Electronic structures of UTSn (T=Ni, Pd) using photoemission spectroscopy

J.-S. Kang¹, S. C. Wi¹, J. H. Kim¹, K. A. McEwen², C. G. Olson³, J. H. Shim⁴, and B. I. Min⁴

¹Department of Physics, The Catholic University of Korea, Puchon 420-743, Korea
²Department of Physics and Astronomy, University College London, WC1E 6BT, UK
³Ames Laboratory, Iowa State University, Ames, Iowa 50011, U.S.A. and
⁴Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea
(Dated: November 9, 2017)

The electronic structures of the localized 5f systems UTSn (T=Ni, Pd) have been investigated using photoemission spectroscopy (PES). The extracted U 5f PES spectra of UTSn (T=Ni, Pd) exhibit a broad peak centered at ~ 0.3 eV below E_F with rather small spectral weight near E_F (N_f/E_F). The small N_f(E_F) in UTSn is found to be correlated with the T d PES spectra that have a very low density of states (DOS) near E_F. The high-resolution PES spectra for UTSn provide the V-shaped reduced metallic DOS near E_F but do not reveal any appreciable changes in their electronic structures across the magnetic phase transitions. A possible origin for the reduced N_f/E_F in UTSn is ascribed to the hybridization to the very low T d DOS at E_F. Comparison of the measured PES spectra to the LSDA+U band structure calculation reveals a reasonably good agreement for UPdSn, but not so for UNiSn.

PACS numbers: 79.60.-i, 71.20.Eh, 71.27.+a

I. INTRODUCTION

Uranium intermetallic compounds often exhibit interesting magnetic behavior that is neither very localized nor very itinerant. UNiSn and UPdSn are considered to be well localized with small linear specific-heat coefficient, \( \gamma \approx 18 - 28 \text{ mJ/mol K}^2 \) and \( \gamma \approx 5 \text{ mJ/mol K}^2 \), respectively, and with the large ordered magnetic moments of ~ 1.55 µB and ~ 2 µB, respectively, which are significantly larger than in other U intermetallic systems. Both UNiSn and UPdSn exhibit interesting phase transitions with the antiferromagnetic (AF) ground states. UNiSn displays an AF order below the Neel temperature \( T_N \approx 43 \text{ K} \), a structural transition from the cubic symmetry to the tetragonal symmetry at \( T_{Nt} \), and a semiconductor-to-metal (S-M) transition around \( T_{MI} \approx 55 \text{ K} \). This multiple phase transition seems to be anomalous because it is an inverse metal-insulator transition with a gap-opening above \( T_N \) and the structural, S-M, and AFM transitions occur concomitantly. Hexagonal UPdSn also displays two AF transitions with concomitant lattice distortions. UPdSn undergoes an AF transition below \( T_N \approx 37 \text{ K} \) with the orthorhombic magnetic symmetry (phase I), and undergoes another AFM transition below \( \approx 25 \text{ K} \) with the monoclinic magnetic symmetry (phase II). Both AF structures in UPdSn are reported to be noncollinear. The resistivity of UPdSn shows a metallic behavior in the whole temperature range but with a feature of rapid drop below \( T_N \approx 37 \text{ K} \).

The underlying mechanism of the peculiar multiple phase transitions in UNiSn and UPdSn has been investigated extensively\(^{9,10,11}\). A quadrupolar ordered phase based on the crystalline electric field (CEF) level scheme for the localized 5f\(^2\) (U\(^{4+}\)) configuration\(^{9}\) has been proposed for the phase transitions in UTSn\(^{11}\), which seems to be consistent with the neutron inelastic scattering data\(^{11}\). In contrast, the localized 5f\(^3\) (U\(^{3+}\)) configuration was proposed based on the neutron diffraction data for UPdSn\(^{12}\). Some electronic structure calculation for UPdSn supports the localized U 5f\(^2\) configuration\(^{13}\), whereas other calculations argue the itinerant character of U 5f electrons in UNiSn\(^{14}\) and UPdSn\(^{15}\).

