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LETTER

Accurate predictions of iron redox state in silicate glasses: A multivariate approach using X-ray absorption spectroscopy

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ABSTRACT

Pre-edge features in the *K* absorption edge of X-ray absorption spectra are commonly used to predict Fe^{3+} valence state in silicate glasses. However, this study shows that using the entire spectral region from the pre-edge into the extended X-ray absorption fine-structure region provides more accurate results when combined with multivariate analysis techniques. The least absolute shrinkage and selection operator (lasso) regression technique yields $\%Fe^{3+}$ values that are accurate to ±3.6% absolute when the full spectral region is employed. This method can be used across a broad range of glass compositions, is easily automated, and is demonstrated to yield accurate results from different synchrotrons. It will enable future studies involving X-ray mapping of redox gradients on standard thin sections at 1 × 1 μm pixel sizes.

Keywords: XANES, EXAFS, silicate glass, lasso, PLS, multivariate analysis, redox state, ferric iron