Experimental Report

Proposal: **5-21-1072** **Council:** 4/2012

Title: Structural investigation of Na3UO4by neutron diffraction

This proposal is a new proposal

Researh Area: Materials

Main proposer: **RAISON Philippe**

Experimental Team: RAISON Philippe
BYKOV Denis
SMITH Anna

Local Contact: SUARD Emmanuelle

Samples: Sodium uranate/ Na3UO4

Instrument	Req. Days	All. Days	From	To
D2B	2	2	26/11/2012	28/11/2012

Abstract:

We are interested in the safety aspects of Sodium-cooled Fast Reactors (SFR) and more specifically by the potential interaction of sodium with the fuel (U, Pu)O2. Indeed, in case of a clad breach, though extremely rare during normal operating conditions, sodium will enter the fuel pin and react with the fuel. Studies carried out in the past in equilibrium conditions have revealed the formation of an urano-plutonate of sodium of general formula Na3MO4 with M = U, Pu. The compound thus formed is of lower density and has a lower thermal conductivity than the fuel leading to local swelling and development of hot spots that could further damage the cladding up to a pin failure. In that regard we would like to revisit the structure of the Na3UO4 compound for which controversial structures have been suggested. Our experiment is aimed to lift the controversy by determining the alpha-form of Na3UO4 by neutron diffraction and possibly also revisit the beta-form which occurs above 975°C.

Report on a structural investigation of Na_3UO_4 by neutron diffraction

On November 27 2012, a powder neutron diffraction experiment was performed on the compound Na_3UO_4 at the Institute Laue-Langevin on the high-resolution diffractometer D2B. The experiment was aimed at determining the crystallographic structure of the compound Na_3MO_4 (M= An, Pu) which is the main product of reaction between the sodium and the fuel in a Sodium-cooled Fast Reactor (SFR) in case of a clad breach. This work is part of A. Smith's PhD. The experiment was a success. Initially reported as cubic in the literature [1] it was determined that the compound actually adopts a monoclinic structure. The Rietveld analysis of the neutron diffraction data is shown in figure 1. The results will soon be published in the literature in conjunction with XANES and ^{23}Na MAS-NMR experimental data.

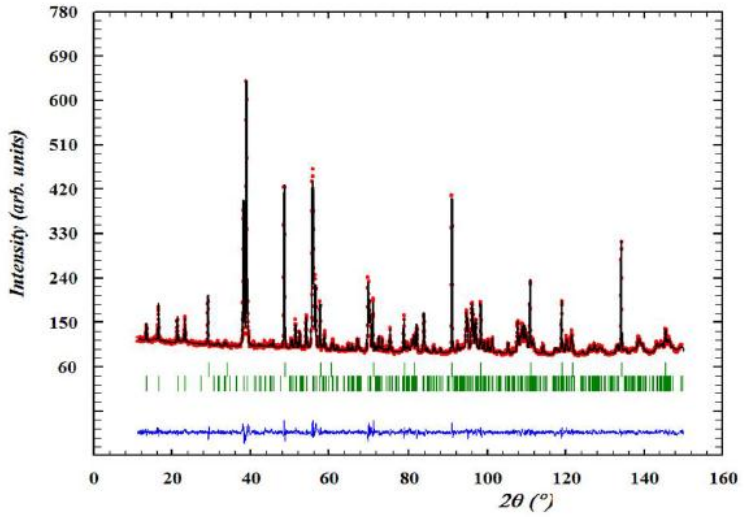

Figure 1*: Comparison between the observed (Y_{obs} in red) and calculated (Y_{calc} in black) neutron diffraction pattern of the α-$Na_{3.2}U_{0.8}O_4$ phase. Y_{obs}-Y_{calc}, in blue is the difference between the experimental and calculated intensities. The Bragg reflections are marked in green. Upper UO_2. Lower α-$Na_{3.2}U_{0.8}O_4$. (λ = 1.594 Å).*

Reference

[1] S.F Bartram and R.E. Frixell, J. Inorg. Nucl. Chem. 32(1970) 3701