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## Interaction Between Metal Fission Products and TRISO Coating Materials: A Study Of Chemical Bonding and Interdiffusion: 3rd Quarter Report, 2004

Clemens Heske

*University of Nevada, Las Vegas*, [clemens.heske@unlv.edu](mailto:clemens.heske@unlv.edu)

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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;

Graduate Students: G. Gajjala, V. Marepally)

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. Using the TRISO coating materials and single crystal references as substrates, interfaces are prepared under controlled conditions in an ultra-high vacuum environment and studied with a variety of different spectroscopic methods. The combination of surface sensitive techniques (e.g., photoelectron spectroscopy) with bulk sensitive methods (e.g., X-ray emission spectroscopy) probes the chemical properties as well as the diffusion behavior in several complementary ways. A variety of surface modification methods is and will be applied ex-situ (e.g., for stressed coating layers) or in-situ (e.g., by ion bombardment or plasma surface treatment) prior to or after the interface formation to study the dependence of the interface properties on the surface/interface morphology and quality of the coating material.

The project utilizes a four-chamber ultra-high vacuum surface science instrument (shown in Fig. 1), which combines several experimental techniques, including X-ray and UV photoelectron spectroscopy (XPS and UPS), X-ray and small-spot-electron-excited Auger spectroscopy

(XAES and AES), low-energy electron diffraction

(LEED), and in-situ

ellipsometry. It

allows the

modification of

surfaces by ion

bombardment,

plasma etching,

annealing, and

metal

evaporation

under strictly

controlled

conditions. The

instrument is

currently in

transit from the

University of Würzburg, Germany, to UNLV. First experiments on the Pd/SiC interface

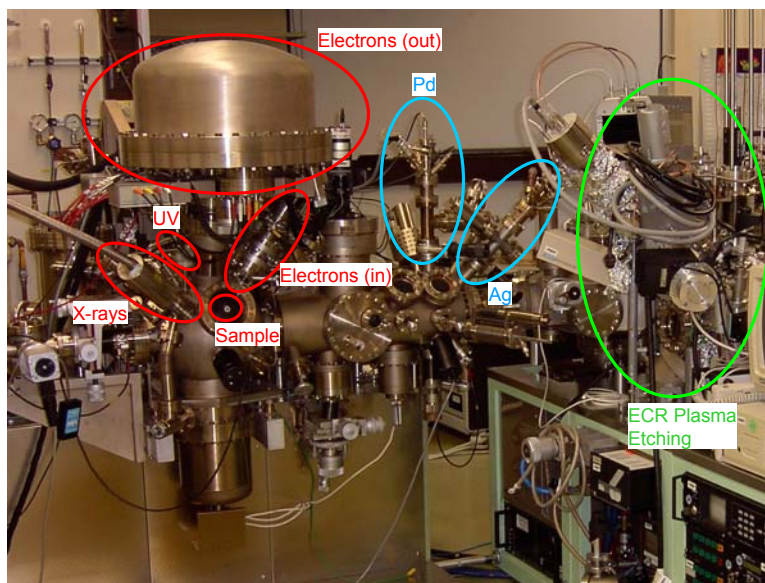


Fig. 1: Picture of the four-chamber ultra-high vacuum apparatus. Red: surface spectroscopy; blue: metal deposition, green: surface modification.

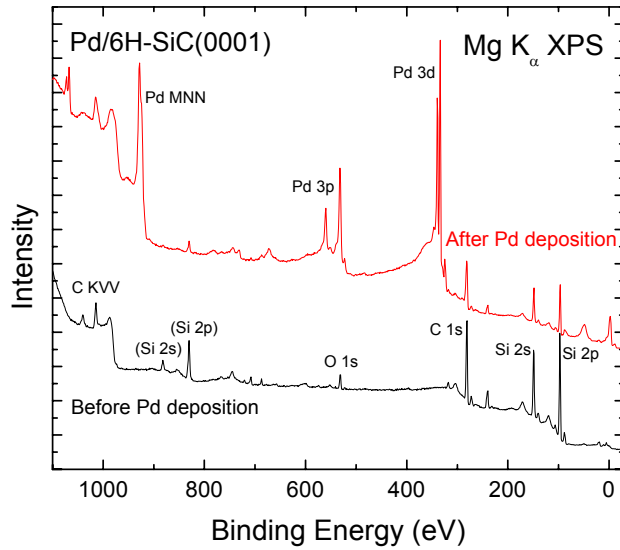


Fig. 2: X-ray photoelectron survey spectrum of a SiC(0001) single crystal before (bottom, black) and after (top, red) Pd deposition.

