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A Data-Driven Workflow for Preprocessing, Anomaly Detection, and Simulation-Guided EXAFS Analysis of Cu in Steel

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We present an integrated workflow for X-ray Absorption Spectroscopy (XAS) data processing, designed for extensible, automated analysis using Python. First, we developed a two-pass rolling median filter (with windows of 21 and 7 points and median absolute deviation thresholds of 6 and 5, respectively) to detect glitches from the incident intensity signal (I_0). The identified glitches are then removed from both I_0 and the fluorescence signal (If), yielding clean spectra for subsequent analysis. Second, we applied Z-score normalization to the absorption spectra, followed by interpolation onto a common energy grid, and then performed Principal Component Analysis (PCA) for unsupervised exploration of spectral variation across measurements. PCA reduces dimensionality, highlights systematic changes, clusters related scans, and flags outliers for inspection. Next, we applied this workflow to Cu K-edge (8.979 keV) XAS in fluorescence mode for 22MnB5 steel sheets with 0.1–0.3 wt.% Cu. Larch-based extended X-ray absorption fine structure (EXAFS) simulations were used to assess the impact of k-range on data quality. Comparing simulated EXAFS data with kmax ≈ 11 $Å^{-1}$ and extended k-ranges shows that higher-k measurements improve amplitude and resolution, enabling better discrimination between structural models. This modular pipeline provides a reproducible framework for XAS analysis, expandable with additional preprocessing and machine learning techniques.

Author: NGUYEN, Duc-Chau (ALBA Synchrotron - CELLS)

Co-authors: Dr PANAHI, Seyedeh Leila (ALBA Synchrotron - CELLS); Dr RAVENTÓS, Marc (ALBA Synchrotron - CELLS); Dr USOLTSEV, Oleg (ALBA Synchrotron - CELLS); Dr BAGUÉS, Núria (ALBA Synchrotron - CELLS); Dr PUJANTE, Jaume (Eurecat, Center Tecnologic de Catalunya Unit of Metallic and Ceramic Materials, Placa de la Ciencia 2, Manresa,08243, Spain); Dr KUMARAN, Surya (Arcelormittal maizieres Research SA, Rue Andre Campra 6 Immeuble Cezanne, Saint Denis, 93200, France); Dr OTÓN, Joaquín (ALBA Synchrotron - CELLS)

Presenter: NGUYEN, Duc-Chau (ALBA Synchrotron - CELLS)

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