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# Interaction between metal fission products and TRISO coating materials: A study of chemical bonding and interdiffusion: 1st quarterly report, 2006

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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, T. Hofmann;  
Undergraduate Students: J. White, K. George, J. Peiser)

- G. Gajjala successfully prepared and defended his Master thesis at the UNLV Dept. of Electrical Engineering
- Constructed new Cs evaporator (for Cs/SiC experimental campaign, to be performed by S. Sudarshanam)
- Reactivated four-chamber UHV instrument after Chemistry department asbestos abatement shutdown, replaced central oil-diffusion pumps by turbomolecular pumps to lower operating costs

This project is devoted to an in-depth study of the chemical and electronic impact of metal fission products on the coating layers in TRISO nuclear fuel. In particular, there is a focus on the investigation of Pd, Cs, and Ag and their interface formation with SiC and carbon-based substrates. A variety of surface and near-surface bulk sensitive probes that investigate the occupied and unoccupied electronic states of the substrate and the metal overlayer have been utilized. By a controlled and stepwise deposition of the metal overlayer, it is possible to gain substantial insight into the formation of interfaces and their intermixing behavior.

In the past quarter, there has been a focus on a detailed analysis and description of the Pd/SiC interface formation process. This description is documented in the Masters thesis of Goverdhan Gajjala, which was successfully defended at the UNLV Dept. of Electrical Engineering. As an example from the thesis, Figure 1 shows a series of X-ray photoelectron spectroscopy (XPS) survey spectra, that were taken for a SiC single crystal substrate after introduction into the system, after sputter-cleaning with Ar<sup>+</sup> ions (2 keV), and after several Pd deposition steps. In this particular case, the Pd deposition was performed at approx. 800 degrees C to simulate elevated temperatures in TRISO fuel. Furthermore, the SiC surface was very strongly sputtered, which induces a significant number of structural defects at the surface and is hence intended to simulate real SiC surfaces. Fig. 2 gives an example of a detailed UV photoelectron spectroscopy (UPS) study of the corresponding samples, indicating how the electronic surface structure is converted from an adsorbate-induced character to a semiconductor (SiC) to a metallic thin film (for increasing Pd overlayer thickness). A detailed analysis of the valence band maxima and Fermi edges shown in Fig. 2, together with a study of the work function (which can be derived from the secondary electron cutoff in the UPS spectra) gives detailed insight into the electronic structure of the Pd/SiC interface, which can be interpreted in view of pronounced intermixing effects, as well as the formation of an electronic Schottky barrier.

