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Variation in XANES in biotite as a function of orientation, crystal composition, and metamorphic history

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ABSTRACT

Microscale analysis of ferrous:ferric iron ratios in silicate minerals has the potential to constrain geological processes but has proved challenging because textural information and spatial resolution are limited with bulk techniques, and in situ methods have limited spatial resolution. Synchrotron methods, such as XANES, have been hampered by the sensitivity of spectra to crystal orientation and matrix effects. In an attempt to break this nexus, biotites from Tanzania were characterized with a combination of optical microscopy, electron microprobe, Mössbauer analysis, electron backscatter diffraction (EBSD) and X-ray absorption near edge structure (XANES) spectroscopy. Pre-edge and edge characteristics of the Fe $K\alpha$ absorption feature were compared to orientation information derived by EBSD and ferric iron content derived from Mössbauer analysis. Statistically significant correlations between measured spectral features and optic/crystallographic orientations did not reduce the uncertainty in Fe³⁺/Fe_{tot}. The observations are consistent with matrix- and ordering-dependency of the XANES features, and further work is necessary if a general formulation for orientation corrections is to be devised.

Keywords: Fe, oxidation, XANES, biotite, orientation