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Deep Learning for the Analysis of Spectroscopic Data

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Abstract

Different measurement techniques in the field of material science generate a large amount of data to evaluate, but still require manual intervention for analysis of the measured signals. For example, in-situ X-ray diffraction (XRD) measures a crystalline powder sample under varying conditions and generates hundreds of one-dimensional signals. Currently, the evaluation process involves a two-stage approach of identifying different phase variants before a refinement model fits the exact parameters. Alternatively, the use of neural networks for the analysis of powder XRD scans proves highly accurate and applicable for measurement techniques that require high-throughput evaluation methods. Similarly, neural networks have been shown to remove artifacts from the spectroscopic signals and work even for two-dimensional diffraction data. We demonstrate that neural networks are well suited to be used with spectroscopic and diffraction data from different techniques within the material science domain and are looking for projects that generate and provide such data.

Data Generation XRD

Crystallite Sample

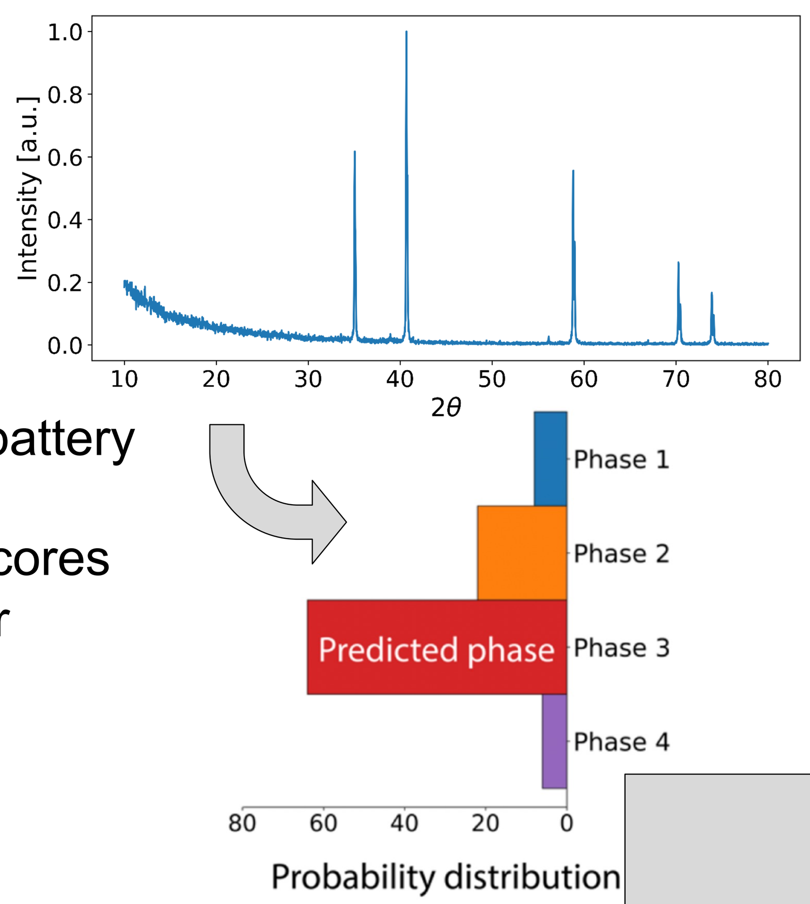
Sample Preparation

1D/2D Scan

Source: Bruker

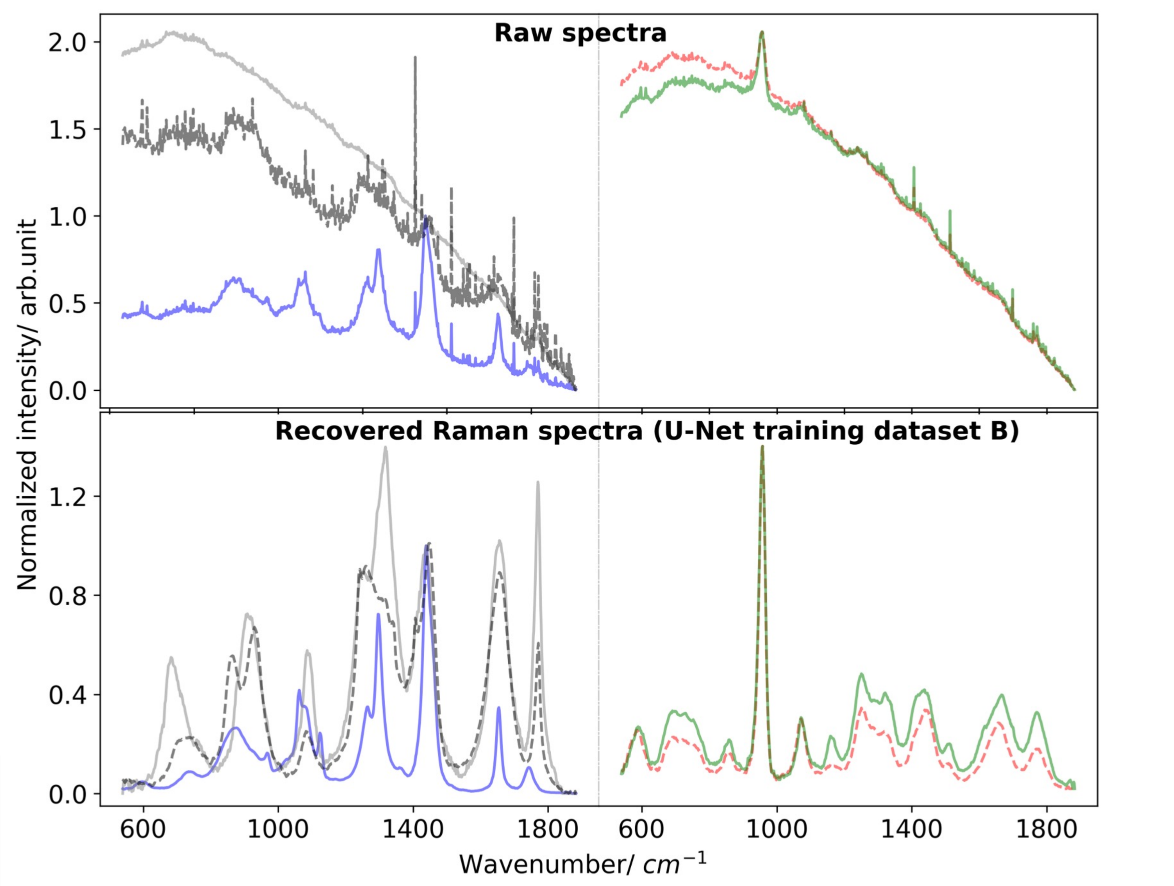
Classification / Identification

- Identification of single-phase or multi-phase diffraction signals
- Applied to different datasets, e.g., iron ores and Mn-based battery cathode materials with high accuracy scores
- Iterative approach for multi-phase samples



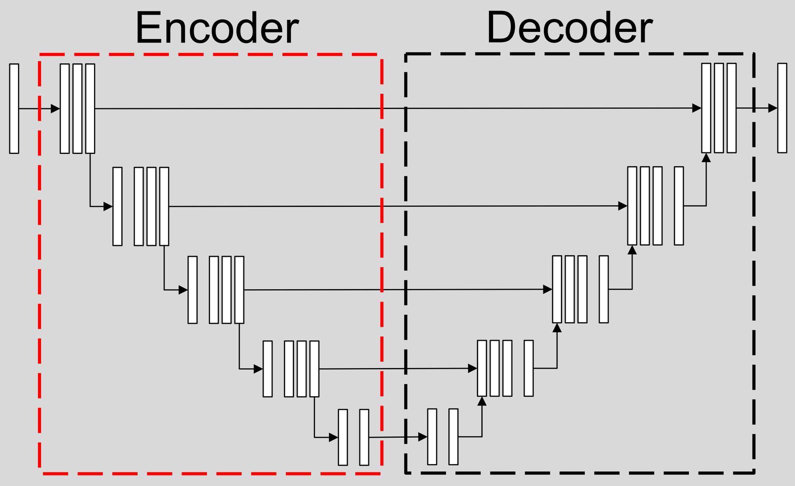
Schuetzke et al., 2021, Enhancing deep-learning training for phase identification in powder X-ray diffractograms
Szymanski et al., 2021, Probabilistic Deep Learning Approach to Automate the Interpretation of Multi-phase Diffraction Spectra

Denoising and Baseline Correction



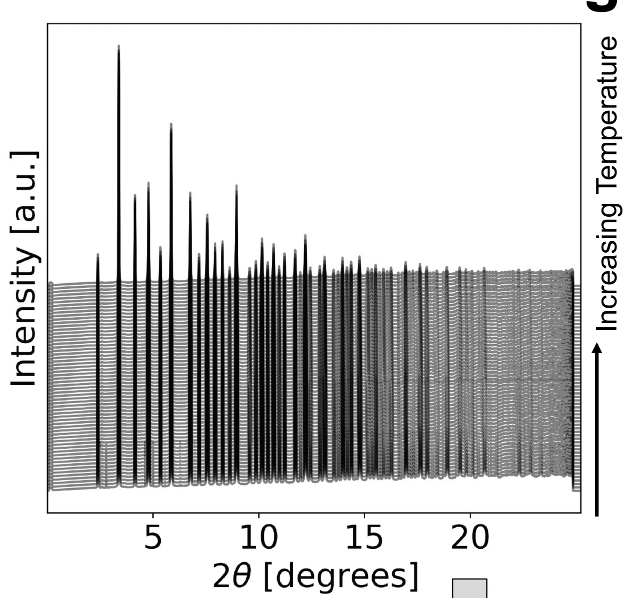
Gebrekidan et al., 2021, Refinement of spectra using a deep neural network: Fully automated removal of noise and background

