STUDY OF CRYSTALLINE AND NON-CRYSTALLINE STRUCTURES USING DIFFRACTION

Studying the crystal structure of a variety of materials

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ABSTRACT

The purpose of the experiment is to determine the crystalline structure of various crystals and to elucidate the structures of non-crystals, possibly determining whether or not they are similar to existing known crystals. By using x-ray crystallography techniques to produce a distinct diffraction pattern, the inner structure of the crystal can be observed indirectly when it is otherwise difficult to quantify on a macroscale. This method forces incident beams through a sample which, through the shape of their periodically recurring unit cells, diffracts the light in a measurable pattern; post analysis of the distance between the resultant diffraction pattern conveys the unit cells' form. Using x-ray diffraction, one can understand these constituent atomic compositions and structures, learn how they correlate to certain properties of the aggregate particle, and draw connections between them and dissimilar elements.

This research was made possible through the Exemplary Student Research Program, supported by Argonne National Laboratory's Educational Programs (HRS), the APS User Office, Bolingbrook High School teacher Lois Emde, and supported by the Argonne National Laboratory, beamline 16 ID-D is supported by NSF grant and DOE grant. Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

MOTIVATION

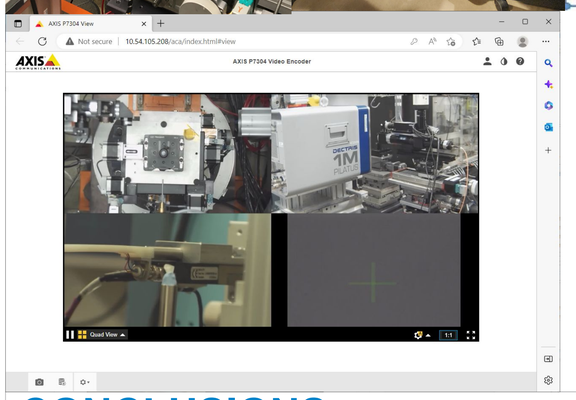
This experiment gives us a better understanding of how to interpret diffraction patterns and how certain factors influence the patterns. Normally, one starts with a diffraction pattern and works from there to attain the lattice parameter, atomic position, and type of atoms, all critical identifying information about the unit cell. However, this requires a strong background in understanding what causes specific diffraction patterns. As we lack this background, we started in the reverse, taking known materials with known unit cells and examining their diffraction patterns to determine how their properties contributed to various anomalies or lack thereof. This gives us a better understanding of future diffraction experiments.

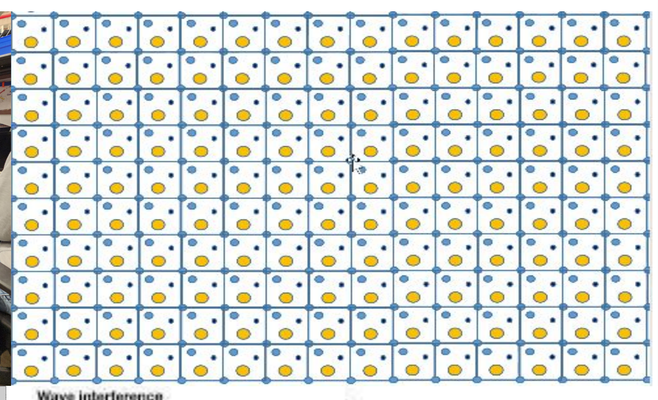
METHODS

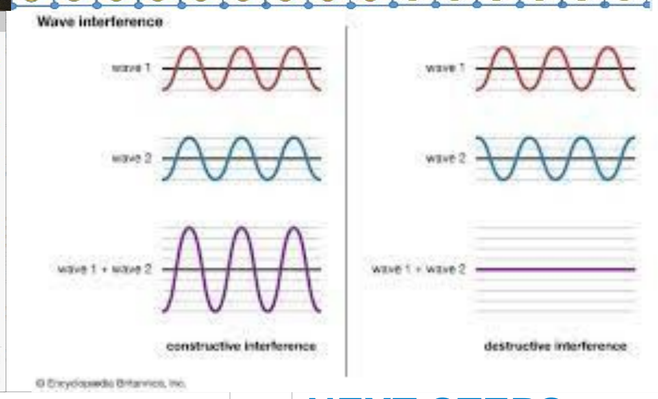
In optics, diffraction is the bending of light as it travels through any narrow aperture. Knowing this property of light and that the wavelength of x-ray photons is the same order of magnitude as the spacing between atoms in a crystal, it is possible to diffract x-ray light through any lattice structure as an x-ray will be absorbed then re-emitted by individual electrons in the lattice. The repeated simultaneous occurrence of this scattering event, characterized as Bragg scattering, creates a series of beams exiting at various angles which constructively or destructively interfere with each other. The resultant intensities at various locations can be mapped onto a screen to produce the sample's diffraction pattern, and the obtained data can help determine certain qualities of the crystal structure.

