

Calibration of XANES for determination of $\text{Fe}^{3+}/\Sigma\text{Fe}$ in garnet

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Fe is the most common multi-valent element in the Earth, occurring as both Fe^{2+} and Fe^{3+} in minerals and melts. Garnet crystallises in peridotite mantle at >60 km depth, and usually contains both Fe^{2+} and Fe^{3+} . $\text{Fe}^{3+}/\Sigma\text{Fe}$ of garnet in equilibrium with the mantle assemblage olivine + opx is sensitive to the oxygen fugacity ($f\text{O}_2$) under which it crystallised (Gudmundsson and Wood 1995), but can currently only be determined by Mössbauer Spectroscopy or by the EPMA-based Flank Method (Höfer et al. 2004). We aim to develop a complementary XANES technique with micron spatial resolution and precision comparable to or potentially better than the existing flank method. The XANES method for determining the $\text{Fe}^{3+}/\Sigma\text{Fe}$ ratio of garnets uses the energy of the 1s-3d transition in the Fe K-edge XANES spectrum (Berry et al. 2003). We used well characterised synthetic garnet samples as standards (Woodland and O'Neill 1993; Woodland and Ross 1994). $\text{Fe}^{3+}/\Sigma\text{Fe}$ was determined previously for these samples from their simple compositions and by Mössbauer spectroscopy, and varies from 0.0 to 1.0. We recorded Fe K-edge XANES spectra from these powdered samples at the Australian National Beamline Facility (Tsukuba, Japan), allowing construction of a calibration curve relating garnet $\text{Fe}^{3+}/\Sigma\text{Fe}$ to 1s-3d energy. The calibration was applied to previously characterised (Mössbauer) natural garnets from garnet peridotites (Woodland and Koch 2003) to test precision. This method has potential for studies of the lithospheric mantle, allowing for example, micron-scale determination of $f\text{O}_2$ profiles in zoned garnet crystals in peridotite, revealing important information about their growth and metasomatic histories.

References

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