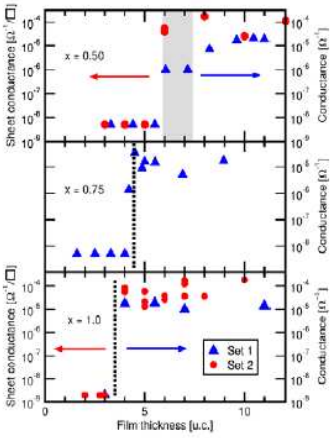
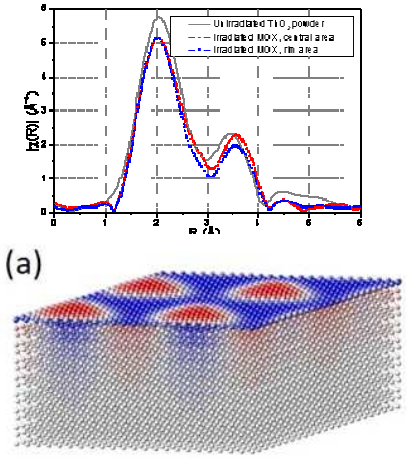
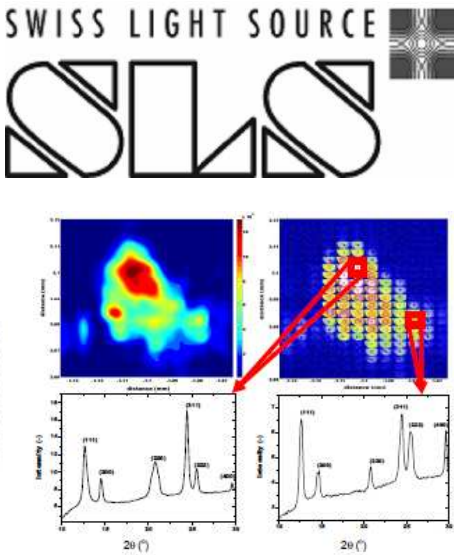






SLS Symposium on

Materials

Tuesday, May 8, 2012

10:00 to 12:15, WBGB/019

10:00 Thorium characterization in plutonium uranium mixed oxide fuel by X-ray absorption
Cedric Cozzo, A. Orlov, C.N. Borca, D. Grolimund and C. Degueldre

10:30 Atomic scale structural changes in an irradiated nuclear fuel
C. Mieszczynsk, G. Kuri, C. Degueldre, M. Martin, J. Bertsch, C. N. Borca, D. Grolimund, Ch. Delafoy, E. Simoni

11:00 Coffee

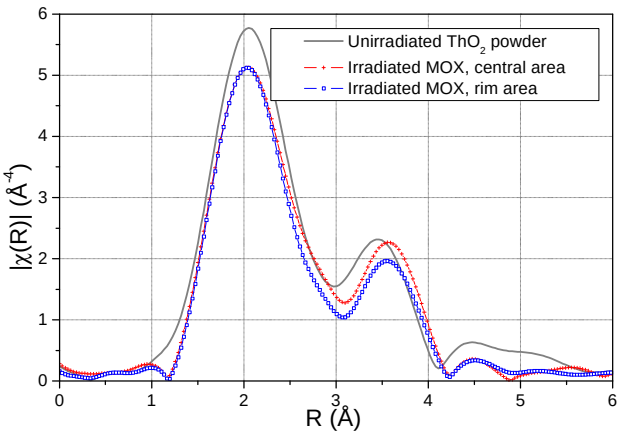
11:15 Surface X-ray diffraction study of graphene and hexagonal boron nitride on transition metal surfaces
I. Kalichava, M. Ianucci, D. Martoccia, S. Leake, Phil Willmott, T. Greber

11:45 Tunable conductivity threshold at polar oxide interfaces: implications for understanding its origin
M. L. Reinle-Schmitt, C. Cancellieri, D. Li, D. Fontaine, M. Medarde, E. Pomjakushina, C. W. Schneider, S. Gariglio, Ph. Ghosez, J.-M. Triscone and P. R. Willmott

Thorium characterization in plutonium uranium mixed oxide fuel by X-ray absorption