Deep Learning

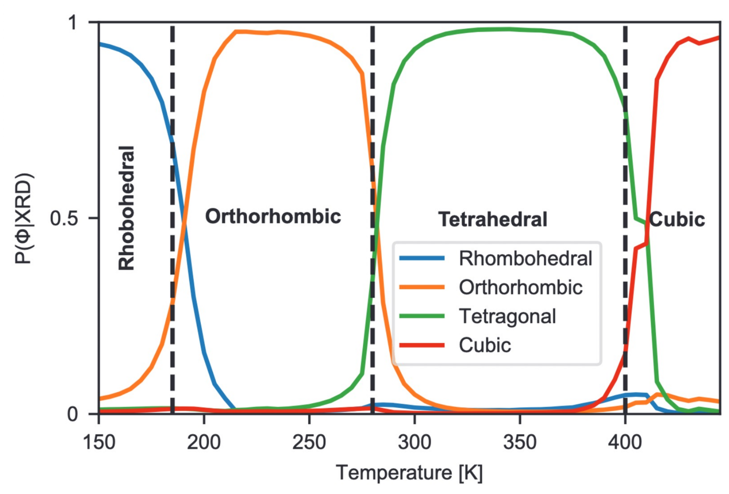


U-Net structure

In-situ High-Throughput

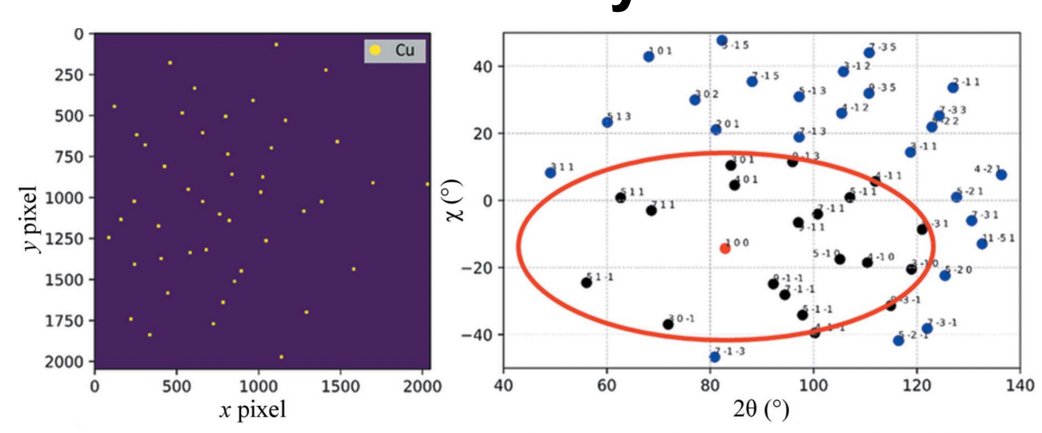


- Determination of present phases in relation of temperature
- More robust than traditional Rietveld refinement

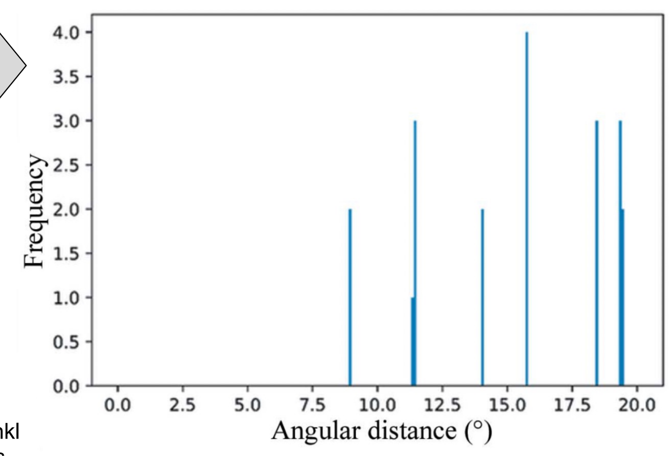


Maffettone et al., 2021, Crystallography companion agent for high-throughput materials discovery

2D XRD Analysis



Laue spots represented in the angular space (scattering angles 2θ, χ)



- Mapping of 2D XRD Laue images to 1D physical features
- Automatic (hkl) indexing of Laue diffraction spots

Purushottam Raj Purohit et al., 2022, LaueNN: neural-network-based hkl recognition of Laue spots and its application to polycrystalline materials

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