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In-situ mapping of ferric iron variations in lunar glasses using X-ray absorption spectroscopy

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Abstract

This paper presents a new X-ray absorption spectroscopy (XAS) method for making two-dimensional maps of Fe^{3+} in-situ in polished glass samples, which opens the door to study redox changes associated with magmatic processes such as crystallization, assimilation, ascent, and eruption. Multivariate analysis (MVA) allows selection of specific channels in a spectrum to inform predictions of spectral characteristics. Here, the sparse model of the least absolute shrinkage and selection operator (Lasso) is used to select key channels in XAS channels that can be used to predict accurate in-situ Fe^{3+} analyses of silicate glasses. By tuning the model to use only six channels, analytical time is decreased enough to allow mapping of Fe^{3+} variations in samples by making gridded point analyses at the scale of the XAS beam (1–2 μm). Maps of Fe^{3+} concentration can then be constructed using freely available, open source software (http://cars.uchicago.edu/xraylarch/). This result shows the enormous potential of using MVA to select indicative spectral regions for predicting variables of interest across a wide variety of spectroscopic applications. Redox gradients in lunar picritic glass beads first observed with point analyses are confirmed through this XAS mapping and suggest degassing processes during ascent and eruption are responsible for the range of Fe^{3+} values measured in these samples.

Keywords: Glass, redox, X-ray absorption spectroscopy, lunar glass