| | | |
|---|---|---|
| ESRF | **Trace-element coordination in carbonate-silicate melts measured in-situ at high pressure and temperature** | **Experiment number**: ES 252 |
| **Beamline**: BM23 | **Date of experiment**: from: 8.4.15 to: 14.4.15 | **Date of report**: 1.3.16 |
| **Shifts:** 18 | **Local contact(s)**: Olivier Mathon | *Received at ESRF:* |


**Names and affiliations of applicants** (* indicates experimentalists):

Julia Pohlenz*, Max Wilke*, Deutsches GeoForschungsZentrum GFZ, Potsdam, Germany
Andrei Shiryaev* IPCE RAS Moscow, Russia
Vadim Murzin*, Kurchatov Institute, Moscow, Russia
Alexej Veligzhanin, Kurchatov Institute, Moscow, Russia
Oleg Safonov, IEM RAS Chernogolovka, Russia
Tetsuo Irifune, Ehime University, Matsuyama, Japan


## Report:

Understanding the structural properties of carbonate-silicate melts builds the basis for understanding magmatic processes in the deep Earth. In order to obtain relevant temperature and pressure conditions for our in-situ experiments, we employed the large volume Paris-Edinburgh press (PEP). A newly designed pressure assembly was tested, which ensured highly stable experimental conditions over several hours of up to 2000 K at 2.5 GPa. Pressure-temperature calibration for this new set-up was determined by using the equation of states of different reference materials to evaluate their volume changes at high temperature / high pressure as detected by XRD (Figure 1). More technical details can be found in Pohlenz et al. (2016).

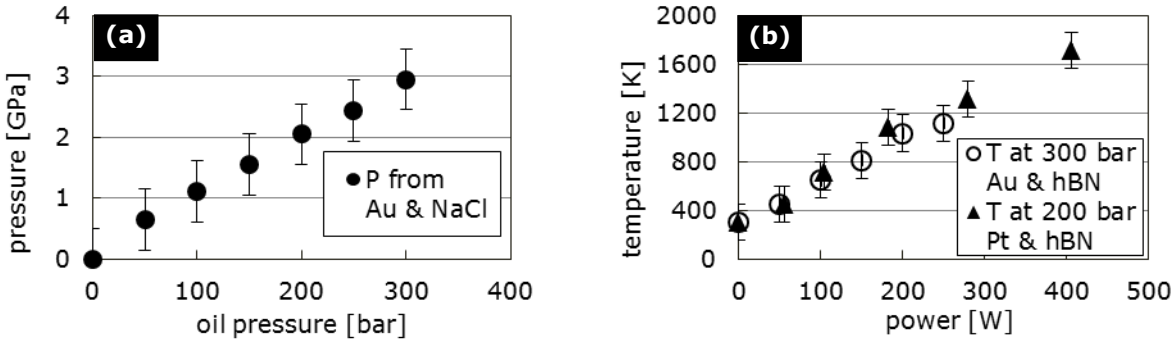


*Figure 1. Pressure (a) and temperature (b) calibration as determined by the equation of states of reference materials (gold (Au), NaCl, hexagonal boron nitrite (hBN), and platinum (Pt)). Volume changes at HT/HP are detected by XRD. Temperature calibration was conducted at ~2 GPa and ~3 GPa sample pressure.*

In continuation to former experiments (ES 191), we used this set-up to investigate structural properties along the join carbonate - silicate melt in-situ and their respective quenched glasses in the system $Na_2O$-CaO-$Al_2O_3$-$SiO_2$-$CO_2$ (doped with ~2 wt% Y and Sr each). We collected transmission EXAFS K edge spectra of Y and Sr (Figure 2), representing heavy rare earth elements and alkali earths, respectively.
EXAFS data was analyzed by the software xafsX (Winterer 1997) using the analytical fit, which accounts for the increased anharmonicity in melts using an asymmetric pair distribution function. Figure 3 shows the results for Y fits, assuming a fixed coordination number of 6 and an S0 of 0.85 (as derived from fitting the

model compound of Y2O3). R, E0, sigma$^2$ and the asymmetry were fitted. In a second step the asymmetry was set to the derived values of 0.12 for melts and 0.04 for quenched glasses. The results imply for a slight change in bond length for carbonate melts compared to silicate melts. Analysis of Sr data is still in progress.

