

In situ characterization of the local coordination, oxidation, and spin state of Earth materials at pressure and temperature

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The knowledge of the spin state, oxidation state, and local coordination is essential to characterize the Earth's mantle materials as they strongly affect macroscopic properties such as density, sound velocity, viscosity, and conductivity. Besides well established methods like Mössbauer spectroscopy, optical spectroscopy, and x-ray diffraction, in recent years inelastic x-ray scattering methods in general [1] emerged to a powerful tool for the in situ study of these properties both at high pressure and high temperature using diamond anvil cell in combination with resistive or laser heating. As an example, x-ray emission spectroscopy was successfully applied to characterize the spin state of iron bearing minerals [2, 3] and x-ray Raman scattering to study e.g. coordination changes in glasses [4]. However, sometimes the experimental results are difficult to interpret and can provide ambiguous results so that complementary spectroscopic information is required. Here, we give some examples on how x-ray Raman scattering can be exploited in order to obtain such complementary information, i.e. on the spin state of a system [5] or on structural changes in the local atomic coordination [6]. Therefore, we present an x-ray Raman scattering study of the high spin to low spin transition of siderite single crystal for pressures between 20 and 50 GPa at the iron M_{2,3}- and L_{2,3}-edges and discuss measurements of the Na L_{2,3}-edge in hydrous silicate melt (Na₂Si₃O₇ with 10 wt% H₂O) at about 1 MPa and 825 K.

References

- [1] W. Schülke, *Electron dynamics by inelastic x-ray scattering*, Oxford Univ. Press (2007).
- [2] C. McCammon et al., *High Press. Res.* 33, 663 (2013).
- [3] J. Badro, *Annu. Rev. Earth Planet. Sci.* 42, 231 (2014).
- [4] S.K. Lee et al., *Proc. Natl. Acad. Sci.* 105, 7925 (2008).
- [5] A. Nyrow, J.S. Tse, N. Hiraoka, S. Desgreniers, T. Büning, K. Mende, M. Tolan, M. Wilke, C. Sternemann, *Appl. Phys. Lett.* 104, 262408 (2014).
- [6] A. Nyrow et al., *Contrib. Mineral. Petrol.* 167, 1012 (2014).

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