

## Tools for Visualizing and Understanding the Structure of Crystalline Ceramics: Expected Course Outline

*Learn about the essential ceramic crystal structures and how we can analyze these structures through X-ray diffraction!*

*X-ray diffraction has been a mainstay of ceramic characterization since its inception. Powder diffraction allows us to determine and refine the crystal structure of ceramics to determine things like lattice parameters, site occupancy, thermal displacement parameters, texturing, weight fraction of multi-phase mixtures, and much more.*

*In recent years, python-based GSAS-II has made this process easier than ever. At the same time, visualization packages like VESTA and Python's Matplotlib allow us to visualize the results of Rietveld refinement and display structures in intuitive and beautiful ways.*

<u>Class Dates</u>	<u>Topics / Activities During Class</u>	<u>Assignments, Notes, Demos</u>
1) 09/17/2025	General introduction to the Rietveld method, Detailed Rietveld refinement tutorials on powder and polycrystalline materials using GSAS-II (pyGSAS), Quantitative phase analysis tutorials and example, Quantitative analysis of amorphous content in multiphase mixtures	Follow along with the refinements by downloading the refinement slides, step-by-step instructions, and diffraction files from <a href="https://github.com/sp8rks/Ceramic_Rietveld_Refinement">https://github.com/sp8rks/Ceramic_Rietveld_Refinement</a>
2) 09/18/2025	Overview of prototypical ceramic structures, General overview of the VESTA software package including tutorials for bonding, planes/directions, multi-phase interfaces, simulated XRD patterns, charge density difference plots, tutorial of Python's Matplotlib library for effectively visualizing diffraction data	Download structure files from <a href="https://github.com/sp8rks/Ceramic_Rietveld_Refinement/tree/main/structure%20examples">https://github.com/sp8rks/Ceramic_Rietveld_Refinement/tree/main/structure%20examples</a>

### Additional References or Resources:

1. Course materials are available for free on GitHub [https://github.com/sp8rks/Ceramic\\_Rietveld\\_Refinement](https://github.com/sp8rks/Ceramic_Rietveld_Refinement)