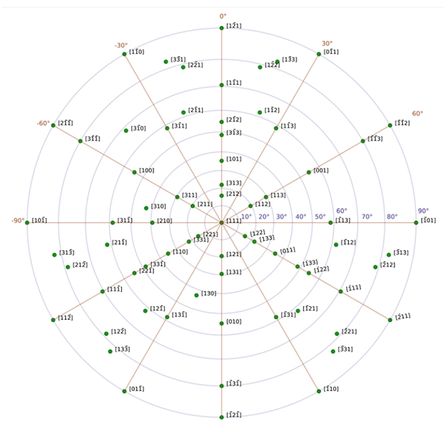
Slice of Intensity



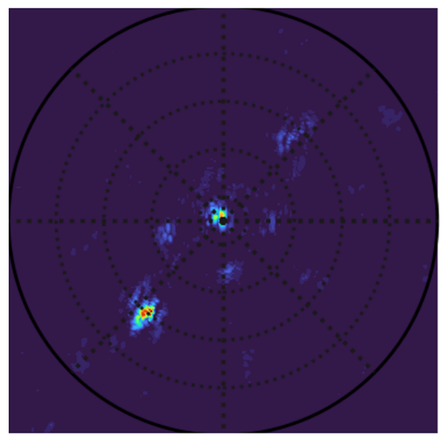
Ex. Stereographic Projection

Mapping

- We define a series of concentric circles with radii of 10, 30, 50, 70, and 90 units to structure our visualization and then change the frame from 3D q-space to a stereographic projection



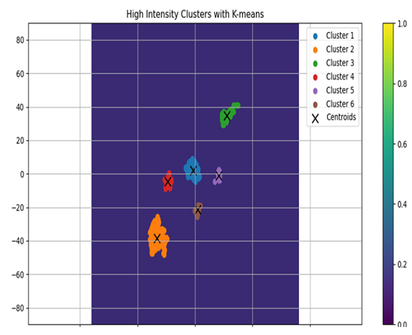
[111] stereographic projection (for a face-centred cubic lattice). The circles describe the angle with the [111] direction from 0 ◦ (centre) to 90◦ (outer-ring).

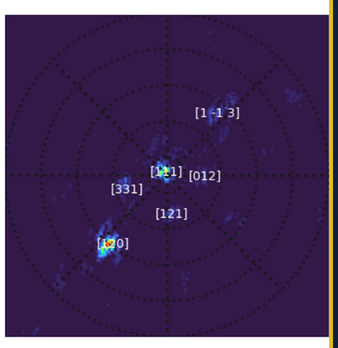


The data mapped on a stereographic projection. (111) Origin

Data

- Use SciPy and K-Means to organize data.
- We identify the clusters and give them azimuthal coordinates.
- Extract the centroids and designate facets
- Map results!!





References

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