Goldschmidt 2026 Abstract 29:188–200.
https://doi.org/10.46427/gold2026.35593

Carbon K Peaks and Iron L Peaks: Toolkits for spectral analysis of C1s and Fe2p X-ray absorption near edge structure data

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Scanning Transmission X-ray Microscopy (STXM) combines nanometer-scale spatial resolution with element-specific chemical sensitivity through X-ray absorption near edge structure (XANES) spectroscopy. A typical STXM workflow involves acquiring a data cube of images across an absorption edge, extracting spatially distinct spectral components via methods such as non-negative matrix factorization, and interpreting the resulting spectra in terms of chemical properties. While mature tools exist for image acquisition, alignment, and data reduction, a gap remains to conveniently extract interpretable and statistically meaningful results, especially from large data sets. For Fe L-edge data, linear combination fitting against reference standards is common, but requires a representative reference database. For C K-edge data, linear combination fitting is uncommon, and interpretation often relies on manual curve fitting in general-purpose software. We present two desktop applications in development that address this gap for two widely measured absorption edges in STXM of natural materials. “CarbonKPeaks” performs constrained Gaussian peak fitting of C K-edge spectra, decomposing the XANES into up to eight functional-group peaks (aromatic, phenolic, aliphatic, carboxyl, carbonyl, hydroxyl, carbonate, and σ*) with physically motivated constraints on peak positions and widths.[1] Two statistical diagnostics assess fitting reliability: a box plot test that evaluates solution uniqueness by randomizing starting conditions, and Monte Carlo analysis that propagates noise to quantify parameter uncertainty.[2] “IronLPeaks” implements two methods for Fe $L_{2,3}$-edge analysis. The first extracts L_3 peak energy separation (ΔeV) and intensity ratio (i_1/i_2) via derivative peak detection and plots on a ΔeV–i_1/i_2 diagram.[3] The second uses a modified integral white-line method to determine $Fe^{3+}/\Sigma Fe$ by integrating Fe^{3+}-sensitive spectral windows (L_3': 708.5-710.5 eV; L_2': 719.7-721.7 eV) after double-arctangent continuum subtraction, then solving a universal calibration polynomial.[4] Together, these methods extract Fe phase and redox state information from a single spectrum. Both tools offer semi-quantitative analysis without requiring a reference standard database and will be distributed as standalone executables to complement existing STXM pipelines.

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