

## REDUPP NEWSLETTER No. 1 September 2011

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### **Latest News in Short**

#### **New post doc at University of Sheffield**

Claire Corkhill has on the 1<sup>st</sup> of September started her new position as postdoctoral researcher at University of Sheffield to work with Neil Hyatt on Work Package 2, Dissolution of CeO<sub>2</sub> and CaF<sub>2</sub>. Claire is taking over after Martin Stennet.

#### **Samples ready**

CeO<sub>2</sub> and ThO<sub>2</sub> samples have been fabricated in Sheffield as a part of Work Package 1. Only a few steps remain until the procedures for the CaF<sub>2</sub> samples have been optimized, and samples will be ready and characterised for a report (Deliverable 1.2) at the end of September. Also, the water samples for Work package 4 has been delivered to VTT.

#### **1<sup>st</sup> Workshop 2/9 in Stockholm**

The first REDUPP workshop was arranged at Stockholm University on September 2 2011. The purpose of the workshop was to meet and greet both internal and external people new to the project. José Godinho (Stockholm University) and Claudio Lousada (KTH) were invited to the workshop and José also demonstrated some analytical equipment to the REDUPP group.

### **General Progress**

The project is proceeding according to plan. Deliverables D7.1 – the web site – and D8.1 – Project presentation – are submitted. The first Milestone, all samples ready and delivered, is soon reached in full.

Deliverables D7.2, Communications Action Plan, and D1.1 , Samples characterised, are pending but will be submitted before the end of September.

The REDUPP project is briefly described in an article in the magazine *Materials World*: Hyatt, N.H. and Evins, L.Z. (2011) Safety - The Swedish Way. *Materials World* 19(7), 20-22. The article summarizes the KBS-3 method, and what materials research is planned to reduce remaining uncertainties.

Collaboration between REDUPP participants (Neil Hyatt , Martin Stennet) and José Godinho at Stockholm University has resulted in a paper, accepted for publication in *Journal of Nuclear Materials*. This paper is part of José's Licentiate thesis, which he defended successfully 13 September.

See overleaf for a short report from the first REDUPP workshop.

See [www.skb.se/REDUPP](http://www.skb.se/REDUPP) for more information on the project.

## Short report: The first REDUPP workshop

### REDUPP Participants:

Peter Oppeneer, Pablo Maldonado, Kaija Ollila, Emmi Myllykylä, Claire Corkhill, Lena Evins

External participants: José Godinho (SU), Cláudio Lousada (KTH)

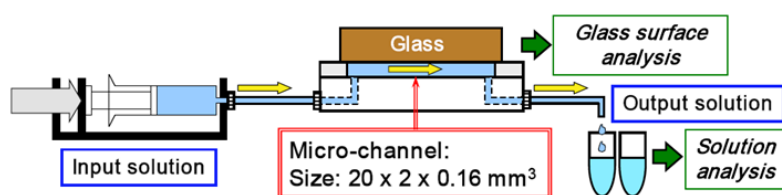


Fig 1. Micro-channel flow through set-up for dissolution experiments

The workshop was arranged at Stockholm university so that we could combine informal presentations of progress in the work packages with demonstrations of instrumentation available for surface analyses at Stockholm university.

José presented his PhD project (at SU), which has many similarities to the REDUPP project. José showed the microstructures of sintered CaF<sub>2</sub> pellets CeO<sub>2</sub> and how he has connected EBSD and Confocal Profilometry to connect surface retreat rates with crystallographic orientations. The data suggests that, during dissolution, the surface adjusts so that the most stable planes are exposed to solution.

Claire presented information on sample preparation and instrumentation set-up for dissolution experiments. The temperature dependence on microstructures was shown for CeO<sub>2</sub> and ThO<sub>2</sub>. Two different dissolution set-ups were described: Single pass flow through, and Micro-channel flow through (Fig 1.).

Emmi showed the first images of the ThO<sub>2</sub> samples produced with Confocal Profilometry and EBSD at SU. The unpolished top of a sintered pellet showed no pores, while the polished inner section did. The plans for the first year include three-month long preliminary dissolution tests to evaluate the resulting Th levels in solution for optimizing HR-ICP-MS analyses.

Kaija presented the first field analyses of the water samples from Olkiluoto. The groundwater was purged with Ar, but was observed to experience an increase in pH and decrease in alkalinity due to CO<sub>2</sub> escape.

Claudio presented his PhD project (at KTH) concerning surface reactions involving radiolysis products on various metal oxides. The project combines experimental and theoretical (DFT) investigations concerning kinetics and mechanisms for H<sub>2</sub>O<sub>2</sub> decomposition on surfaces of ZrO<sub>2</sub>, TiO<sub>2</sub>, and Y<sub>2</sub>O<sub>3</sub>.

Pablo distributed before the workshop a first report (unpublished) on the CaF<sub>2</sub> and CeO<sub>2</sub> *ab initio* study. This was presented and explained. The first results show the number of layers required for a stable surface model (6-8) and the relative surface stabilities for different planes. The (100) has a low stability and is a polar surface in CeO<sub>2</sub>. Results from modelling H<sub>2</sub> adsorption on CeO<sub>2</sub> were presented.

José guided the REDUPP group to the EBSD and Confocal Profilometry laboratories. ThO<sub>2</sub> was being analysed by EBSD during our visit.

The workshop was finished with a short discussion concerning collaboration and deliverables, with a focus on joint publications.

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