AUTONOMOUS EXPERIMENT DESIGN: Machine-Learning Guided X-Ray Powder Diffraction for Efficient Phase Tracking

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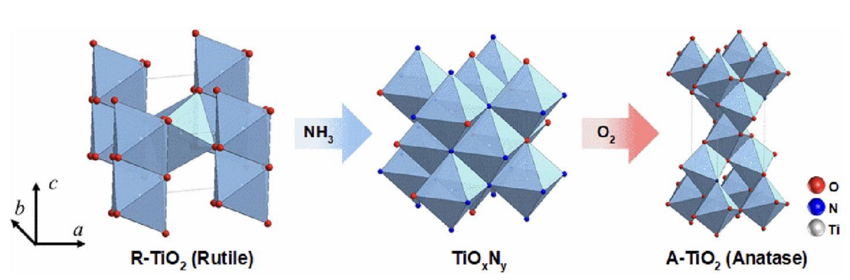
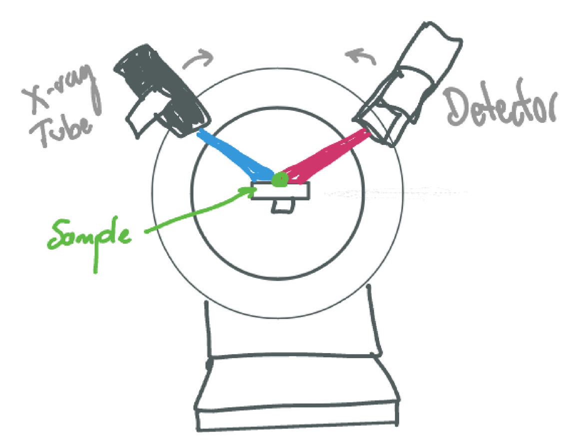
INTRODUCTION

- **Motivation:** Synchrotron experiments demand time, resources, and constant operator input.
- **Goal**: Develop a Python-automated, ML-driven system for autonomous beamline control.



