Advances in X-ray spectroscopy of geomaterials at high pressure and temperature

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In the last decades, synchrotron radiation (SR) has become an indispensable tool for studying geomaterials using X-ray spectroscopic techniques. The continuous spectrum and the high brilliance produced by SR sources not only enable the acquisition of high quality spectral data in short time, but also provide the possibility to focus the SR beam into a small spot with very high photon flux. Particularly the latter feature is a prerequisite for many applications in Earth sciences. In this contribution, applications of X-ray spectroscopy are presented to study materials and processes in-situ at high pressure and temperature.

Due to the rather low absorption of hard X-rays, SR opens up the possibility to perform measurements in high-pressure or reaction cells. SR micro-XRF is now generally used for obtaining trace element concentrations in aqueous fluids in-situ at high P and T using XRF-optimized diamond anvil cells, with detection limits in the lower ppm range, e.g. [1]. This high-pressure setup was used to investigate element complexation in aqueous fluids by acquiring X-ray absorption spectra at conditions of the Earth's crust as shown for lanthanides or Zr at low concentrations in aqueous fluids, e.g. [2], [3]. Such data cannot be achieved on quenched samples at all and illustrate the importance for the understanding of processes involving fluids at high P and T.

The range of elements accessible by XAFS techniques at in-situ conditions is usually limited by the absorption of X-rays due to the sample environment. The indirect measurement of XAFS spectra by inelastic X-ray Raman scattering provides a workaround to access absorption edges at low energies (e.g. low Z elements). This enables studying the local structure, oxidation state and spin state for edges at low energy in-situ at high P and T, e.g. B K-edge, O K-edge, Fe M or L-edge ([4], [5], [6], [7]).

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