Master thesis proposal

# Real-Time XRD Analysis Using Deep Learning

**Keywords :** Deep Learning, High Energy X-Ray Diffraction, Steel, Phase transformation

## SCIENTIFIC DESCRIPTION :

**Context**

High-energy X-ray diffraction (XRD) plays a crucial role in material characterization, offering insights into crystallographic structures, phase fractions, and other microstructural features [1]. However, with the advent of fourth-generation synchrotrons and high-throughput experiments, the volume and complexity of XRD data have significantly increased, presenting challenges for traditional analysis methods like Rietveld refinement [2,3]. These conventional analysis methods rely on iterative least-squares fitting and require extensive manual processing, often taking weeks or even months to extract meaningful information from in situ experiments. Furthermore, these traditional methods struggle in low signal-to-noise scenarios, particularly when detecting very low phase fractions, where manual intervention becomes unavoidable.

Recent advances in deep learning have shown considerable promise in rapid image recognition and data classification across various scientific fields. In the context of XRD, previous studies have largely focused on using convolutional neural networks (CNNs) for tasks like crystal structure prediction, space group classification, and phase identification—typically determining the presence or absence of specific phases [4].

**Objective**

The present project aims to improve and validate an existing deep learning model tailored to process XRD data in real time. To achieve robust performance, we will implement a hybrid data strategy that combine experimental datasets with synthetically generated XRD patterns. Synthetic data will enhance the model's precision in quantifying low-phase fractions and enable it to operate across a broader parameter space. Meanwhile, experimental data will ensure that the model accurately captures real-world diffraction signals, particularly the complex noise patterns encountered in practical measurements.

**Techniques/methods in use :** CNN model written in python for predicting phase fractions from the XRD profiles. FullProf to test and validate the results from the CNN.

**Applicant skills :** Master's student in AI, Data Science, Materials Science, Physics, or related fields. Good foundation in machine learning and programming. Familiarity with diffraction techniques. Experience with data analysis tools.

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