Reduction of Kondo lattice effects in Yb$_{1-x}$Lu$_x$Al$_3$ observed by soft x-ray photoelectron spectroscopy

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Abstract. We have carried out the bulk-sensitive and high-resolution soft x-ray photoelectron spectroscopy on Lu substituted intermediate-valence compound Yb$_{1-x}$Lu$_x$Al$_3$ ($x = 0.4$) at temperatures from 200 to 20 K. The temperature dependences of the bulk Yb 4f photoelectron spectra revealed in our preceding works on high purity YbAl$_3$ have not been observed in this Lu substituted system. The temperature dependences of the bulk Yb 4f peak positions and the Yb valence in this system can be well reproduced by the single impurity Anderson model (SIAM), whereas the spectral behaviors in YbAl$_3$ were not at all reproduced by the SIAM. These results confirm the importance of the Kondo lattice effects for YbAl$_3$, for which the coherent lattice periodicity plays essential roles.

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1. Introduction

The single impurity Anderson model (SIAM) could often explain the 4f spectral behavior observed by photoelectron (or photoemission) spectroscopy (PES) in rare-earth intermediate-valence (IV) compounds \([1]–[4]\). However, it has recently been revealed that the bulk 4f PES spectra of CeRu\(_2\), whose Kondo temperature \(T_K\) is higher than 1000 K, cannot be well reproduced by the SIAM \([5, 6]\) \((T_K\) represents the hybridization strength between the 4f and conduction electrons). In addition, behaviors of the 4f electrons in the systems with lattice coherence (Kondo lattice effects or Anderson lattice effects) are also thought to deviate from the SIAM predictions, since the SIAM can be applicable only to an isolated 4f impurity ion with ignoring the influence of the periodicity of the lattice on the 4f state. In our preceding work \([7]\), we have performed high-accuracy soft x-ray PES (SXPES) measurements of Yb-based IV compound YbAl\(_3\). This compound has the relatively high \(T_K\) (\(\sim 500\) K) among Yb-based IV compounds and the Kondo lattice effects are suggested below the coherence temperature \(T_{coh} \sim 40\) K \([8, 9]\). From the SXPES measurements, unusual temperature dependences of the Yb 4f spectra have been revealed for YbAl\(_3\). These temperature dependences of the Yb 4f spectra in YbAl\(_3\) have not been reproduced within the framework of the SIAM. Thus, the limitation of the SIAM has been unambiguously clarified for the first time for YbAl\(_3\).

In Lu substituted compounds Yb\(_{1-x}\)Lu\(_x\)Al\(_3\), the temperature \(T_{max}\) of the broad maximum in the magnetic susceptibility shifts to higher temperatures with increasing \(x\), i.e. \(T_K\) (estimated as \(T_K \sim (4–6)T_{max}\)) increases with increasing \(x\) \([10]\). The anomalies in both susceptibility and specific heat below \(T_{coh}\) attributed to the Kondo lattice effects in YbAl\(_3\) are also suppressed for \(x \geq 0.05\) in Yb\(_{1-x}\)Lu\(_x\)Al\(_3\) \([10, 11]\). By increasing \(x\), the SIAM predictions are expected to be applicable to the Yb 4f spectra of Yb\(_{1-x}\)Lu\(_x\)Al\(_3\) in accordance with the suppression of the Kondo lattice effects. Therefore, SXPES studies of Yb\(_{1-x}\)Lu\(_x\)Al\(_3\) attract much attention to discuss the Kondo lattice effects.

In this paper, we present a SXPES study of Yb\(_{0.6}\)Lu\(_{0.4}\)Al\(_3\). We have confirmed that the temperature dependences of the Yb 4f spectra in Yb\(_{0.6}\)Lu\(_{0.4}\)Al\(_3\) can be well reproduced by the non-crossing approximation (NCA) calculation based on the SIAM irrespectively from the increased \(T_K\) induced by the Lu substitution.

\(^7\) Below \(T_{coh}\), the electrical resistivity exhibits \(T^2\) Fermi-liquid behaviors \([12]\) and the magnetic susceptibility (with a peak at 15 K, as well as a broad maximum at \(T_{max} \sim 125\) K governed by the SIAM Kondo temperature) and the specific heat (with an up turn saturating toward \(T = 0\) K) show anomalies unexpected by the SIAM \([8]\).
Figure 1. Valence-band SXPES spectra of Yb\textsubscript{0.6}Lu\textsubscript{0.4}Al\textsubscript{3} and YbAl\textsubscript{3} [7] measured at 200 K. The Yb\textsuperscript{3+} 4f multiplet structures are indicated by the vertical bars predicted by the atomic multiplet calculation [16]. For the spectrum of Yb\textsubscript{0.6}Lu\textsubscript{0.4}Al\textsubscript{3}, the two arrows show the Lu\textsuperscript{3+} 4f\textsubscript{7/2} and 4f\textsubscript{5/2} peaks at 6.7 and 8.1 eV, respectively.