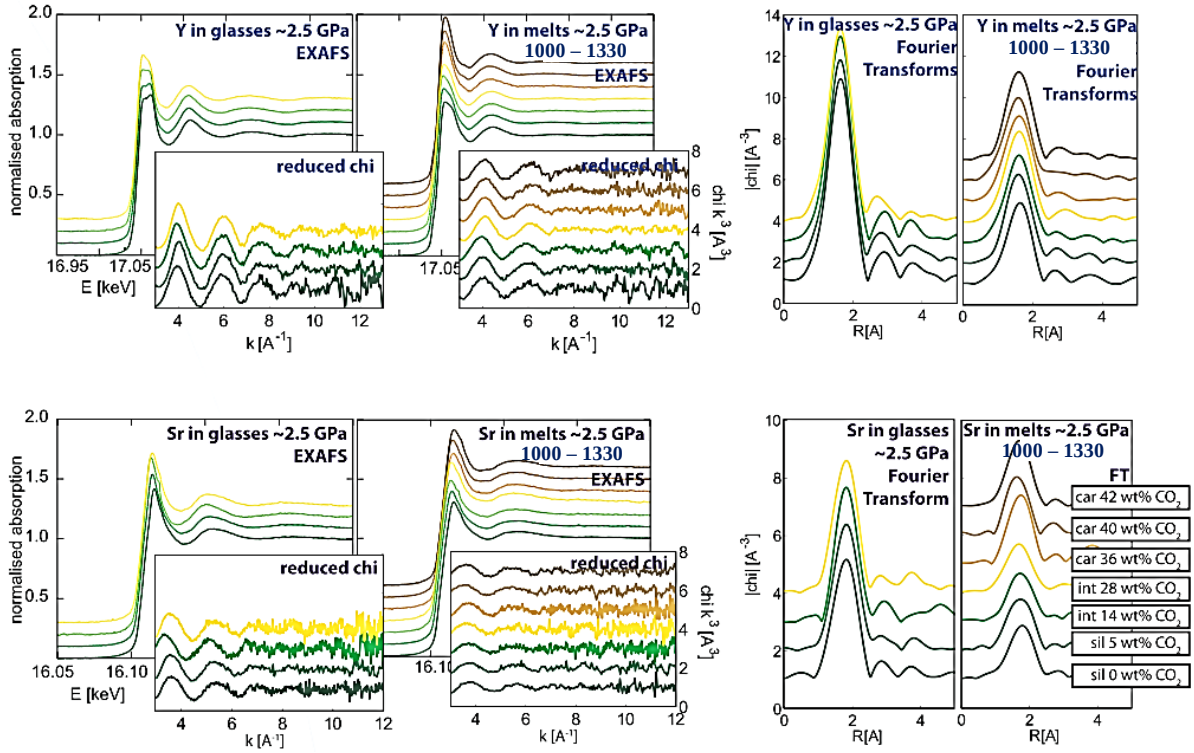


*Figure 2. Normalized XANES and reduced EXAFS (χ) of Y and Sr K edge and their Fourier Transforms (FT) along the join silicate (green) to carbonate (brown) melt (respectively quench).*

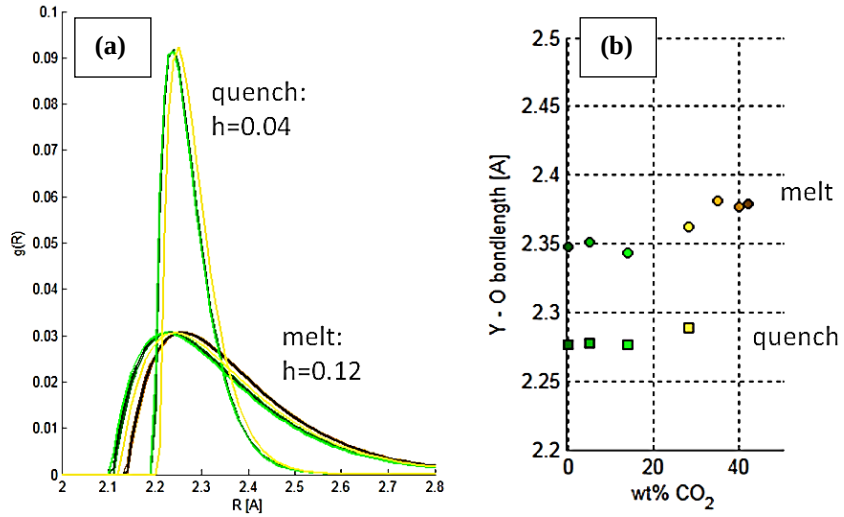


*Figure 3: (a) Fitted pair distribution function of Y–O in the melts and quench products of the join along silicate (green) to carbonate (brown) composition. The asymmetry parameter h was determined by best fits and then fixed.*

*(b) Y – O bond length as a function of CO2 content of the investigated compositions for melts (circles) and quenched glasses (squares).*


Refernces:

Pohlenz, J, Pascarelli, S, Mathon, O, Belin, S, Shiryaev, A, Safonov, O, Veligzhanin, A, Murzin, V, Irifune, T, Wilke, M. 2016. „Structural properties of sodium-rich carbonate-silicate melts: An in-situ high-pressure EXAFS study on Y and Sr*". J. Phys.: Conf. Ser.* in press.

Winterer, M. 1997. „XAFS - A Data Analysis Program for Materials Science". *Le Journal de Physique IV* 7 (C2): C2–243 – C2–244. doi:10.1051/jp4/1997182.



## Acknowledgements:

The great help and support of Olivier Mathon, Sakura Pascarelli, Innokenty Kantor, Sebastian Pasternak, Mohamed Mezouar and the BM23-team is highly appreciated.