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Title: Optimization of depth resolved X-ray absorption spectroscopy in grazing emission mode for characterizing compositionally complex alloys

Abstract

Layered materials are fundamental to technological advancements, offering distinct properties that differentiate them from bulk materials. In electronics, for instance, thin-film transistors (TFTs) are used to enhance charge transport and flexibility, thereby improving device performance. In the same way, thin-film photovoltaic devices used in renewable energy use strategic layering to absorb light more efficiently and separate electron-hole pairs more effectively, which leads to higher energy conversion efficiency. In recent decades, the development of new alloys has highlighted the importance of layered materials in another context. Compositionally complex alloys, for example, form multiple oxide layers on their surfaces when they oxidize. Studying these corrosion layers is crucial for understanding material-environment interactions.

Typical surface analysis techniques, including X-ray photoelectron spectroscopy (XPS), secondary ion mass spectrometry (SIMS), and Meitner-Auger electron spectroscopy (M-AES), provide valuable insights but are constrained by their requirements for high vacuum conditions and their limited depth analysis. In contrast, X-ray absorption near-edge structure (XANES) spectroscopy presents a versatile and advantageous alternative. It operates effectively under ambient conditions and allows time-resolved measurements, enhancing the analysis of materials in real-time as they undergo structural and compositional changes. This adaptability broadens the scope for material analysis, allowing for a more comprehensive understanding of dynamic processes.

Grazing Emission X-ray Fluorescence (GEXRF) spectroscopy stands out as a non-destructive, depth-resolved, element-specific characterization technique important for collecting depth-resolved information at the nanometer scale. Its ability to collect in-depth resolved information based on the grazing emission angle of the fluorescence radiation makes it ideal for investigating thin films, corrosion layers, and interfaces within layered materials. The integration of XANES in emission mode with GEXRF enables detailed exploration of the chemical states of the analyzed atom and provides depth-resolved information. This study discusses grazing emission X-ray absorption near-edge structure spectroscopy (GEXANES), a novel layer analysis technique that is created by integrating these two methods.

This study also innovatively combines machine learning with GEXANES spectroscopy to reduce experimental times. By using active learning, a subset of machine learning, it refines the data acquisition process, enabling more efficient and streamlined methods. The application of active learning in this context illustrates the potential of data-driven approaches to transform experimental methodologies, particularly in resource-limited environments such as synchrotron facilities, thereby accelerating scientific research and discovery.