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ROBL CRG at the ESRF

ROBL-CRG

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beamtime for measurements on ROBL (BM 20) at the ESRF. This double-page report will be reduced to a one page, A4 format, and will be published in the Annex to the ROBL Bi-Annual Report. The report may be put on the Web-pages of the FZR. If necessary, you may ask for an appropriate delay between report submission and publication.

Should you wish to make more general comments on the experiment, enclose these on a separate sheet, and send both the Report and comments to the FZR or ROBL team.

Published papers

All users must give proper credit to ROBL staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to ROBL (will be submitted to the Joint ESRF/ ILL library) the complete reference and the abstract of all papers appearing in print, and resulting from the use of ROBL.

Deadlines for submission of Experimental Report

Normally, reports should be submitted not later than 6 month after the experiment.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal / experiment to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.
- bear in mind that the double-page report will be reduced to 71% of its original size, A4 format. A type-face such as “Times” or “Arial” , 14 points, with a 1.5 line spacing between lines for the text produces a report which can be read easily.

Note that requests for further beam time must always be accompanied by a report on previous measurements.

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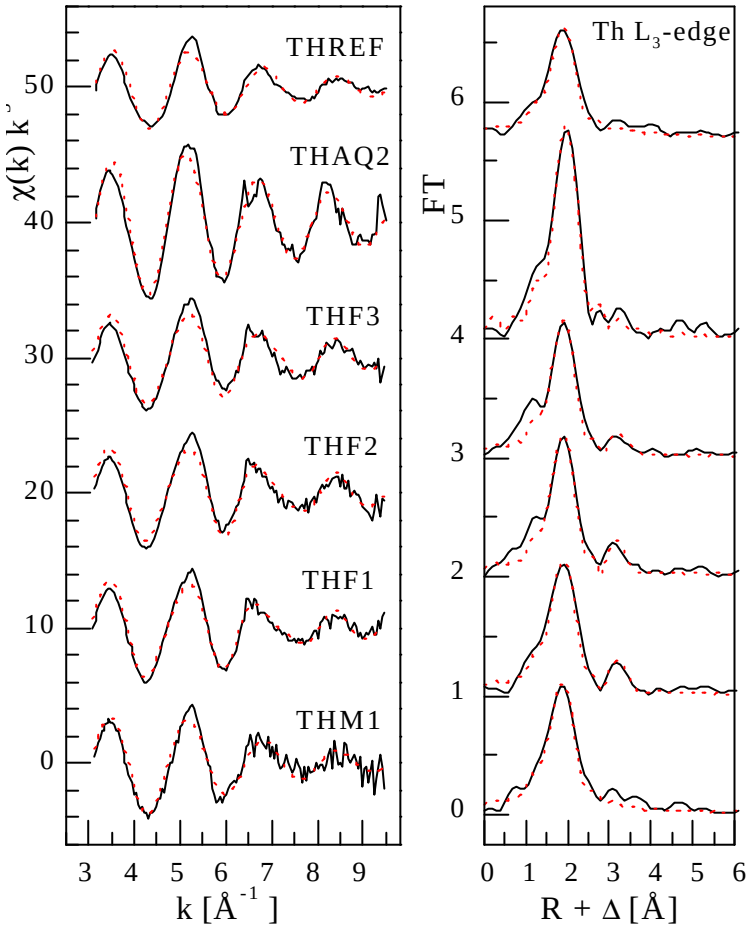
ROBL-CRG	**Study of the surface complexes formed between thorium and iron corrosion products.**	**Experiment number**: ME-815
Beamline: BM 20	**Date of experiment**: from: 25/02/04 to:27/02/04	**Date of report**: March , 2004
Shifts: 6	**Local contact(s)**: Christoph Hennig	*Received at ROBL:*
Names and affiliations of applicants (* indicates experimentalists):Mireia Grivé*, Lara Duro, Ferran Seco, Frederic Clarens*, Isabelle Bonhour*, Joan de Pablo, Jordi Bruno		

INTRODUCTION: The objective of this work is the spectroscopic study of surface interaction mechanisms between a tetravalent actinide, Th, and the products of corrosion of the steel canister used in a HLNW repository. The selection of Th as metal to study is straigthfoward. Under the reducing environment expected to develop in the vicinity of the spent nuclear fuel stored in the repository, the most stable redox states for the long-lived actinides is the tetravalent state (Th(IV), U(IV) and Pu(IV) mainly). The elucidation of the structure of the surface species formed between the surface of the corrosion products and these metals will help in the understanding of their sorption mechanims, what can lead to a better and more proper assessment of the concentrations of these metals likely to occur when in contact with the mineral. This can have important implications in risk assessment given that normally the sorption processes are conceptualised as distribution coefficients in the mentioned risk assessments, what poses important limitations to the confidence-building process necessary to ensure in this type of safety exercises.

EXPERIMENTAL: sorption experiments onto ferrihydrite (THF) and magnetite (THM) samples have been conducted at pH 3-4 and initial concentrations below the solubility of the most amorphous Th oxides reported. In order to maximize the surface coating of the solid, several enrichment cycles have been followed. Surface coating has been conducted from supersaturation and from undersaturation

experiments. EXAFS spectra of standard $ThO_2 \cdot xH_2O(s)$ (THREF) pellet and an aqueous reference sample at pH=3 (THAQ2) have been also recorded .

RESULTS:



Preliminary data analysis was performed using the EXAFSPAK software. Theoretical scattering amplitudes and phases for each adsorber and backscattered pair were calculated with the program FEFF8. In general, the Th-O distance (around 2.4 Å) seems to be much shorter in the sorption samples than in the aqueous sample while in this later case the coordination number of the oxygen shells is higher. In some cases a shell at ~3.9Å showing Th-Th interactions is obtained. The ~3.5 Å shell seems to correspond to the interaction Th-Fe, which has not been previously reported as far the authors are aware.