II. EXPERIMENTAL AND CALCULATIONAL DETAILS

UNiSn and UPdSn polycrystalline samples are made by arc melting constituent elements of high purity. Our magnetization measurements taken on the sample after one month annealing showed clear antiferromagnetic transitions in agreement with previous results\(^{8,16}\). Photoemission experiments were carried out at the Ames/Montana ERG/Seya beam-line at the Synchrotron
Radiation Center. The details of PES experiment are the same as those described in Ref.\textsuperscript{17}. The total instrumental resolution [FWHM: full width at half maximum] was about 80 meV and 250 meV at $h\nu \sim 20$ eV and $h\nu \sim 100$ eV, respectively. High resolution photoemission spectra were taken with the FWHM of about 30 meV. The photon flux was monitored by the yield from a gold mesh and all the spectra were normalized to the mesh current. Temperature (T)-dependence of PES was also investigated below and above the AF transition temperature. For T-dependent PES measurements, the chamber pressure stayed below $7 \times 10^{-11}$ Torr during heating. The low-T PES spectra were reproduced after the heating-cooling cycle.

The electronic structures of UTSn have been calculated by employing the self-consistent LMTO (linearized muffin-tin-orbital) band method. The partial densities of states (PDOS) have been calculated by using the LSDA+$U$ band method incorporating the spin-orbit (SO) interaction, so that the orbital polarization is properly taken into account.\textsuperscript{18} The von Barth-Hedin form of the exchange-correlation potential has been utilized.

\section{RESULTS AND DISCUSSION}

\subsection{U 5f and T d PSWs}

Figure 1 shows the valence-band spectra of UTSn (T=Ni, Pd) in the photon energy ($h\nu$) range of $22 - 110$ eV. At low $h\nu$‘s ($22-30$ eV), the contribution from the Sn sp electron emission is non-negligible ($10 - 15\%$), and the cross-sections ($\sigma$) of U 6$d$ and T d electrons are comparable to one another ($\sim 40\%$).\textsuperscript{20} $h\nu = 92$ eV, $h\nu = 98$ eV, and $h\nu = 110$ eV correspond to the off- and on-resonance energies due to the U 5$d_{5/2} \rightarrow 5f$ and U 5$d_{3/2} \rightarrow 5f$ absorptions, respectively. Therefore the emission enhanced at $h\nu = 98$ and $h\nu = 110$ eV can be identified as the U 5$f$ emission. The off-resonance spectrum at $h\nu = 92$ eV is dominated by the Ni and Pd d emission because, at this $h\nu$, the Sn sp electron emission is negligible with respect to the T d emission ($< 1\%$ of the Ni/Pd d emission) and the U 5$f$ electron emission is suppressed. Using the U 5$d$ $\rightarrow$ 5$f$ RPES, we have determined the U 5$f$ PSWs of UTSn. Before subtraction, the off-resonance spectra have been multiplied by a factor of 0.94 and 0.6 for UNiSn and UPdSn, respectively, in order to account for the $h\nu$ dependence of other conduction-band electrons.