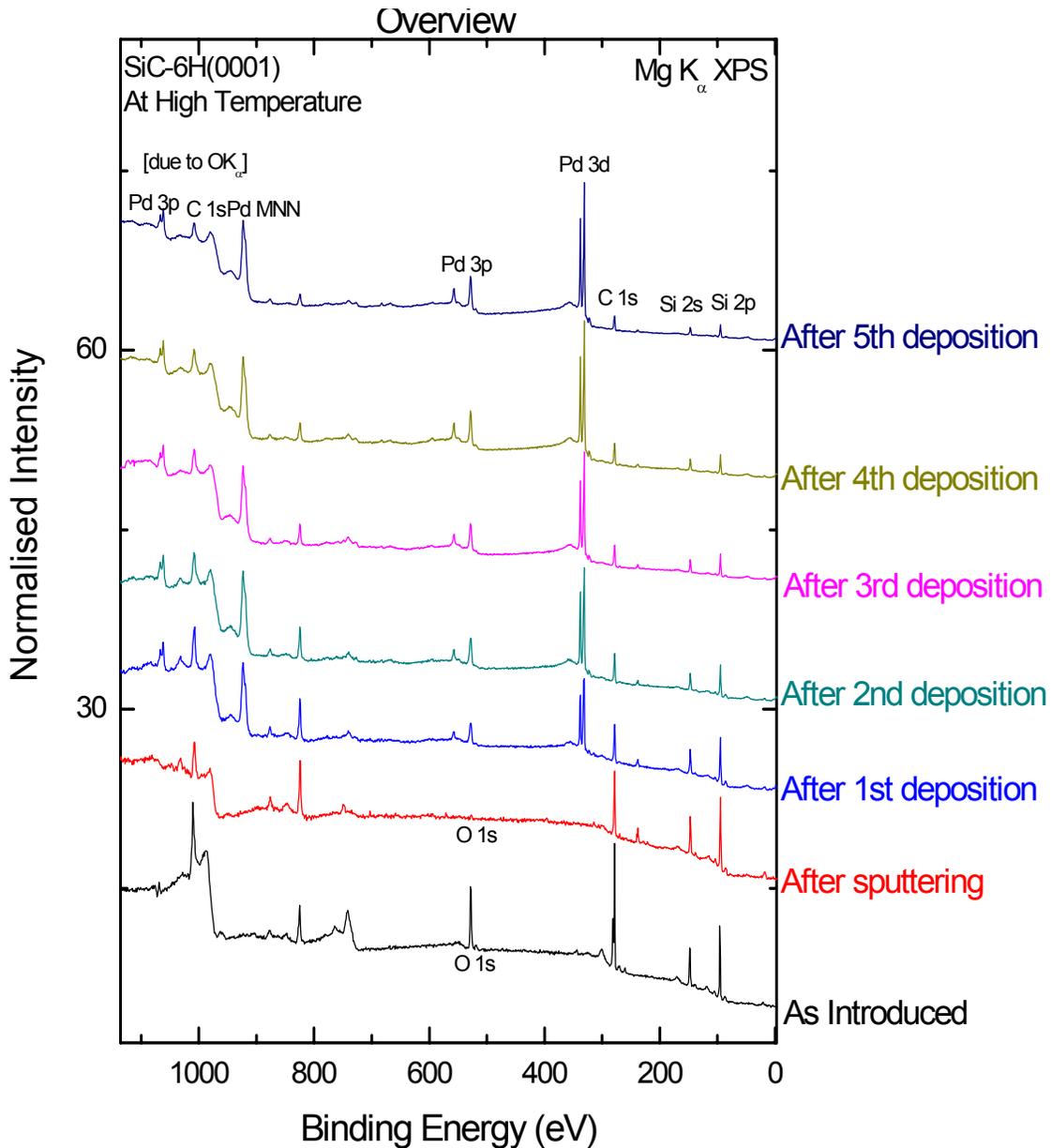
