 ROBL-CRG	Experiment title: Interaction of uranium with microorganisms relevant to nuclear waste disposal in clay and granite formations using X-ray absorption spectroscopy	Experiment number: 20-01-711
Beamline: BM 20	Date of experiment: from: 22.06. to: 28.06.2011	Date of report: 26.01.2012
Shifts: 18	Local contact(s): A. Rossberg	<i>Received at ROBL:</i>
Names and affiliations of applicants (* indicates experimentalists): H. Moll, L. Lütke*, A. Geissler, S. Selenska-Pobell, E. Krawczyk-Bärsch, A. Rossberg*, A. Scheinost*, Ch. Hennig*, G. Bernhard		

Report: Synchrotron-based XAS is a powerful technique to obtain structural information on uranium in bacterial systems. Within this proposal we explore structural parameter of U(VI) after interaction with Mont Terri Clay Isolates and the Äspö-Strain *Pseudomonas fluorescens* (planktonic cells and cells fixed in a biofilm). The present report is focussed on our first XAS measurements, where we investigated the speciation of U(VI) bound by planktonic cells of *P. fluorescens* (see Fig. 1) and *P. fluorescens* biofilms; and by the Mont Terri isolates *Sporomusa* sp. and *Paenibacillus* sp..

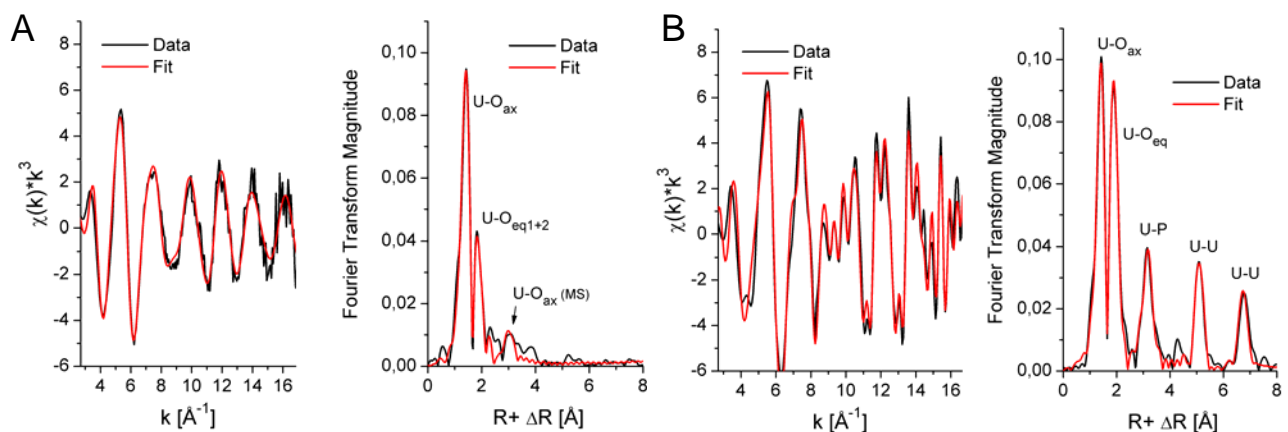


Fig. 1: U L_{III}-edge k^3 -weighted EXAFS spectra (left) and the corresponding Fourier transforms (right) and the theoretical fits (red line) of 0.2 mM U(VI) with 0.2 g/L *P. fluorescens* at pH 7.0 A: in 0%-P-SSM and B: in 0.5%-P-SSM .

Experimental. U L_{III}-edge XAS measurements were carried out with wet pastes of the U(VI) loaded biomasses with a fixed pH. These samples were

measured at 15 K either in fluorescence or in transmission mode. For comparison a solution containing only UO_2^{2+} (0.05 M at pH 2.0) was measured at room temperature.

Results. An example of the measured EXAFS oscillations and corresponding Fourier transforms are presented in Fig. 1. Selected structural parameters are summarized in Table 1.

Table 1: Summary of selected structural parameters.

Sample	Shell	N	R (Å)	σ^2 (Å ²)	ΔE_0 (eV)
0.05 M UO_2^{2+} , pH = 2.0	U=O	2f	1.77	0.0013	10.6
	U-O _{eq}	5.1	2.41	0.0071	
<i>P. fluorescens</i> + 0.2 mM U(VI); 0%-P-SSM; pH 7 metabolically active	U=O	2f	1.79	0.0018	14.9
	U-O _{eq1}	5.5	2.34	0.0097	
	U-O _{eq2}	0.5	2.54	0.0010	
<i>P. fluorescens</i> + 0.2 mM U(VI); 0.5%-P-SSM; pH 7 metabolically active	U=O	2f	1.79	0.0016	13.0
	U-O _{eq}	4f	2.29	0.0018	
	U-P	4f	3.63	0.0049	
	U-U	4f	5.24	0.0032	
<i>P. fluorescens</i> + 0.1 mM U(VI); 0.1 M NaClO_4 ; pH 7 metabolically inactive	U=O	2f	1.79	0.0018	17.9
	U-O _{eq1}	4.6	2.36	0.0094	
	U-O _{eq2}	1.0	2.53	0.0028	
	U-U	4f	6.88	0.0016	
<i>Sporomusa</i> + 0.2 mM U(VI) pH 4	U=O	2f	1.78	0.0023	8.7
	U-O _{eq1}	3.7	2.38	0.0061	
	U-O _{eq2}	1.1	2.53	0.001	

f: fixed parameter.

The analysis of the data obtained with planktonic cells of the Äspö-strain *P. fluorescens* showed that depending on availability of PO_4^{3-} and metabolic activity of the cells the formation of highly crystalline meta-autunite-based structure occurred. If no PO_4^{3-} added then the U(VI) biosorption on functional groups of the cell envelope dominates. Our results of the biofilm samples brought us to the conclusion that the meta-autunite formation was enhanced in comparison to planktonic cells. The biofilm is more efficient in terms of U(VI) detoxification. In case of U(VI) interactions with *Paenibacillus* sp. at pH 7 indications were found for a polynuclear U(VI) surface complex at the cell envelope. *Sporomusa* sp. was able to reduce U(VI) to U(IV) at pH 7 without any added e- donor. However, no reduction occurs at pH 4. The data evaluation is still in progress.

Acknowledgements. This work is supported by the BMWi (no. 02E10618).