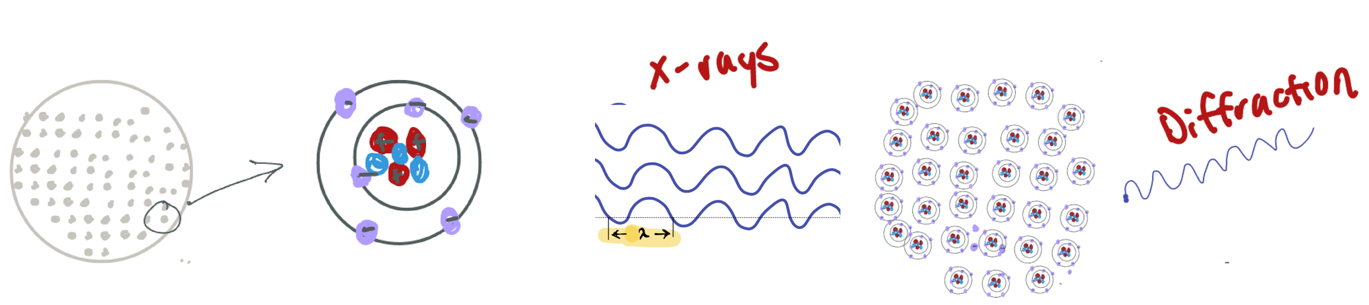


Research Questions

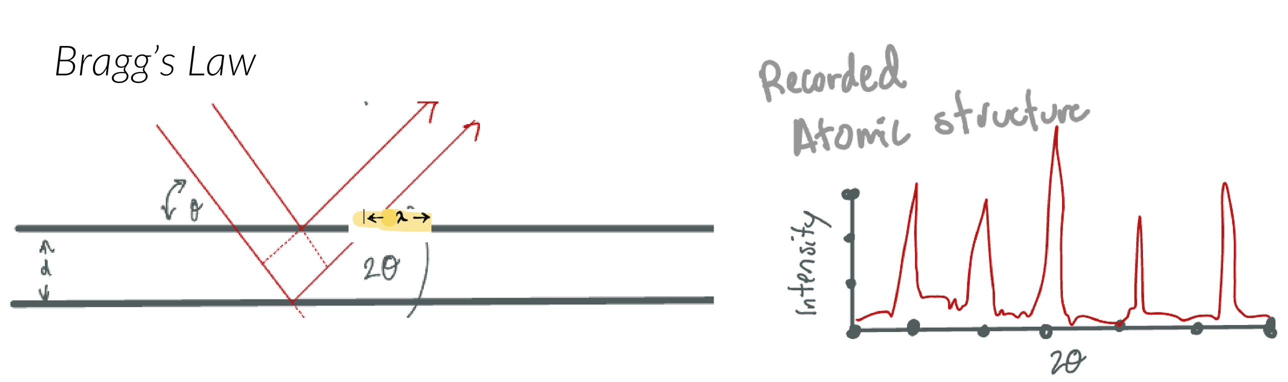
1. How can we direct the computer to scan only information-rich regions?
2. Can intelligent scan selection save time, storage, and materials *without losing structural data*?

BACKGROUND

X-rays have wavelengths comparable to atomic spacings, making diffraction a powerful probe of crystal structure.



Powder diffraction: X-rays scatter from tiny grains; a two-detector setup records unique diffraction patterns.

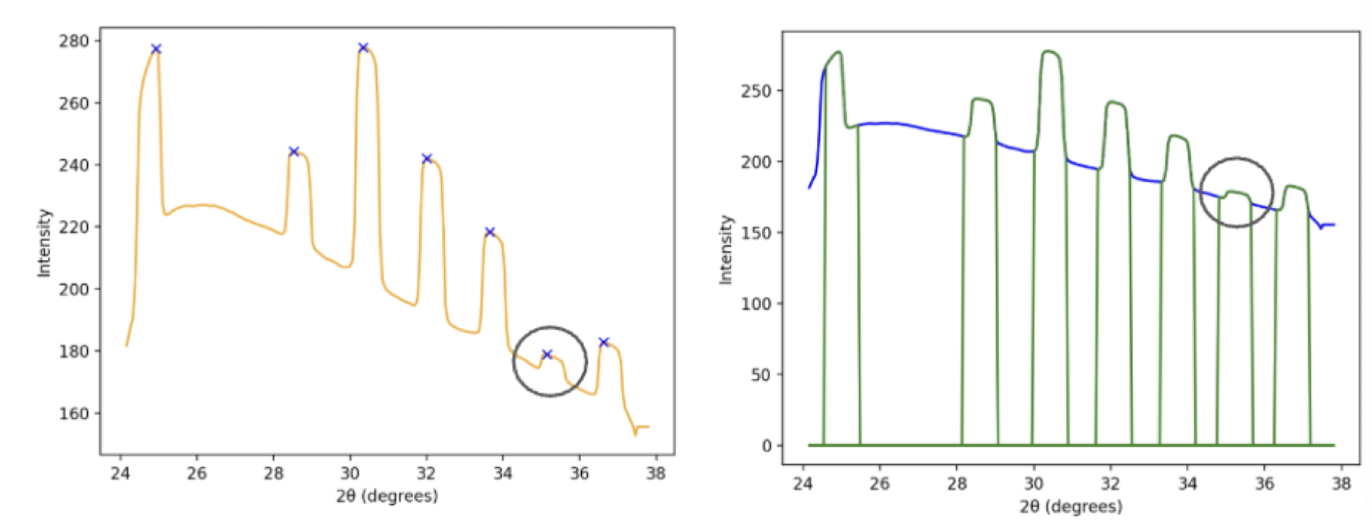


References: [1] Cullity & Stock, *Elements of X-Ray Diffraction*, 3rd ed., 2014. [2] Diebold, *Surf. Sci. Rep.*, 48, 53–229 (2003). [3] Sivia & Skilling, *Data Analysis: A Bayesian Tutorial*, 2nd ed., 2012. [4] SSRL BL 2-1 User Documentation, 2025. [5] Pease, D. M., "What is X-Ray Diffraction?" YouTube, 2020.

