



**Understanding structural properties of carbonate-silicate melts:
EXAFS studies on Y and Sr in the melt system of Na₂O-CaO-
Al₂O₃-SiO₂-CO₂**

**Experiment
number:**
ES 126

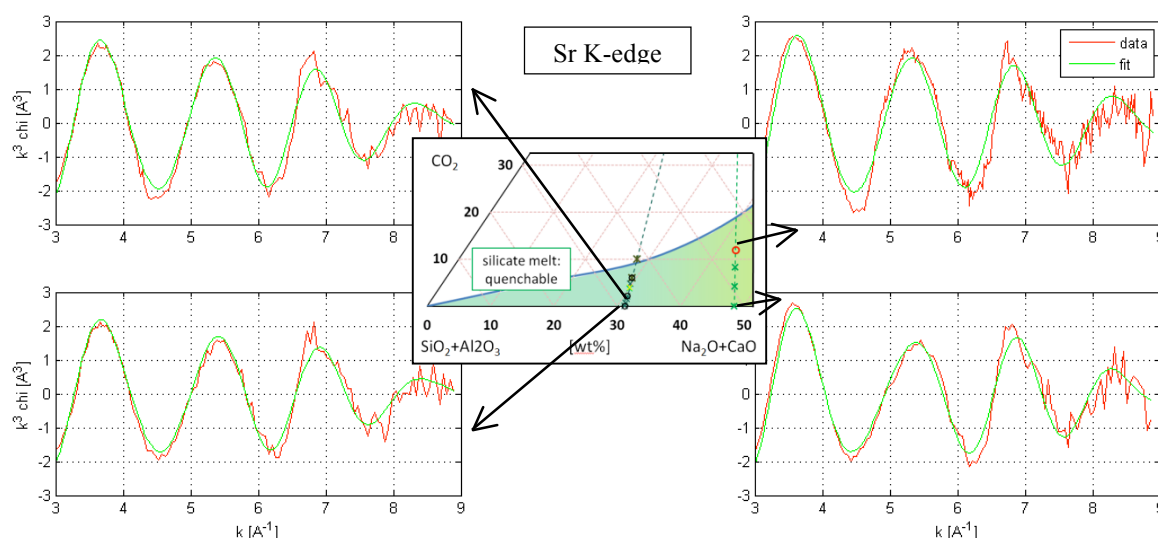
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Report:

This study aims at understanding the structural properties of carbonate-silicate melts relevant to magmatic processes in the deep Earth. Carbonate melts show extraordinary properties, especially in regard to their low melt viscosities and densities, high surface tensions and electrical conductivities as well as distinct geochemical affinities to a wide range of trace elements¹. Understanding the structural properties of carbonate-bearing melts is fundamental to explaining their chemical and physical behaviour as well as the processes operating in the deep Earth. This study focuses on elucidating the local structural environment of Y, Sr and Zr in silicate melts in the system with varying CO₂ contents. Whereas Sr is expected to represent the alkaline earth metals, Y is expected to represent the role of heavy rare earth elements. Glasses containing Y and Sr of around 5000 ppm were quenched from high temperature and pressure (1200°C and 0.7 GPa), assuming comparability to structural properties found in corresponding melts². We aim at tracking the dependence of the structural incorporation of the trace elements on the varying CO₂ content.



We collected Y, Sr and Zr K-edge EXAFS on glass samples at BM23 using an Si(111) double-crystal monochromator in transmission and fluorescence mode. Rb spectra formerly measured proofed to be

distorted by multi-electron excitation and were therefore not taken. K^3 -weighted Sr EXAFS spectra of selected measurements on samples in the system $\text{Na}_2\text{O}-\text{CaO}-\text{Al}_2\text{O}_3-\text{SiO}_2-\text{CO}_2$ are plotted in Figure 1. Fitting the data requires fitting procedures based on an asymmetric distribution functions. First investigative fitting shows only minor variations in the local structure of Sr in glasses of different chemical composition in terms of atomic distances ($\sim 2.7 \text{ \AA}$), σ^2 ($\sim 0.003 \text{ \AA}^2$) or asymmetry at fixed coordination number (7). Even less variation is found for Y coordination. More refined data fitting, also including the effect of multi-electron-excitation (seen in spectra around a k of 7 \AA^{-1} in Figure 1), is still in process. These first results might indicate only a minor influence of the CO_2 content in silicate melts on trace elements coordination. However, the invariability of the coordination may also be related to the quench as it only reflects the structure at the melt – glass transition.

The Zr K-edge of the samples synthesized in the system $\text{CaCO}_3\text{-CaSiO}_3$ shows similarity to spectra of partially polymerized silicate glasses, indicating that Zr is six-fold coordinated as in catapleite³. There are minor sample-dependent variations observed (Figure 2). This indicates that at conditions of samples' synthesis (at least 90 minutes at 4 GPa and 1550 C) Zr is likely present in the silicate glass.

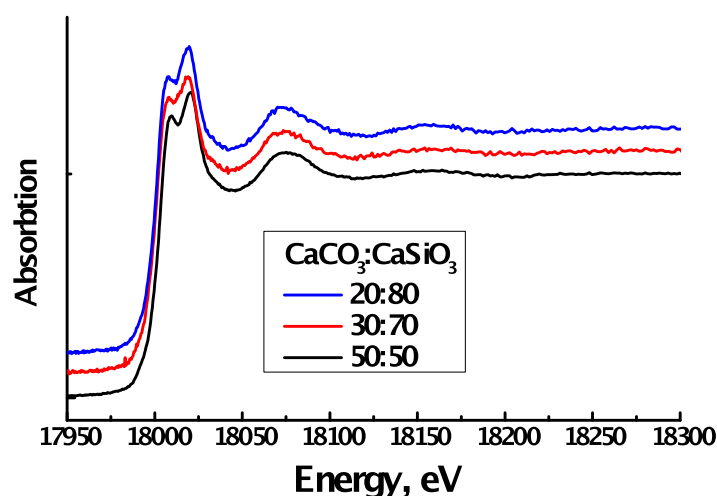


Figure 2: Absorption spectra of Zr K-edge with chemical compositions in the range of $\text{CaCO}_3\text{:CaSiO}_3$ 50:50, 30:70, 20:80, 10:90.

These measurements of quenched melts will serve as reference for later in-situ experiments at high pressure and temperature, also executed at carbonatitic compositions, which are non-quenchable. The ultimate goal is to gain insight into the structural control on chemical fractionation processes in carbonate-bearing magmatic systems in the deep Earth.

1. Jones, A. P., Genge, M. & Carmody, L. *Rev. Mineral. Geochem.* 75, 289–322 (2013).
2. Seifert, F. A., Mysen, B. O. & Virgo, D. 1879–1884 (1981).
3. Farges, F., Rossano, S. *Eur. J. Mineral.* 12, 1093–1107 (2000).

Acknowledgements:

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