Contribution ID: 111 Type: Oral

Iterative energy self-calibration of Fe XANES spectra

Monday, 2 December 2019 12:35 (15)

Determining the oxidation state of Fe through parameterisation of XANES spectral features is highly dependent on accurate and repeatable energy calibration between spectra. Small errors in energy calibration can lead to vastly different interpretations. While a simultaneous measurement of a reference foil is often undertaken on X-ray spectroscopy beamlines, other beamlines measure XANES spectra without a reference foil and therefore lack a method for correcting energy drift. Here we propose a method that combines two measures of Fe oxidation state taken from different parts of the spectrum to iteratively correct for an unknown energy offset between spectra. We show that the method is applicable even when the two spectra have been collected at different times and different beamlines, potentially eliminating the need to collect standard reference spectra during every beamtime.

Speakers Gender

Travel Funding

No

Level of Expertise

Do yo wish to take part in the poster slam

No

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Track Classification: Technique Development