Figure 2(a) compares the extracted 5$f$ PSWs of UTSn (T=Ni, Pd) to those of a nearly heavy fermion system UAl\textsubscript{2}\textsuperscript{21} and a typically localized 5$f$ system UPd\textsubscript{3}\textsuperscript{22}. All the spectra are scaled at the peak. UPd\textsubscript{3} is known to be a tetra-valent (U$^{4+}$) intermetallic uranium compound with a localized 5$f^2$ configuration, and so the 5$f$ peak in UPd\textsubscript{3} is assigned as the 5$f^2 \rightarrow 5f^1$ transition.\textsuperscript{22} On the other hand, 5$f$ electrons in UAl\textsubscript{2} is expected to be itinerant, and so the 5$f$ peak close to E\textsubscript{F} in UAl\textsubscript{2} is considered to represent the fully relaxed 5$f^{n}e^{m-1}$ final states ($n=2$, 3, 4), under the assumption of the 5$f^{n}e^{m}$ ground state configuration. Interestingly the extracted U 5$f$ spectra of UNiSn and UPdSn are very similar each other, even though the on- and off-resonance spectra are very different. They have common features, such as a pronounced peak centered at about 0.3 eV binding energy (BE) and a tail to about 3 eV below E\textsubscript{F}.\textsuperscript{23} It is found that, as one moves from UAl\textsubscript{2} to UTSn and UPd\textsubscript{3}, the centroid of the 5$f$ electron peak moves away from E\textsubscript{F} and its width becomes wider. This trend is accompanied by the decreasing 5$f$ spectral
weight at the Fermi level, $N_f(E_F)$. Compared to the large 5$f$ spectral weight near $E_F$ in UAl$_2$, $N_f(E_F)$ in UTSn is lower than that in UAl$_2$, suggesting that U 5$f$ electrons in UTSn are more localized than in UAl$_2$. This finding is consistent with the fact that UNiSn and UPdSn have large ordered magnetic moments (1.55 – 2$\mu_B$).

The U 5$f$ PSW of UNiSn is very similar to that of UPdSn. The similarity in the U 5$f$ PSW between UNiSn and UPdSn suggests that the interaction between U 5$f$ electrons in UTSn (T=Ni, Pd) is mediated mainly by the hybridization to conduction-band electrons, rather than by the direct $f$-$f$ hopping, as explained below. The average U-U separation $d_{U-U}$ in UPdSn (3.63$\AA$) is much shorter than that in UNiSn (4.53$\AA$), but is rather close to that in UAl$_2$ (3.22$\AA$). $d_{U-U} = 3.63$Å in UPdSn lies on the border of the Hill limit ($d_{Hill} = 3.3-3.5$Å), beyond which the U 5$f$ electrons are observed to form local moments. If we consider the average U-U separation only, the direct $f$-$f$ hopping among U 5$f$ electrons is expected in UPdSn (even if it may be weak), while it is expected to be negligible in UNiSn. Thus the interaction between U 5$f$ electrons in UTSn should be mediated by the hybridization to conduction-band electrons, such as U 6$d$, Sn $sp$, and T $d$ electrons. This conclusion is consistent with the fact that UNiSn and UPdSn have significantly larger ordered magnetic moments than in other U intermetallic systems. The inelastic neutron scattering study also found rather well-defined CEF excitations in UTSn (T=Ni, Pd).

Figure 2(b) compares the $h\nu = 92$ eV off-resonance spectra of UNiSn and UPdSn, which can be considered to represent the experimental Ni 3$d$ and Pd 4$d$ PSWs, respectively. To find a correlation between the U 5$f$ PSW and the hybridization effect, we compare the off-resonance spectrum ($h\nu = 92$ eV) of UAl$_2$ for which $N_f(E_F)$ is very large. The spectrum for UAl$_2$ is reproduced from Ref. and it is scaled so that the area $E_F$ and $\sim$7 eV BE is comparable with that in UNiSn. It is shown that the Pd 4$d$ peak lies at a higher BE ($\sim 4$ eV BE) than Ni 3$d$ peak ($\sim 2$ BE) and its FWHM ($\sim 2$ eV) is much wider than that of Ni 3$d$ peak ($\sim 1$ eV). The latter difference reflects the less localized nature of Pd 4$d$ states than Ni 3$d$ states. Then the more spread wave functions of the Pd 4$d$ electrons than those of the Ni 3$d$ electrons would yield the larger spatial overlap between U 5$f$ and Pd 4$d$ wave functions. On the other hand, due to a higher BE of Pd 4$d$ peak, the energy overlap between U 5$f$ and Pd 4$d$ wave functions would be small so as to weaken the hybridization. It is thus expected that the effective hybridization in UNiSn and UPdSn becomes more or less similar.

