

## **APS WK#10: Training Workshop on X-ray Spectroscopy Data Analysis with Larch (Data Analysis Tools for X-ray Spectroscopy) and AXEAP (Argonne X-ray Emission Analysis Package)**

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With the upgraded spectroscopic beamlines at APS-U era, it is essential to achieve the real-time interpretation of the spectroscopic data and the capability to change experimental conditions during a beam run correspondingly. This one-day workshop will focus on x-ray absorption and emission spectroscopy data analysis with Larch (Data Analysis Tools for X-ray Spectroscopy)<sup>1</sup> and AXEAP (Argonne X-ray Emission Analysis Package)<sup>2</sup>, respectively.

Larch is an open-source library and set of applications for processing and analyzing x-ray absorption and fluorescence spectroscopy data and x-ray fluorescence and diffraction image data from synchrotron beamlines. Larch aims to provide a complete analysis toolkit for x-ray absorption fine-structure spectroscopy (XAFS), including both x-ray absorption near-edge spectroscopy (XANES) and extended x-ray absorption fine-structure spectroscopy (EXAFS). Larch also provides visualization and analysis tools for x-ray fluorescence (XRF) spectra and XRF and x-ray diffraction (XRD) images as collected at scanning x-ray microprobe beamlines.

Argonne X-ray Emission Package (AXEAP), a singular purpose software package for processing x-ray emission (XES) images collected with a 2-dimensional position sensitive pixel array detector, has been developed. AXEAP can rapidly convert XES image files into a spectral form by applying parallel computation and unsupervised machine learning to compute vast amount of image data. Special focus has been placed on designing user-friendly-interface for processing multiple edges, non-resonant and resonant x-ray emission image analysis, in order to make data processing quick and easy. AXEAP is free software and is written in MATLAB, armed with powerful libraries and toolboxes. The software runs on all common operating systems such as Linux, Window, and Mac.

The workshop will start with an overview of spectroscopic beamlines and a brief introduction to XAFS<sup>3</sup>, followed by the demonstration of the Larch in the morning; in the afternoon, we will provide outline on x-ray emission techniques, then provide the demonstration of XES data analysis with AXEAP.

### References:

- 1) Newville M. 2013 J. Phys.: Conf. Ser. 430 012007
- 2) Hwang, I-H. etc. Journal of Synchrotron Radiation 29, no. 5 (2022).
- 3) Kelly, S. D.; Hesterberg, D.; Ravel, B.; Ulery, April L.; Richard Drees, L. (2008), SSSA Book Series. Soil Science Society of America. doi:10.2136/sssabookser5.5.c14