Cedric Cozzo, A. Orlov, C.N. Borca, D. Grolimund and C. Degueldre
NES & SYN, Paul Scherrer Institute, 5232 Villigen, Switzerland

In non-extreme redox environment, thorium presents only one stable oxidation state (IV). Therefore, thorium in pristine and irradiated MOX samples has been used as a reference. Its characterization can be used as a solid base for the study of the other actinides with the same oxidation state An(IV).
In a current work, the structure and next-neighbour atomic environment of thorium within irradiated (60 MWd kg^{-1}) MOX samples was analyzed by micro-X-ray absorption fine structure (µ-XAFS) spectroscopy measured in fluorescence mode. The experimental spectra were obtained from the peripheral (rim) and central zones on the fuel cross-section. In addition, spectra of non irradiated pure thoria (ThO_2) powder samples were recorded to provide the spectrum of pristine ThO_2. The number of next neighbours as well as their distances from the absorber atom are discussed. The experimental data were also compared to XAFS calculations for thorium.



Atomic scale structural changes in an irradiated nuclear fuel

C. Mieszczynski[1,*], G. Kuri[1], C. Degueldre[1], M. Martin[1], J. Bertsch[1], C. N. Borca[1], D. Grolimund[1], Ch. Delafoy[2], E. Simoni[3]

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Uranium dioxide nuclear fuel, UO_2, with fissile ^{235}U enrichment is normally used in commercial power plants. Fission of ^{235}U generates light and heavy fission fragments and disturbs both cation-cation and cation-anion network in the fuel matrix. The overall fuel performance, however, is associated with many parameters under high temperature oxidizing conditions in the reactor. Due to incorporation of fission products in the UO_2 matrix, fuel swelling, a modification to the local chemical composition of the fuel and/or structural damage leading to polygonization of the original 'mother' grains may occur [1,2]. Therefore, in order to improve the properties of nuclear fuels it is considered necessary to understand micro- and atomic-scale structural changes taking place in irradiated UO_2.

In this work micro-focused X-ray diffraction (μ-XRD) and X-ray absorption fine structure (μ-XAFS) spectroscopy are used to examine the lattice structure of UO_2 and the next neighbor atomic environment in a UO_2 pellet irradiated to a medium burn-up at a Swiss nuclear power plant. Micro-structures, having evolved at two different radial positions, such as the center-region and the rim-zone [2], of the irradiated fuel pellet are examined. Measurements are also carried out on a fresh (pristine) UO_2 pellet of the same batch used for the irradiation experiment. Structural changes in the irradiated UO_2 grains, grain subdivision, lattice parameters, local distortion and lattice dilation in the irradiated material are measured from XRD data. XAFS has been applied to identify element specific local atomic structure of this irradiated material. The possibility of fission product segregation and their local enrichment when incorporated in the UO_2 lattices have been explored in the data analysis. All these results will be presented and discussed.

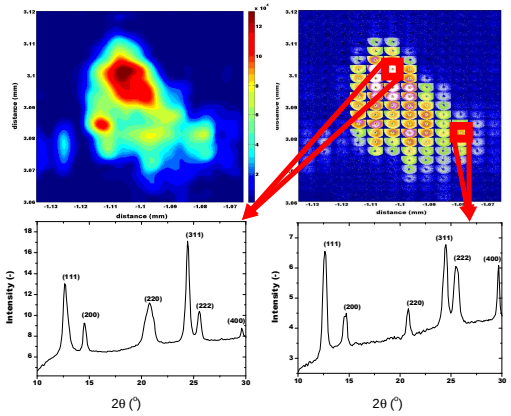

Figure 1: Examples of micro-XRF and micro-XRD maps of the irradiated fuel particle, and integrated diffraction intensity plots from two different regions in the fuel particle are shown.

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[2] C. Mieszczynski et al., Prog. Nucl. Eng. 57 (2012) 130-137.