Note that both the Pd 4$d$ and Ni 3$d$ PSWs reveal a very low spectral intensity near $E_F$, $I(E_F)$, which is of comparable magnitude if the main d peaks are scaled at their maxima. In contrast, UAl$_2$ reveals a much larger $I(E_F)$ than UTSn. This finding indicates that the reduced $N_f(E_F)$ in UTSn arises from the energy-dependent hybridization matrix elements $M_{fd}(h\nu)$ between the U 5$f$ states and the T $d$ states that have a very low DOS at $E_F$. This interpretation implies that the energy-dependent hybridization, instead of the average hybridization strength, plays an important role in determining $N_f(E_F)$ in uranium compounds.

B. High-resolution PES across phase transitions

Figure 3 shows the temperature dependence of the high-resolution PES spectra of UTSn (T=Ni, Pd) in the vicinity of $E_F$, obtained at $h\nu = 22$ eV with FWHM $\sim 30$ meV. All the spectra were obtained with the same measurement conditions except for temperature. The top panel compares the high-resolution T=15 K PES spectra of UTSn and Pt metal. Pt is chosen as representing the typical metallic Fermi-edge spectrum. In this comparison, all the spectra are scaled at about 300 meV below $E_F$. The solid line along the measured spectrum of Pt metal is the result of the flat DOS with a non-zero slope.
FIG. 4: The calculated PDOS per spin and per atom of UNiSn, obtained from the LSDA+U calculation for the AF ground state. The spin-up and spin-down PDOS are denoted with black and grey lines, respectively. From top are shown U 5f, U 6d, Ni d, and Sn 5p PDOSs.

Figure 3 shows that the high-resolution PES spectra of UTSn in the vicinity of \( E_F \) are almost identical each other and that there is certainly a finite metallic DOS at \( E_F \) in UTSn. It is clearly shown that the slope of the PES spectrum of UTSn just below \( E_F \) is lower than that of Pt, indicating a lower DOS at \( E_F \). In contrast to a flat DOS with a non-zero slope for Pt, the 15 K spectra of UTSn are described well by the V-shaped metallic DOS near \( E_F \). The V-shaped metallic DOS represents a model with a reduced but finite DOS at \( E_F \) which is usually formed in semi-metallic systems. This difference confirms that UTSn have a lower DOS at \( E_F \) than a typical metal, in agreement with a low \( N_f(E_F) \) (See Fig. 2).

The middle panel compares the spectra of UNiSn, obtained at \( T = 15 \)K (black line), which belongs to the AF metallic phase, to that at \( T = 90 \)K (gray line) which belongs to the paramagnetic semi-conducting phase. Similarly, the T-dependence of the spectra of UPdSn is shown in the bottom panel, obtained at \( T = 15 \)K (black lines), the monoclinic AF phase, \( T = 30 \)K (gray lines), the orthorhombic AF phase, and \( T = 60 \)K (open dots), the paramagnetic phase, respectively. Nearly no changes have been observed in the PES spectra of UTSn across magnetic phase transitions, except that due to the temperature broadening. Therefore the same V-shaped metallic DOS is expected to provide a reasonably good fit to the measured spectra for UPdSn at 30K, 60K, and 90 K. Our study indicates that both UNiSn and UPdSn have finite metallic DOSs at \( E_F \) in different magnetic phases, suggesting that there are no appreciable changes in their electronic structures across the magnetic phase transitions.