conducted to optimize the surface cleaning procedures for commercial SiC(0001) single crystal substrates. Fig. 2, bottom, shows an XPS survey spectrum taken after a series of ion-sputter/annealing cycles to remove surface contaminants from the surface polishing process and the air exposure (in particular Ca, O, and water). As can be seen, only a small residual signal of oxygen is present, while all other prominent peaks are associated with the SiC bulk material. This surface was used to collect first data on the room temperature Pd/SiC interface formation by depositing a thin (less than 1 nm) layer of Pd (top spectrum in Fig. 2). This leads to the observation of Pd-related lines and an attenuation of the SiC peaks. In order to gain insight into the chemical interaction at the Pd/SiC interface, a detailed analysis of the individual XPS peaks is currently being conducted. As an example, Fig. 3 shows a close-up of the Carbon 1s peak. Again, the bottom

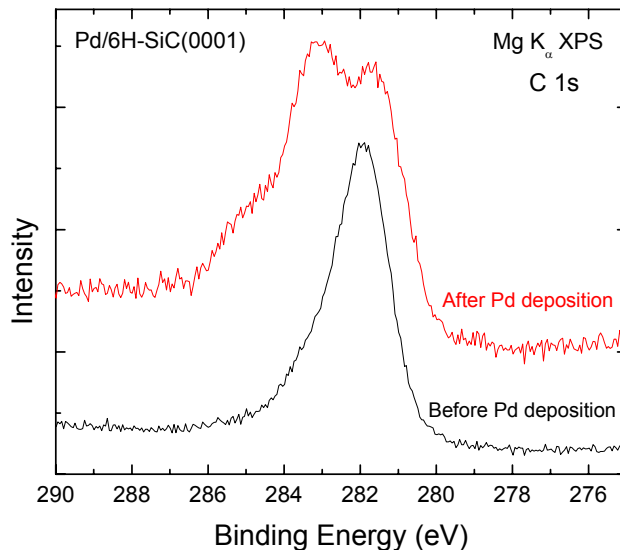


Fig. 3: X-ray photoelectron spectra of the C 1s peaks before (bottom, black) and after (top, red) Pd deposition.

could be conducted in Würzburg during the summer of 2004 before dismantling the system for shipment (see results below).

A second line of experiments is being conducted at the Advanced Light Source, Lawrence Berkeley National Laboratory (Beamline 8.0, SXF endstation). The first experimental campaign, in which the Pd/SiC interface will be studied by soft X-ray emission spectroscopy, is scheduled for the end of November.

### First Results

After getting all researchers acquainted with the operation of the ultra-high vacuum equipment, several experimental runs were

conducted to optimize the surface cleaning procedures for commercial SiC(0001) single crystal substrates. Fig. 2, bottom, shows an XPS survey spectrum taken after a series of ion-sputter/annealing cycles to remove surface contaminants from the surface polishing process and the air exposure (in particular Ca, O, and water). As can be seen, only a small residual signal of oxygen is present, while all other prominent peaks are associated with the SiC bulk material. This surface was used to collect first data on the room temperature Pd/SiC interface formation by depositing a thin (less than 1 nm) layer of Pd (top spectrum in Fig. 2). This leads to the observation of Pd-related lines and an attenuation of the SiC peaks. In order to gain insight into the chemical interaction at the Pd/SiC interface, a detailed analysis of the individual XPS peaks is currently being conducted. As an example, Fig. 3 shows a close-up of the Carbon 1s peak. Again, the bottom spectrum pertains to the clean SiC surface, while the upper spectrum was derived from the carbon atoms at and near the Pd/SiC interface. Even without a detailed peak-fitting analysis, which is currently in progress, it is evident that at least two additional chemical carbon species exist after Pd deposition. In an initial-state picture, the fact that the new species appear at higher binding energies indicates a charge transfer away from the carbon atoms. This effect is currently being further analyzed (e.g., by investigating the Si 2p spectra) and will be further

studied after the reassembly of the instrument at UNLV is completed.