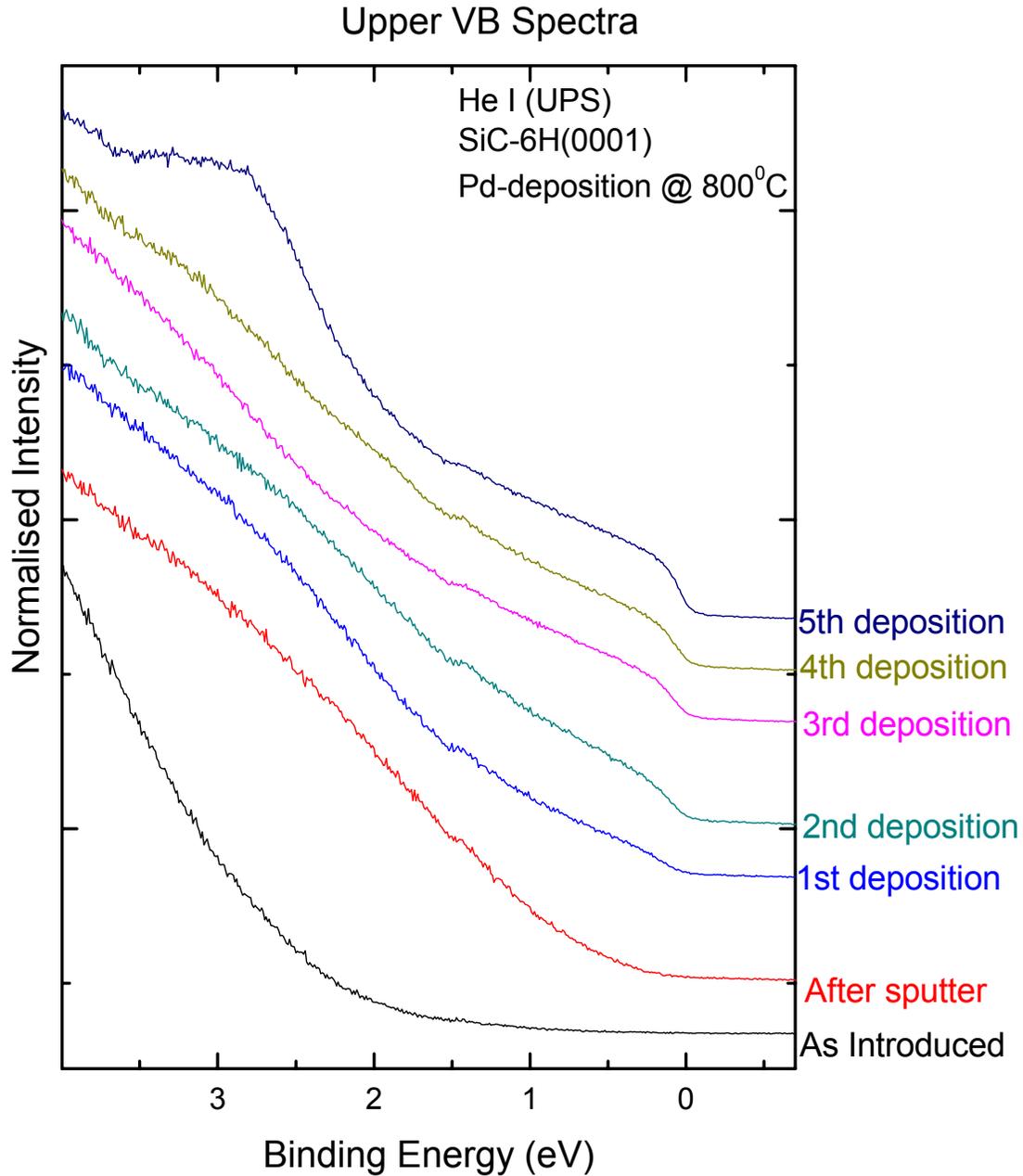


