X-ray Raman scattering: A spectroscopic tool for in-situ studies of low Z element's absorption edges at high pressure and high temperature

Christian Sternemann[1], Kolja Mende[1], Alexander Nyrow[1], Christoph J. Sahle[1], Max Wilke[2], Christian Schmidt[2], Laura Simonelli[3], Marco Moretti Sala[3], and Metin Tolan[1]
[1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany.
[2]Deutsches GeoForschungsZentrum GFZ, 14773 Potsdam, Germany.
[3]ESRF, 38043 Grenoble Cedex, France.

The Earth's mantle is composed of silicate compounds containing low and intermediate Z elements such as oxygen, silicon, magnesium, iron, aluminum, calcium and sodium. In-situ studies of these compounds at conditions of geological relevance, i.e. pressures up to 130 GPa and temperatures up to 3000°C for the deep Earth's mantle, require the use of diamond anvil cells in combination with resistive or laser heating. To study changes in the local atomic and electronic structure at extreme conditions x-ray absorption spectroscopy can be applied in the hard x-ray regime to intermediate and high Z elements. However, the study of absorption edges for binding energies between several eV and 2 keV is hardly possible using electrons or soft x-rays as a probe due to the highly absorbing sample environment. Here, x-ray Raman scattering (XRS), an energy loss spectroscopy using hard x-rays as a probe, provides a unique experimental method which can be used for in-situ experiments employing heated diamond anvil cells. XRS yields similar information as soft x-ray absorption and electron energy loss spectroscopy. It is sensitive to changes of the electronic and local atomic structure and allows to study different excitation channels by variation of the momentum transfer in such measurements. The partial unoccupied density of states can be determined utilizing this momentum transfer dependence. Often XRS measurements are focused on the near edge structure but also studies of the extended x-ray absorption fine structure are feasible. Different computational methods are available to model XRS spectra both for crystalline and amorphous systems, as liquids and melts, latter using cluster calculations often based on molecular dynamics simulations. The capabilities of this experimental technique for geophysical applications will be discussed and selected examples will be presented.

References:
W. Schülke, (Oxford University Press, Oxford, 2007).
J.P. Rueff, A. Shukla (2010), Rev. Mod. Phys., 82, 847-896.
S.K. Lee, Y-F. Lin, Y.Q. Cai et al. (2008), PNAS, 105, 7925-7929.
A. Sakko, C. Sternemann, Ch.J. Sahle et al. (2010), Phys. Rev. B, 81, 205387.