



	Experiment title: <u>Site location of trace level Nd and Ce in natural garnets by K edge XAFS</u>	Experiment number: CH 825
Beamline: BM 08	Date of experiment: from: 19/6/00 to: 24/6/00	Date of report: 17/8/00
Shifts: 12	Local contact(s): F. D'Acapito	<i>Received at ESRF:</i>
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Report:

Garnets represent an important group of rock-forming minerals. They are stable over a wide range of physico-chemical conditions, and the complexity of their crystal chemistry and thermodynamic behavior has been the subject of many investigations. Garnets in lower crustal mafic and ultra-mafic rocks usually contain rare-earth elements (REE) in trace concentrations. The diffusion coefficients of REE between garnets and the co-existing phases are used to interpret the crystallization and metamorphic history of the crustal rocks. An understanding of REE diffusion in garnets cannot be obtained without a characterization of their structural behavior. Despite their geochemical importance, a direct crystallochemical characterization of REE at trace levels in natural garnets is not available in the literature, because of the difficulty of obtaining structural information by means of conventional diffractometric methods. XAFS has already been successfully used in the study of Yb^{3+} in 1% weight in synthetic pyrope and grossular (Quartieri *et al.*, 1999a, b) highlighting that Yb^{3+} enters the structural X-site of garnet causing a strong localized structural relaxation.

In order to address this issue, we have proposed K edge XAFS measurements of Nd and Ce at trace levels (300 – 1200 ppm) in a set of natural garnets occurring in carbonatitic rocks from the Kola peninsula and from Siberia. Measurements at the commonly used REE L_{III} edge are impossible in these samples because of

- a) the presence of interfering fluorescence lines ($\text{Ti } K_{\beta}$ from the matrix and $\text{Ce } L_{II}$ from other REE) which cannot be resolved by the fluorescence detector;
- b) the presence of the $\text{Ce } L_{II}$ edge near the $\text{Nd } L_{III}$ edge, with a Ce concentration similar to that of Nd.

These problems can be overcome with the use of the Nd and Ce K edges because at these energies there are no problems of overlapping absorption edges and fluorescence lines; a high photon flux at these energies can be obtained at the GILDA beamline at ESRF, which also has a state-of-the-art fluorescence detector and electronics.

The measurements have been successfully performed in June 2000. We have collected spectra of Nd_2O_3 and CeO_2 standard compounds and of three natural garnets. The raw data for samples and standard compounds are shown in Figs 1 and 2.

A qualitative inspection of the the data indicates that:

- a) the local structural environment of Nd is the same in the three natural garnets differing by the Nd concentration (from 300 to 1100 ppm) and it is different from that found in Nd_2O_3 ;
- b) the local structural environment of Ce is different from that found in CeO_2 .

These results suggest that the REE enters a structural garnet site and not a matrix defect. Moreover there seems to be no dependence of the local structure on the REE concentration.

Quantitative data analysis is in progress. The extended spectra is being analysed with the FEFF package while the near-edge data is treated by means of full multiple scattering theory in collaboration with Dr. Chaboy (University of Zaragoza, Spain) following the procedure outlined by Chaboy and Quartieri (1995) and Quartieri *et. al.* (1999b).

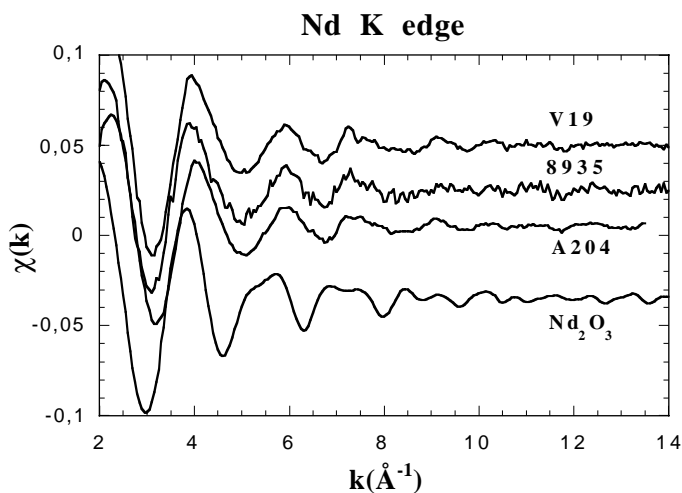


Fig. 1: Nd raw data

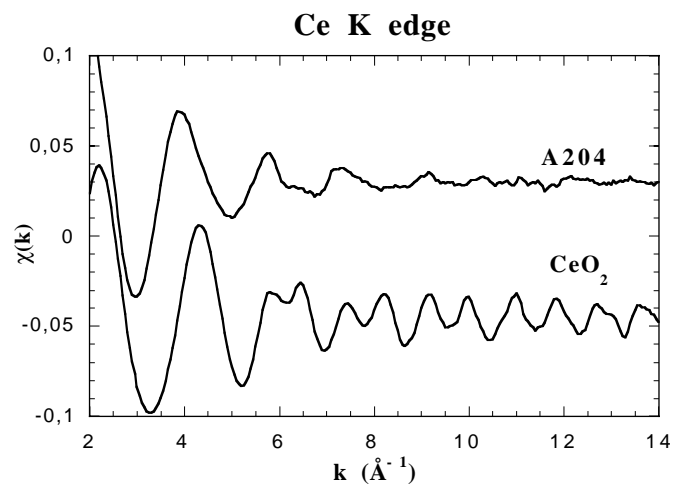


Fig. 2: Ce raw data

References

- Chaboy J. and Quartieri S. (1995) *Phys. Rev. B* 49, 6349 – 6357.
 Quartieri S., Antonioli G., Geiger C.A., Artioli G., Lottici P.P. (1999a) *Phys. Chem. Min.* 26, 251 – 256.
 Quartieri S., Chaboy J., Antonioli G., Geiger C.A. (1999b) *Phys. Chem. Min.* 27