Fig. 1: XPS survey spectra of an as-introduced SiC-6H(0001) single crystal surface, after 2 keV  $Ar^+$  ion sputtering, and after several Pd deposition steps at approx. 800°C. The spectra indicate the removal of oxygen species due to the sputter process and the gradual increase in Pd emission intensity as a function of Pd coverage. Likewise the C 1s and Si 2s and 2p signal are decreasing with increasing Pd coverage.

In the thesis of Goverdhan Gajjala, the results obtained from the sample series in Figs. 1 and 2 are compared with a similar series that was obtained at room temperature. Furthermore, the first experimental series, which was taken at the University of Wuerzburg (before relocation of instrument to UNLV), can be well compared. In all cases, the presence of two additional carbon species at the interface are found, one associated with a short-range charge transfer (the actual chemical bonding) and a longer-range interdiffusion species (in addition to the expected SiC bulk species). Combining all spectral regions (in XPS and UPS), a detailed picture of the Pd/SiC interface formation can be painted.



*Fig. 2: UPS spectra of the upper valence band as a function of Pd deposition. The as-introduced sample exhibits a large separation between valence band maximum (VBM) and Fermi energy, which is ascribed to surface contaminations. These contaminations can be effectively removed by the sputter cleaning, revealing the actual position of the SiC VBM. Upon deposition of Pd, a metallic Fermi edge is formed, which exhibits a shift towards lower binding energy due to the increased size of Pd islands on the surface.*

The Pd/SiC results are currently being prepared for publication in a peer-review journal. For this purpose, some additional data must be collected in order to allow a reliable quantitative analysis of the bonding and interdiffusion processes. This is necessary, because our old electron analyzer (ESCALab MkII) showed irreproducible background problems, as previously reported. At the time of writing of this report (mid-April), the

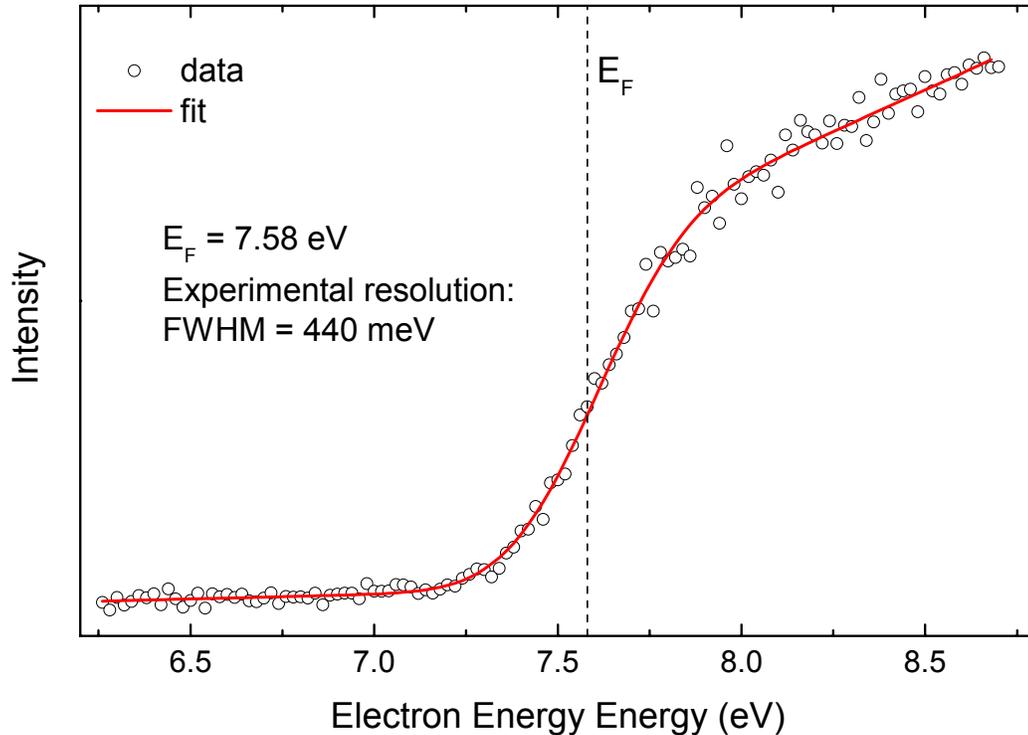


Fig. 3: Inverse Photoemission (IPES) spectrum of the Fermi edge of a Ag reference foil, indicating excellent signal-to-noise-ratio and a very good energy resolution of 0.44 eV.

electron analyzer has been replaced by a modern state-of-the-art instrument (SPECS PHOIBOS 150MCD) that not only allows a much more reliable quantitative analysis, but also a significantly improved energy resolution, shorter accumulation time, and drastically enhanced signal-to-noise ratio.

Finally, the new Inverse Photoemission set-up has been put to routine use. Figure 3 shows, as an example, an IPES spectrum of a Ag reference foil, indicating both an excellent signal-to-noise ratio as well as very good energy resolution. In all further experimental series, IPES can thus now be included to give complementary information about the unoccupied electronic states, in particular the conduction band minimum (CBM).

In addition to completing the existing Pd/SiC data set, the investigation of the Cs/SiC interface is being prepared – a Cs evaporator has been designed and is currently being constructed by Sharath Sudarshanam.