C. Comparison to the LSDA+U Calculation

Figures 4 and 5 show the calculated PDOSs per atom of UNiSn and UPdSn, respectively, obtained from the LSDA+U calculations. Tetragonal and orthorhombic AF structures are considered for UNiSn and UPdSn, respectively, and the collinear spin configurations are assumed for both systems. The on-site Coulomb correlation parameter \( U \) for the U 5f electrons is included in these calculations. The parameters used in this calculation are the Coulomb correlation \( U = 2.0 \) eV and the exchange \( J = 0.95 \) eV and \( J = 0.8 \) eV for UNiSn and UPdSn, respectively. The on-site Coulomb correlations for the Ni 3d and Pd 4d electrons have been neglected. The
LSDA+U yields the correct metallic ground states for the AF phase of UTSn (T=Ni, Pd), and the correct semiconducting and metallic ground states for the paramagnetic phases of UNiSn and UPdSn, respectively. The major effect of including U in the LSDA+U is to shift both the occupied 5f peaks and the unoccupied 5f peaks away from $E_F$. The second effect of the LSDA+U is to shift the U d, T d, and Sn p PDOSs toward $E_F$. The larger the U value is, the larger the peak shifts. For UTSn (T=Ni, Pd), the calculated orbital and spin magnetic moments for U ions are $4.53\mu_B$ and $-2.25\mu_B$ (UNiSn), and $4.53\mu_B$ and $-2.24\mu_B$ (UPdSn), respectively, and so the total magnetic moments of U ions become $2.28\mu_B$ (UNiSn) and $2.29\mu_B$ (UPdSn). These values are in reasonable agreement with experiment.\(^\text{34}\) The spin magnetic moments of U 5f states, $\approx 2\mu_B$ for both UNiSn and UPdSn, reflect that the number of occupied 5f-electrons is close to two ($5f^2$) with U$^{4+}$ configuration. Note, however, that the f-electrons in UNiSn and UPdSn are not so localized as in UPd$_3$ due to the large hybridization with the neighboring elements. Therefore the f-electron count is not really meaningful in these intermetallic compounds.

For both UNiSn and UPdSn, the U f states exhibit the exchange-split 5f bands, separated from each other by about 4 eV and 3 eV, respectively. The other states (U d, T d, Sn p) exhibit nearly no exchange splitting, indicating that the spin-polarization in UTSn is mainly due to the U f electrons. The Ni and Pd d bands are nearly filled with a very low DOS at $E_F$, in agreement with the PES data (see Fig. 2). The Sn p states are spread over the whole valence band, but relatively more concentrated at 1 – 2 eV below $E_F$. The U d, T d, and Sn p PDOSs share common features, indicating the large hybridization among them. The DOS at $E_F$ is low for UNiSn, but high for UPdSn. It is because that the Fermi level in UNiSn cuts the valley of U f DOS, while the Fermi level in UPdSn is located near the second peak of the U f DOS. This difference arises from the different crystal structures of UNiSn and UPdSn.

Figure 6 compares the extracted PSWs (dots) of UTSn (T=Ni, Pd) to the calculated PDOS, obtained from the LSDA+U calculations (solid lines) . In the comparison to the PES spectra, only the occupied part of the calculated PDOS was taken, and then convoluted by a Gaussian function with 0.2 eV at the FWHM. The Gaussian function has been used to simulate the instrumental resolution. The effects of the lifetime broadening and photoemission matrix elements are not included in the theory curves. At the bottom panels, the theoretical spectra correspond to the sum of the U d, T d, and Sn 5p PDOSs. See the text for details.