Surface X-ray diffraction study of graphene and hexagonal boron nitride on transition metal surfaces

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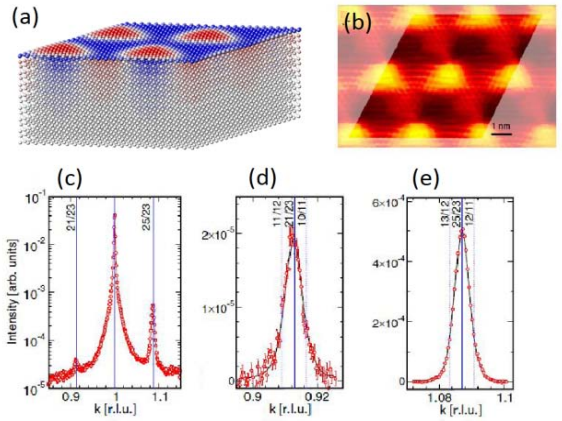
Graphene is a one of the carbon allotrope representing single sp2-hybridized layer of carbon atoms arranged as a honeycomb structure. Graphene grown epitaxialy on transition metals forms single-domain large superstructures with high structural perfection [1]. The lattice mismatch between the substrate and a carbon layer causes periodically varying strength of chemical bond with the substrate across the surface, the monolayers tend to corrugate and morph into a highly ordered periodic supercell [2]. The graphene superstructures may provide template functionality for nanocluster array grow, catalytic or biological applications.

We perform Surface X-ray diffraction (SXRD) studies of graphene on different transition metal substrates. SXRD as a non-destructive sub-angstrom resolution tool allows directly observe graphene reconstruction signals and provides information about registry between graphene and the underlying substrate. It will be shown that the model fitting based on SXRD data gives quantitative information about graphene on Ru(0001) surface structure.

Another object of interest is a single layer of hexagonal boron nitride (h-BN) which forms a regular superstructure (nanomesh) on transition metals. We are concentrated to study such h-BN nanomesh structures on PtRh(111) single crystal where nanomesh induces lateral metal segregation of PtRh substrate.



(a) The 3D model of the structure. (b) The STM image of the graphene superstructure. (c),(d) and (e) The in-plane scans along the k direction in reciprocal space detailing 25-on-23 reconstruction signal.

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Tunable conductivity threshold at polar oxide interfaces: implications for understanding its origin

M. L. Reinle-Schmitt[1], C. Cancellieri[1], D. Li[2], D. Fontaine[3], M. Medarde[1], E. Pomjakushina[1], C. W. Schneider[1], S. Gariglio[2], Ph. Ghosez[3], J.-M. Triscone[2] and P. R. Willmott[1]

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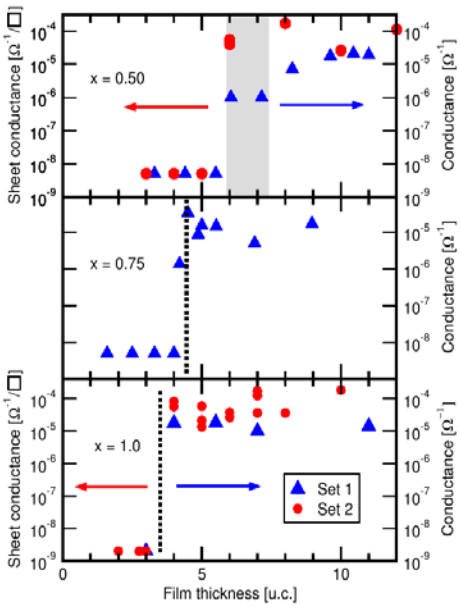
The prototypical system of $LaAlO_3/SrTiO_3$ exhibits, among other unexpected properties [1-4], a transition from an insulating to a metallic interface at a critical thickness of $LaAlO_3$ of 4 unit cells, in agreement with an *intrinsic* polar catastrophe scenario [5, 6, 7]. However, models explaining the conductivity in terms of *extrinsic* effects caused by structural deviations from a perfect interface, such as oxygen vacancies and interfacial intermixing, have also been proposed [8, 9].



The physical properties of ultrathin films of the solid solution $(LaAlO_3)_x$ $(SrTiO_3)_{(1-x)}$ grown on $SrTiO_3$ were investigated as a function of film thickness and x. We observe an insulating interface for the thinnest films that becomes conducting above a critical thickness which depends on x in a predictable way (see figure).

These results can be best described in terms of the i*ntrinsic* polar-catastrophe model, hence providing the most compelling evidence to date in favour of this mechanism.

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