Realizing Autonomous, Real-Time, AI-Driven Multimodal Studies at X-Ray Light Sources

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As new and upgraded x-ray light sources are established alongside advances in detector technology, the data generation rates at beamlines are skyrocketing. Data collected in fractions of a second to minutes at such facilities may take weeks to months to process and understand. New streaming analysis methods, particularly those employing Artificial Intelligence (AI), have demonstrated the ability to expedite data analysis to the speed and scale required for the light source community.

Beyond the ability to accelerate researchers real-time understanding of their ongoing experiment at the beamline, these methods offer the potential to run fully automated experiments that are driven by directed scientific inquiry; for example, searching for a boundary in a phase-map or tuning synthesis conditions to maximize product. Bringing these methods to bear at large-scale user facilities has the potential to increase scientific output. This level of automation does not need to be limited to a single measurement. Increasingly, the use of multimodal characterization is required to fully understand the structure and function of complex materials. The inherent information content from one measurement can be used to inform and drive others, such as using relatively fast diffraction measurements to drive slower, but equally critical, spectroscopy studies. Just as human researchers can look at the full range of available information on a material to inform their understanding, we have begun to use AI-methods that leverage multifaceted data from different measurement techniques.

We have recently performed a fully autonomous multimodal study of high entropy alloys (HEA) using diffraction, PDF, and X-ray Absorption Fine Structure (XAFS). In this experiment, a wafer film deposited with a complex, unknown phase-map of high-entropy alloys was simultaneously studied using the Pair-Distribution Function (PDF) and Beamline for Materials Measurements (BMM) beamlines at NSLS-II. As measurements proceed on each beamline,

AI-agents coordinated the next sequence of measurements by identifying regions of interest on the sample. Thus, information derived in real-time from both techniques was leveraged and applied to drive the automated decision making behind the experiment control. This new method of approaching multi-beamline studies may pave the way for an entirely new class of access proposal that leverages our user facilities in simultaneous multimodal approaches.

In this contribution, we will present the technical details of how the experiment was designed and realized, demonstrate the AI-driven analysis and decision making agents, present results of recent experiments, and discuss the future of this approach.