METHODS

Workflow Development

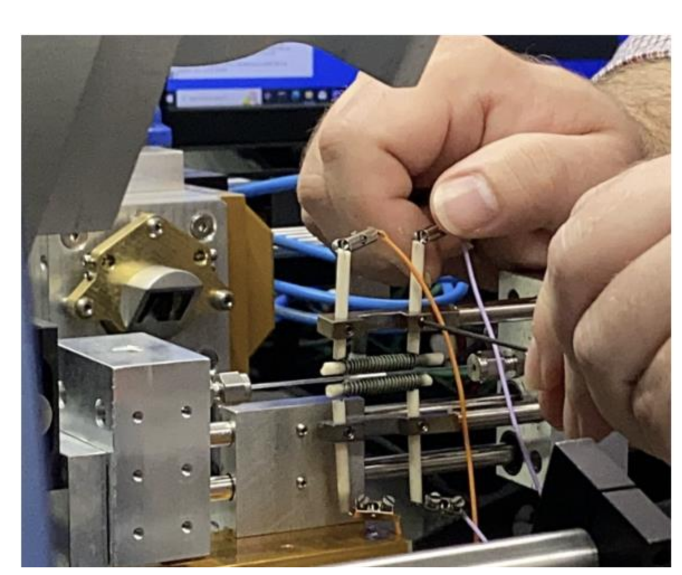
- Six scanning strategies (top peaks, intensity change, shifting, growth, shrinkage, max-change regions).

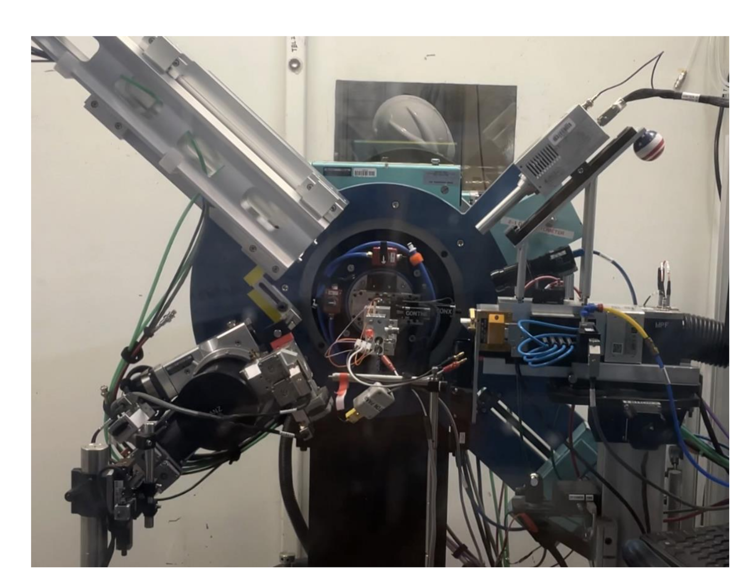


- Integrated low-res → 1D patterns; local maxima & peak thresholds.
- High-res scans only where meaningful change is expected.

Beamline Setup (SSRL 2-1)

- TiO_2 nano powder in quartz capillaries.
- Controlled heating (20 °C → 820 °C).
- Dual-detector system: fast continuous monitoring + high-resolution targeted scans.