IV. CONCLUSIONS

The electronic structures of UTSn (T=Ni, Pd) have been investigated by performing the photoemission experiment and the LSDA+U electronic structure calculation. The extracted U 5f spectra of UTSn are very similar to each other, showing the U 5f peaks at $\approx 0.3$ eV BE. Compared to the U 5f PSWs of a nearly heavy fermion system UAl$_2$ and a typically localized 5f system UPd$_3$, the...
the centroid of the 5f electron peak moves away from \( E_F \) from \( \text{UA}l_2 \) to \( \text{UTSn} \) and \( \text{UPd}_3 \), accompanied by the decreasing 5f spectral weight at the Fermi level, \( N_f(E_F) \), which suggests that the localization of U 5f electrons in \( \text{UTSn} \) is between those in \( \text{UA}l_2 \) and \( \text{UPd}_3 \). The similarity in the U 5f PSW between \( \text{UNiSn} \) and \( \text{UPdSn} \) suggests that the interaction between U 5f electrons in \( \text{UTSn} \) is mediated mainly by the hybridization to conduction-band electrons, rather than by the direct \( f-f \) hopping. Both the Ni 3d and Pd 4d PSWs show the main peaks well below \( E_F \) and a very low DOS at \( E_F \). The high-resolution PES spectra of \( \text{UTSn} \) are also very similar each other, with the slope just below \( E_F \) being lower than that of Pt. They are described well by a V-shaped metallic DOS near \( E_F \), consistent with the reduced 5f DOS at \( E_F \). The similarity of PSWs shows the main peaks of \( \text{UNiSn} \) and \( \text{UPdSn} \) suggests that the reduced \( N_f(E_F) \) in \( \text{UTSn} \) is ascribed to the hybridization to the very low \( T \) DOS at \( E_F \). Our work suggests that the energy-dependent hybridization plays an important role in determining the U 5f electronic structure. The calculated spin magnetic moments of U 5f states, \( \sim 2\mu_B \) for both \( \text{UNiSn} \) and \( \text{UPdSn} \), reflect that the number of occupied 5f-electrons is close to two \( (5f^2) \) with the \( U^{4+} \) configuration. Comparison of the measured PES spectra to the LSDA+U band structure calculation reveals a reasonably good agreement for \( \text{UPdSn} \), but not for \( \text{UNiSn} \), indicating the importance of the on-site Coulomb interaction not only for U 5f electrons but also for \( T \) \( d \) electrons.

## Acknowledgments

This work was supported by the KRF (KRF-2002-070-C00038) and by the KOSEF through the CSCMR at SNU and the eSSC at POSTECH. The SRC is supported by the NSF (DMR-0084402).

