ROBL-CRG	**Experiment title:** **Determination of Ni Sorption Mechanisms on Montmorillonite**	**Experiment number**: 20_01_003
Beamline: BM 20	**Date of experiment**: from: 4.2.1999 to: 11.2.1999 2.6.1999 08.06.1999	**Date of report**: 14.7.1999
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Report:

Aims of the experiment and scientific background

Sorption of heavy metal ions on mineral surfaces is an important process for maintaining environmental quality. A thorough level understanding of sorption mechanisms of heavy metal sorption on mineral surfaces is therefore of fundamental importance. On smectitic clay minerals Ni(II) can sorb as surface complex on edge sites and/or interlayer sites.
The aim of this study is to use EXAFS to determine sorption mechanisms of Ni on montmorillonite. Montmorillonite is an important smectitic mineral responsible for the retention of metals in the geosphere. Furthermore, the clay is used as a backfill material in the Swiss concept for a high level radioactive waste repository and thus, metal sorption on montmorillonite has been investigated in our laboratory in great details [1].

Experiments + Results

Samples were prepared in a glove box by reacting Ni and montmorillonite at pH 8.0 and at high ionic strength 0.2M $Ca(NO_3)_2$ to block cation exchange processes. The initial Ni concentrations for the samples varied from 0.03 mM to 0.92 mM Ni. After a reaction time of 1-90 days the samples were centrifuged and the wet paste was transferred into a Plexiglas sample holder. Ni K-edge fluorescence EXAFS spectra were recorded for samples containing 4 - 96 µmol/g Ni sorbed onto the montmorillonite. Figure 1 shows the dependence of different Ni concentrations sorbed onto montmorillonite after a reaction time of 90 days.

With increasing Ni loading a characteristic shoulder at 5.3 $Å^{-1}$ appears in the EXAFS spectra. The corresponding radial distributions function are shown in Figure 2. The first peak represents an oxygen shell and its position and height does not depend on the Ni concentration. The second peak shifts with increasing Ni concentration to lower R values (from 2.9 Å to 2.7 Å) and its peak height is increasing. The dashed line characterises the position of a Ni-Ni shell in an α-$NiOH_2$ and suggests the presence of a Ni-hydroxide like phase in the most concentrated sample. The sample with the lowest concentration suggests specific bounds of Ni to the montmorillonite surface and the absence of a Ni-nucleation. To date, however the structural origin of the second peak of the lowest concentration is still under investigation using theoretical approaches.

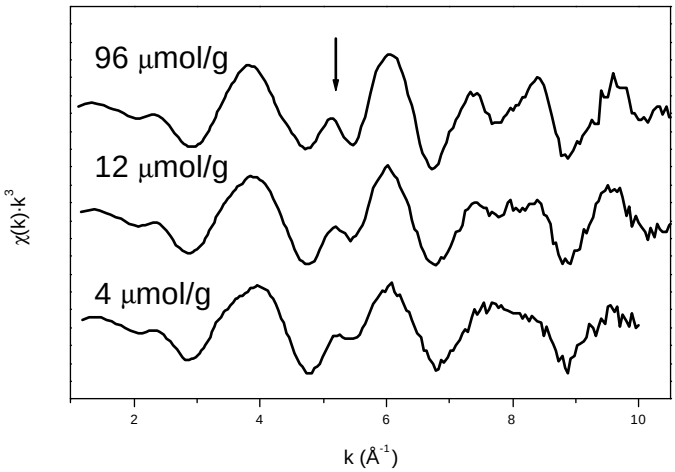

Figure 1: k^3-weighed Ni K-edge EXAFS spectra for different Ni-concentrations sorbed onto montmorillonite

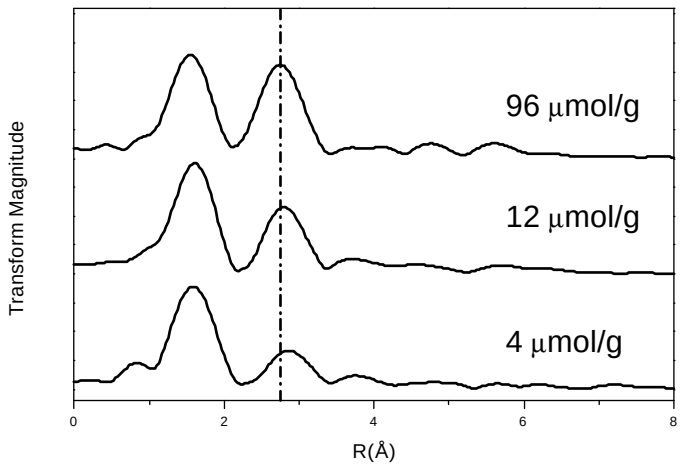

Figure 2: Concentration dependence of the Ni K-edge RDF of Ni sorbed onto montmorillonite

References

[1] Baeyens B, and Bradbury M. H. 1997. *J. Contam. Hydrol.* **27**, 199-222.