Geophysical Research Abstracts
Vol. 16, EGU2014-16578, 2014
EGU General Assembly 2014

Iron M-edge x-ray Raman scattering spectroscopy – a tool to determine Fe speciation at conditions of deep Earth

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We present a spectroscopic study of the iron $M_{2,3}$-edge for several minerals and compounds to reveal information about the oxidation state, local coordination and spin state of iron. We describe a novel approach to probe the iron M-edge bulk sensitively using non-resonant inelastic x-ray scattering. Significant changes in the onset and shape of the Fe M-edge were observed demonstrating the capabilities of x-ray Raman scattering spectroscopy to extract information on the Fe^{3+}/Fe_{tot} ratio and local coordination. In-situ measurements of the pressure-induced spin transition in FeS even demonstrate that this technique allows for detection of the spin cross-over as well as characterization of the electronic properties of the low-spin phase. Thus, x-ray Raman spectroscopy is suitable for obtaining detailed insights to the properties of Fe in-situ at high pressure and temperature providing indispensable information for many physical and chemical processes of the deep Earth.