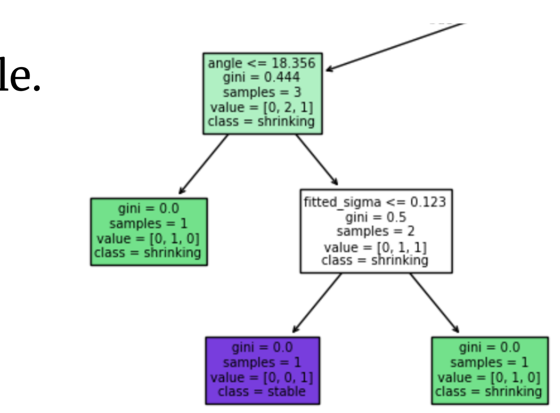




RESULTS

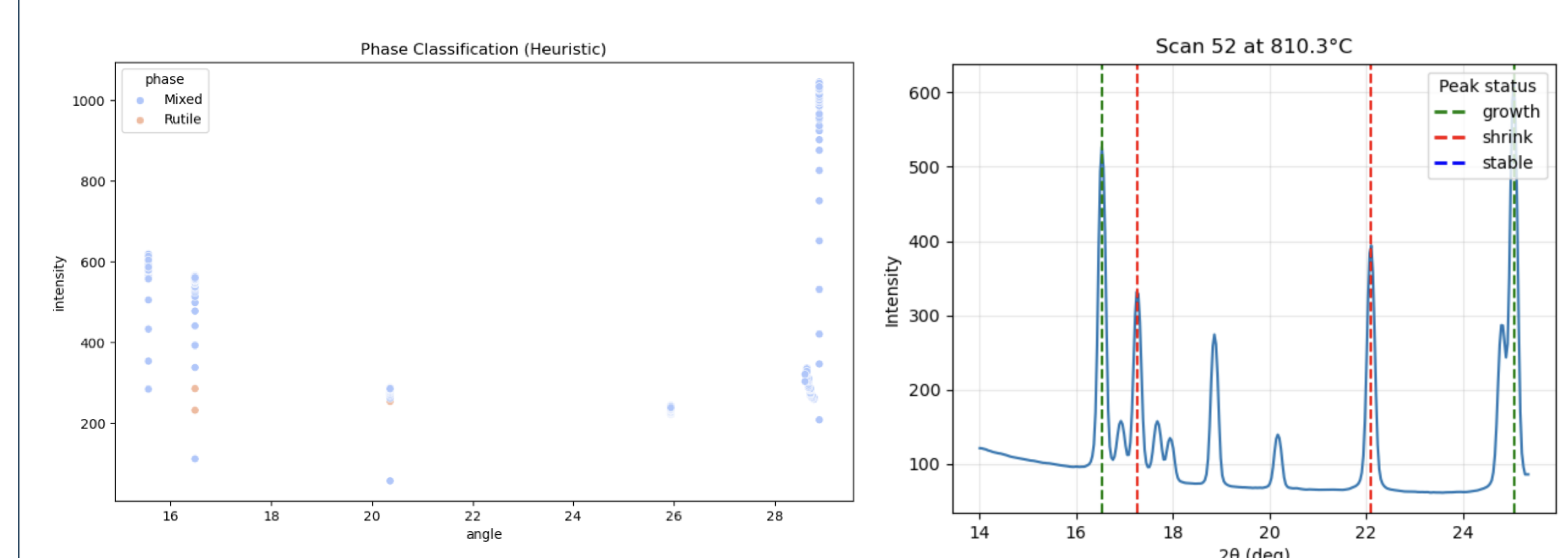
Algorithm Improvements

- Peak classification: growing, shrinking, stable.
- Phase assignment (anatase vs rutile).
- Gaussian fits for precision.



Machine Learning Integration

- **Decision Tree Classifier** trained on labeled peaks.
- Prioritized scans of relevant phase changes.



- **Beamtime efficiency ↑**: Reduced unnecessary scans.
- **Phase tracking**: Captured anatase → rutile transition.
- **High-quality data**: Combined raw intensity + categorical descriptors.
- **Adaptability**: Framework extendable to other materials.

CONCLUSION

- ML-driven scan selection improves efficiency and scientific value of synchrotron experiments.
- Interpretable models (decision trees) enhance reliability and real-time decision-making.

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