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Machine Learning-Based XRD Analysis for Nanostructure Characterization

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Problem statement

- High-throughput XRD produces hundreds/thousands of diffractograms
- Traditional methods (CMWP, WPPM) are accurate but slow and computationally intensive
- Manual analysis is a bottleneck in materials discovery

ML-Based Solution (ML-XLPA)

What is ML-XLPA

- Uses machine learning to predict microstructural parameters directly from XRD patterns.

- Fast: reduces analysis time from hours/days to second.

How it works

Combines:

1. Physical diffraction modeling (for training data)
2. Background subtraction (e.g., ARPLS)
3. ML regression (e.g., XGBoost)

Limitations & Goals

Limitations

- Current ML-XLPA works only for cubic (FCC) materials.
- Not yet extended to hexagonal (HCP) structures.
- Real data challenges: noise, peak shifts, overlapping peaks.

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Goals of project

- Extend ML-XLPA to HCP and multiphase materials.
- Improve preprocessing for noisy/real data.
- Enable fast microstructure mapping for combinatorial libraries.

Working Plan

This semester

- Focused on theoretical understanding of ML-XLPA foundations.
- Studied diffraction modeling, background correction, ML methods.
- No implementation yet—groundwork laid for next phase.

Next semester

- Implement ML-XLPA for HCP structures.
- Improve handling of experimental artifacts and multiphase systems
- Test on synthetic and experimental datasets

Why it matters?

- Enables high-throughput microstructure mapping
- Supports accelerated materials discovery (e.g., composition–property links).

Future impacts

- Can be applied to complex alloy, ceramics, batteries, etc
- Bridges XRD experiments with ML-driven analysis.

Thank You

References

[1] P. Nagy et al. “Machine learning-based characterization of the nanostructure in a combinatorial Co-Cr-Fe-Ni compositionally complex alloy film.” Nanomaterials, 2022.

[2] B. Kaszas et al. “Diffault: Simulation of diffraction patterns of faulted crystals.” SoftwareX, 2024.

[3] G. Ribarik et al. “Correlation between strength and microstructure of ball-milled Al-Mg alloys determined by X-Ray diffraction.” Materials Science and Engineering: A, 2004.

[4] S.-J. Baek et al. “Baseline correction using asymmetrically reweighted penalized least squares smoothing.” Analyst, 2015.

[5] P. Nagy et al. “Microstructure, hardness, and elastic modulus of a multibeam-sputtered nanocrystalline Co-Cr-Fe-Ni compositional complex alloy film.” Materials, 2021.

[6] J. Gubicza. X-Ray Line Profile Analysis in Materials Science. IGI Global, 2014.