---

1. T. T. M. Palstra, G. J. Nieuwenhuys, R. F. M. Vlastuin, J. van den Berg, J. A. Mydosh, and K. H. J. Buschow, J. Magn. Magn. Mater. 67, 331 (1987).
2. F. R. de Boer, E. Brück, H. Nakotte, A. V. Andreev, V. Sechovsky, L. Havela, P. Nozar, C. J. M. Denissen, K. H. J. Buschow, B. Vaziri, M. Meissner, H. Maleta, and P. Rogl. Physica B 176, 275 (1992).
3. H. Kawanaka, H. Fujii, M. Nishi, T. Takabatake, K. Motoya, Y. Uwatoko, and Y. Ito. J. Phys. Soc. Jpn. 58, 3481 (1989).
4. R. A. Robinson, A. C. Lawson, K. H. J. Buschow, F. R. de Boer, V. Sechovsky, and R. B. Von Dreede. J. Magn. Magn. Mater. 198, 147 (1991); R. A. Robinson, A. C. Lawson, J. W. Lynn, and K. H. J. Buschow. Phys. Rev. B 45, 2939 (1992).
5. T. Akazawa, T. Suzuki, F. Nakamura, T. Fujita, T. Takabatake, and H. Fujii. J. Phys. Soc. Jpn. 65, 1471 (1996).
6. H. Fujii. H. Kawanaka, T. Takabatake, M. Kurisu, Y. Yamaguchi, J. Sakurai, H. Fujiwara, T. Fujita, and I. Oguro. J. Phys. Soc. Jpn. 58, 2495 (1989).
7. J. Diel, H. Fischer, R. Köhler, C. Geibel, F. Steglich, Y. Maeda, T. Takabatake, and H. Fujii. Physica B 166-188, 708 (1993).
8. H. Nakotte, R. A. Robinson, A. Purwanto, Z. Tun, K. Prokes, E. Brück, and F. R. de Boer. Phys. Rev. B 58, 9269 (1998).
9. Y. Aoki, T. Suzuki, T. Fujita, H. Kawanaka, T. Takabatake, and H. Fujii. Phys. Rev. B 47, 15060 (1993).
10. T. Akazawa, T. Suzuki, H. Goshima, T. Tahara, T. Fujita, T. Takabatake, and H. Fujii. J. Phys. Soc. Jpn. 67, 3256 (1998); T. Akazawa, T. Suzuki, T. Tahara, T. Goto, J. Hori, H. Goshima, F. Nakamura, T. Fujita, T. Takabatake, and H. Fujii. Physica B 259-256, 248 (1999).
11. K. A. McEwen, M. J. Bull, and R. S. Eccleston, Physica B 281-282, 600 (2000).
12. S. W. Johnson, R. A. Robinson, H. Nakotte, E. Bruck, F. R. de Boer, and A. C. Larson. J. Appl. Phys. 73, 6072 (1993).
13. J. Trygg, B. Johansson, and O. Eriksson, Phys. Rev. B 49, 7165 (1994).
14. P. M. Oppeneer, A. N. Yaresko, A. Ya. Perlov, V. N. Antonov, H. Eschrig. Phys. Rev. B 54, R3706 (1996).
15. L. M. Sandratskii and J. Kübler. J. Phys.: Condens. Matter. 9, 4897 (1997).
16. H. Höchst, K. Tan, and K. H. J. Buschow, J. Magn. Magn. Mater. 54-57, 545 (1986).
17. J.-S. Kang, J.-G. Park, K. A. McEwen, C. G. Olson, S. K. Kwon, and B. I. Min. Phys. Rev. B 64, 085101 (2001).
18. V. I. Anisimov, F. Aryasetiawan, and A. I. Liechtenstein. J. Phys. : Condens. Matter 9, 767 (1997).
19. S. K. Kwon and B. I. Min. Phys. Rev. Lett. 84, 3970 (2000).
20. J.J. Yeh and I. Lindau. Atom. Data Nucl. Data Tables 32, 1 (1985).
21. J. W. Allen, Y.-X. Zhang, L. H. Theng, L. E. Cox, M. B. Maple, and C.-T. Chen. J. Elec. Spec. Relat. Phenom. 78, 57 (1996).
22. J.-S. Kang, J. W. Allen, M. B. Maple, M. S. Torikachvili, W. P. Ellis, B. B. Pate, Z.-X. Shen, J. J. Yeh, and I. Lindau. Phys. Rev. B 39, 13529 (1989).
23. There some uncertainties in determining the U 5f PSW, such as the resonating U 6d emission and the 5f emission from the surface states (L. Duo, Surf. Sci. Rep. 32, 233 (1998); A. Sekiyama, T. Iwasaki, K. Matsuda, Y. Saitoh, Y. Onuki, and S. Suga, Nature 403, 398 (2000)). However, it is likely that the resonating U 6d intensity is normalized out in subtracting the off-resonance spectrum from the on-resonance spectrum because it usually mimics the ligand d and sp density of states. Further, the surface effects have not been observed explicitly in uranium systems in contrast to Ce systems for which surface effects have been well established.
24. L. Duo, Surf. Sci. Rep. 32, 233 (1998).
25. A. Sekiyama, T. Iwasaki, K. Matsuda, Y. Saitoh, Y. Onuki,
and S. Suga, Nature 403, 398 (2000).

26 H.H. Hill "Plutonium 1970 and Other Actinides", Nucl. Met. 17, edited by W.N. Miner (AIME, New York, 1970) pp. 2-19.

27 The U-Ni separation (2.77Å) and the U-Pd separation (2.92Å) are much smaller than the U-U separations.

28 J.-S. Kang, J.-G. Park, K. A. McEwen, Y. Onuki, C. G. Olson, and B. I. Min, Physica B 312-313, 882 (2002).