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Interaction Between Metal Fission Products and TRISO Coating Materials: A study of Chemical Bonding and Interdiffusion: 4th Quarter Report, 2004

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Task 17: Interaction between metal fission products and TRISO coating materials:

A study of chemical bonding and interdiffusion

(PI: C. Heske, Department of Chemistry, UNLV;
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Undergraduate Student: J. White)

The goal of this project, which started in May 2004, is to elucidate the chemical bonding and interface formation of metal fission products with the coating materials used in state-of-the-art TRISO fuel particles. Particular emphasis is placed on an analysis of intermediate chemical phases at the interface, the intermixing/diffusion behavior, and the electronic interface structure as a function of material choice (metal and coating materials), temperature, and external stress. In detail, this project is devoted to studying the interface formation of Pd, Ag, and Cs with SiC and pyrolytic carbon. In order to study the properties of the relevant interfaces, we prepare such interfaces under controlled conditions in an ultra-high vacuum environment and study them with a variety of different spectroscopic methods, i.e., surface sensitive techniques (in particular photoelectron spectroscopy – XPS and UPS) and bulk sensitive methods (in particular X-ray emission spectroscopy - XES).

In the last quarter, our efforts were focused on two areas, namely (1) to organize the arrival and reassembly of the four-chamber ultra-high vacuum surface science instrument on the UNLV campus and (2) to conduct first XES experiments at the Advanced Light Source, Lawrence Berkeley National Laboratory.

As shown in Fig. 1, the instrument has arrived safely on the UNLV campus after an 8 week transit from the University of Würzburg, Germany, and several weeks in customs.

Currently, almost all components are reinstalled and first vacuum tests were successfully conducted on Jan 14, 2005. It appears that transit-related damage is minimal, in large parts due to an excellent packing job of the group members from UNLV and the University of Würzburg. First experiments will be conducted within the next two months.



Fig. 1: Picture of the four-chamber ultra-high vacuum apparatus during set-up in the UNLV lab, showing graduate students T. Hofmann (left), V. Marepally (center), G. Gajjala (not shown), and undergraduate student J. White (right).

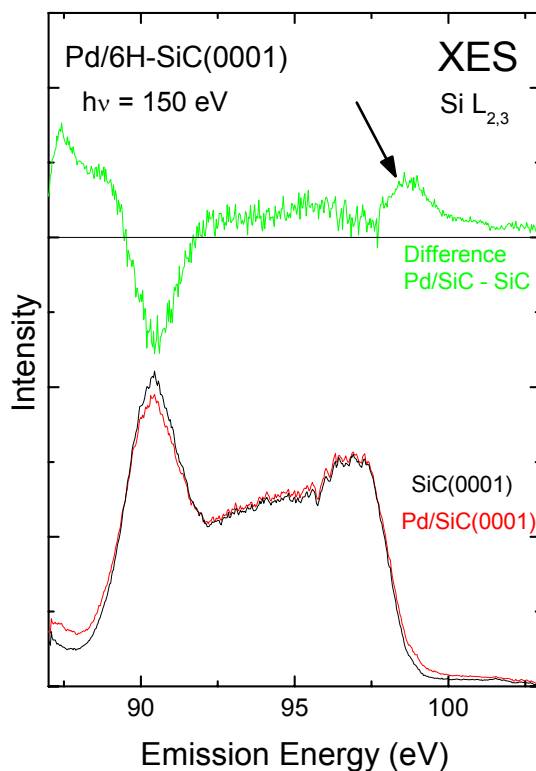


Fig. 2: Si $L_{2,3}$ x-ray emission spectra of a SiC(0001) single crystal (black) and a Pd/SiC interface (red). The difference between both spectra is shown in green (magnified by a factor of five). The arrow indicates an enhanced spectral weight near the Fermi energy, suggesting an increased metallic character of the local environment of silicon atoms at the Pd/SiC interface.

chemical carbon species at the Pd/SiC interface. In order to shed more light on this effect, we analyzed both C and Si emission spectra for the two different samples with varying excitation energies (generally called “resonant inelastic x-ray scattering” – RIXS). Two spectra taken from these series are shown in Fig. 2. When comparing the two Si $L_{2,3}$ spectra at an excitation energy of 150 eV, it becomes apparent that, due to the Pd/SiC interface formation, spectral weight is lost around 91 eV (i.e., near the bottom of the valence band) and gained between 98 and 100 eV. This is more clearly shown in the difference spectrum (green) in Fig. 2. As indicated by the arrow, we find an increase in the electronic density-of-states at these energies, which, based on a thorough energy calibration (not shown here), lie close to the Fermi energy. Note that XES is a bulk sensitive probe and hence the contribution of the interface to the overall signal is rather small (but nevertheless easily discernible in the present case). The finding of an increased electronic density of states near the Fermi edge needs further confirmation and analysis, but at present suggests that the local electronic and chemical environment of the Si atoms at the interface is strongly influenced by the interface formation and now exhibits a significantly more “metallic” character. The complete analysis of the XES and RIXS data is currently in progress, both for the Si $L_{2,3}$ spectra as well as for the C K line. The next experiments at the ALS (May 2005) will utilize “fresh” (ideally: in-situ prepared) samples as well as sample systems involving realistic SiC-layers from the TRISO coating process, and will strongly build on the student expertise gained in the November 2004 beamtime.

During the reporting period, we were able to conduct first experiments at Beamline 8.0 of the Advanced Light Source (ALS) in Berkeley. The main goal of this beamtime, apart from taking first data on Pd/SiC interfaces (see below), was to acquaint the graduate students in this project (at the time of the beamtime: G. Gajjala and V. Marepally) with the cutting-edge research environment at the ALS. This includes the operation of a soft x-ray undulator beamline, a high-end soft x-ray spectrometer, ultra-high vacuum sample transfers, radiation safety, high-efficiency 24-hour data taking, etc.

Moreover, first X-ray emission spectroscopy (XES) data could be collected using the SiC and Pd/SiC samples produced during the summer research campaign at the University of Würzburg prior to the relocation of the instrument. As described in the previous report, we there found (using photoelectron spectroscopy) that a thin Pd overlayer induces at least two new