



	Experiment title: Phosphorus in magmas: relations between geochemical role and magma rheology	Experiment number: HD100
Beamline: ID21	Date of experiment: from: 15 november to: 20 november 2006	Date of report: 28-Feb-07
Shifts: 18	Local contact(s): Jean Susini	<i>Received at ESRF:</i>

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Report:

A set of XAS spectra at the P K-edge has been successfully collected for a wide group of silicate glasses representing different magma compositions spanning from granitic to ferrobaltic, with various alkali to Aluminum ratio, different bulk chemistry, and synthesised over different oxygen fugacities. One of the two ferrobaltic set, has been already characterised by Fe K-edge XAS spectroscopy to provide Fe oxidation state, coordination numbers and Fe-O bond distances.

Averaging up to 50 scans allowed to obtain spectra with a very good signal to noise ratio. For the most important samples, also short EXAFS spectra have been collected up to $K=7 \text{ \AA}^{-1}$.

A set of synthetic and natural P model compounds have been collected as well in order to interpret some spectral features (presence/absence of a pre-edge peak, and variations of the white-line intensity and energy position).

Theoretical XANES calculations are being performed by means of the mxan code in order to reproduce the spectral features found in the experimental data.

Preliminary results allowed to find that PO_4 tetrahedra in the silicate network are bonded by the corners to AlO_4 and FeO_4 tetrahedra.

No detectable changes are observed in a series of glasses where Fe is known to vary from five-fold coordinated Fe^{2+} to four-fold coordinated Fe^{3+} . As literature data indicate that P K-edge data are sensibly affected by a variation of second coordination shell cations chemistry and oxidation state, this imply that Fe is not the main cation bonded to PO_4 units.

Further XANES theoretical calculations, along with analysis of EXAFS data are currently in progress in order to better constrain the local chemistry and structure around PO_4 units in the studied glasses.