METHODS (Continued)

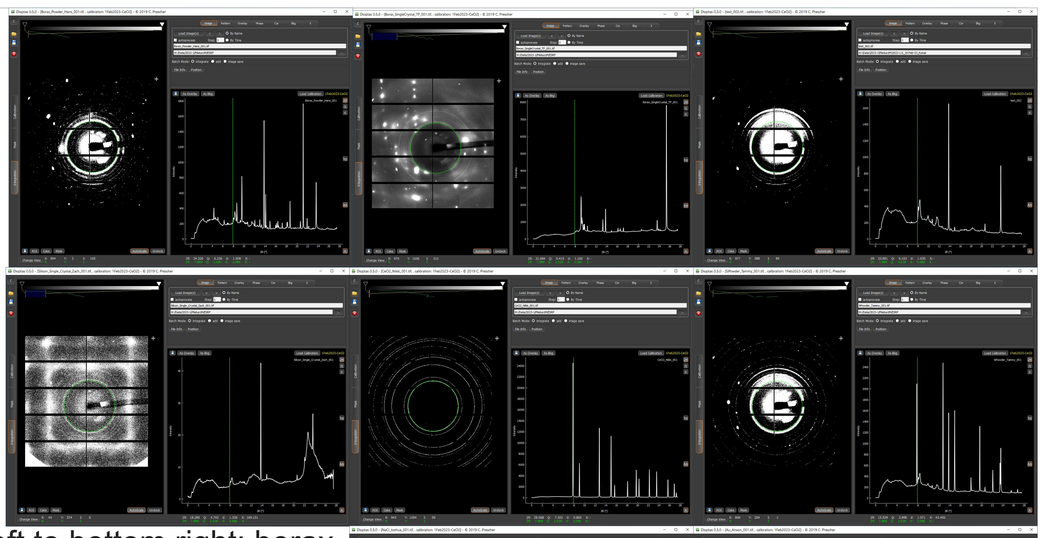
1. Unseal door
2. Fix sample onto adjustable kinematic mount.
3. Search out hutch, seal door.
4. Remotely align the PIN diode.
5. Align the sample on x, y, and z axes and adjust using scanner.
6. Release x-ray beams for 5 seconds.
7. Load diffraction pattern, adjust intensity.
8. Download and save in an online document.

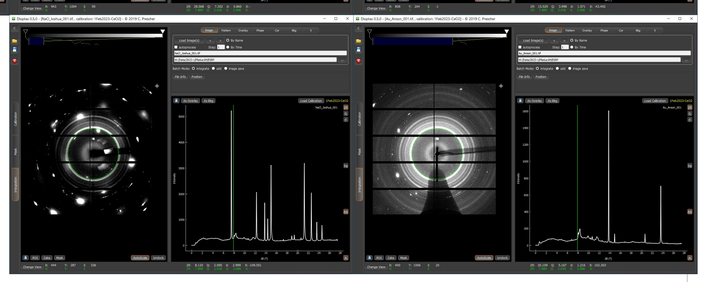






DATA





From top left to bottom right: borax powder, borax single crystal, calibration of glass tube, Germanium single crystal wafer, cerium dioxide, silicon powder, NaCl crystals, and gold wire.

The width, height, number, and angle value of peaks all contain information about the material. When calibrated, the software determines the position which will produce the maximum constructive interference. In a perfect crystal powder, there will be small crystallites in every orientation, producing all angles of emitted photons from the sample, which appear on the detector as a circle. This requirement to have crystallites in every orientation can explain some irregularities. For example, a number of large chunks of salt were used for the NaCl sample. Because this wasn't a powder, there are some spots in discontinuous circles where the Bragg condition was fulfilled but not in every orientation. The gold wire also contains certain irregularities in the pattern. This is due to preferred orientation of the crystals as the gold is drawn into a wire.

CONCLUSIONS

The results of this experiment demonstrate that various materials with known and different structures produce different diffraction patterns, and that these diffraction patterns reflect, through various properties of the peaks, information about the structure of the experimental material. The patterns affirmed our knowledge that the more perfect a powder a sample was, the more contiguous the rings would be, and that irregularities in the pattern carry information about flaws in the crystal structure of the sample.

NEXT STEPS

Not only would the use of a broader range of materials allow for more information to analyze about otherwise unknown structures, but it would also strengthen the bond between the aforementioned concepts. Furthermore, determining the use of some crystals already employed may allow such applications to be extended to crystals of similar structures and constitution, and processing data through functions such as the formula for diffraction patterns would provide numerical elements to supplement our findings.

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