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Machine Learning-driven Quantification of XRF Data: Integrating Sample Generation and Simulation for Enhanced Analysis

Tuesday 9 April 2024 18:30 (20 minutes)

This poster presentation will introduce the development and application of machine learning techniques for elemental concentration quantification of X-ray Fluorescence (XRF) spectra collected by a laboratory setup and the surrounding techniques needed, with a focus on sample generation and simulation. XRF analysis is a powerful tool for elemental sample characterization, yet the accuracy, reliability and performance of analytical approaches will be influenced by complex sample composition and matrix effects.
Our approach involves the development and utilization of machine learning models for the quantification process in order to overcome challenges associated with traditional analytical methods. The poster will explain the design and implementation of these models, highlighting their capacity to adapt and learn from complex datasets.
A main part of our machine learning approach is the utilization of sample generation, ensuring diversity and the representativeness of the training dataset to the real world. By simulating a broad range of samples with varying elemental compositions, we aim to enhance the robustness and generalization ability of the machine learning model. This addresses directly the challenge of limited experimental data, allowing for more comprehensive and reliable model training.
Based on the sample generation we will discuss the simulation of XRF spectra. They serve as a essential component in training and refining our machine learning models. Additionally through the generation of synthetic datasets, we aim to assess the models performance under various experimental setup conditions, ensure their robustness and adaptability to real-world scenarios.
The presented work is still under progress but will finally contribute a significant tool for elemental analysis with XRF and will open up a path for broader applications of machine learning in XRF in order to overcome challenges associated with complex sample systems. The integration of machine learning, sample generation, and data simulation offers a comprehensive approach to enhance the robustness, accuracy, reliability and speed of XRF quantification.

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