2. Experimental

Single-crystalline Yb\textsubscript{0.6}Lu\textsubscript{0.4}Al\textsubscript{3} samples (cubic AuCu\textsubscript{3}-type structure) were grown by the self-flux method with excess aluminium [9, 12] and characterized by magnetic susceptibility and specific heat measurements [11]. The Kondo temperature suggested from \( T_{\text{max}} \sim 250 \) K in the magnetic susceptibility is \( T_{K} \sim 1000 \) K [10, 11]. The bulk-sensitive and high-resolution SXPES measurements were performed with synchrotron radiation (\( h\nu = 700 \) eV) at beamline BL25SU of SPring-8 [13, 14], by using the SCIENTA SES200 analyzer. The samples were fractured \textit{in situ} in a vacuum with a base pressure of better than \( 3 \times 10^{-8} \) Pa and the SXPES were measured at temperatures from 200 to 20 K. The surface cleanliness was confirmed by the absence of the O 1s and C 1s SXPES signals. Energy calibration was performed for Au Fermi-edge at each measuring temperature. The total resolution of the SXPES measurement was set to 65 meV.

3. Results and discussion

Figure 1 compares the valence-band SXPES spectra of Yb\textsubscript{0.6}Lu\textsubscript{0.4}Al\textsubscript{3} and YbAl\textsubscript{3} [7] measured at 200 K. The spectra have been normalized by the integrated intensity of the Yb\textsuperscript{3+} 4f multiplet structures. At \( h\nu = 700 \) eV, the cross-sections of the Yb and Lu 4f states are dominant while the contributions from the valence-bands are almost negligible [15]. Two groups of characteristic features derived from the Yb divalent (Yb\textsuperscript{2+}) and trivalent (Yb\textsuperscript{3+}) states for Yb-based IV
compounds are observed in both Yb$_{0.6}$Lu$_{0.4}$Al$_3$ and YbAl$_3$. The Yb$^{3+}$4f$^{12}$ final-state multiplet structures (shown by the vertical bars after a proper energy scaling ($\sim$1.1) for the calculated atomic multiplet structures [16]) are observed between 5 and 11 eV. Meanwhile two sharp peaks just below the Fermi level ($E_F$) and at 1.3 eV are derived from the Yb$^{2+}$ 4f$^{13}$ $J = 7/2$ (abbreviated as 4f$_{7/2}$) final-state and its spin–orbit partner $J = 5/2$ (4f$_{5/2}$) final-state from the Yb$^{2+}$ 4f$^{14}$ initial-state in the bulk. In addition, rather broad peaks centered around 0.9 and 2.2 eV in the Yb$^{2+}$ 4f region are observed, which are derived from the surface layer. Surface electronic configurations are often different from those of bulk in many strongly correlated electron systems [5, 17]. In the present SXPES results, however, the spectral intensity of the surface components is much weaker compared with the previous low-energy (20 < $h\nu$ < 130 eV) PES results [18]–[21]. Therefore, we can discuss the intrinsic peak energy positions in the bulk 4f spectra and the Yb valence with much higher accuracy. For Yb$_{0.6}$Lu$_{0.4}$Al$_3$, one can see the prominent doublet peaks derived from the Lu 4f$^{13}$ final-states (shown by the two arrows) from the Lu$^{3+}$ 4f$^{14}$ initial-state overlapping with the Yb$^{3+}$ 4f multiplet structures.

Figure 2(d) shows the temperature dependence of the first peak ($^3H_6$) of the Yb$^{3+}$ 4f$^{12}$ multiplet structures and the Yb$^{2+}$ 4f$^{13}$ $J = 7/2$ peak (so-called Kondo peak) near $E_F$ in Yb$_{0.6}$Lu$_{0.4}$Al$_3$. For comparison, the temperature dependence of the Yb 4f spectra of YbAl$_3$ [7] is reproduced in Figure 2(b). Here, all spectra have been normalized by the integrated intensity of the $^3H_6$ peak. As shown in Figure 2(a), the $^3H_6$ peak and also the whole peaks of the Yb$^{3+}$ 4f multiplet structures) is found to shift toward higher binding energies ($E_B$) with decreasing the temperature from 200 to 20 K. On the other hand, the shift of the Yb$^{2+}$ 4f$_{7/2}$ peaks is found to be almost negligible (the Yb$^{2+}$ 4f$_{5/2}$ peaks also exhibit a similar behavior) in Yb$_{0.6}$Lu$_{0.4}$Al$_3$. In contrast to Yb$_{0.6}$Lu$_{0.4}$Al$_3$, however, the shift of the $^3H_6$ peaks is found to be almost negligible in YbAl$_3$. On the other hand, the Yb$^{2+}$ 4f$_{7/2}$ peak is found to shift toward lower $E_B$ with decreasing the temperature in YbAl$_3$. Thus the temperature dependence of the Yb 4f spectra of Yb$_{0.6}$Lu$_{0.4}$Al$_3$ is in a strong contrast to that of YbAl$_3$.

In order to estimate the accurate peak positions of the Yb 4f spectra and the Yb valence of Yb$_{0.6}$Lu$_{0.4}$Al$_3$, we have carried out a numerical fitting. For simplicity, calculated PES line spectra are convoluted with the Gaussian function for the instrumental resolution and the Lorentzian function for the lifetime broadening. The Yb valence can be estimated from the intensity ratio of the bulk Yb$^{2+}$ and Yb$^{3+}$ 4f components after subtraction of the surface components (the Yb valence of which is assumed to be 2+) observed in the Yb$^{2+}$ 4f region. In addition, it has been reported that a subsurface layer with more Yb$^{2+}$-rich properties than the bulk exists in some Yb-based IV compounds [19], [22]–[25]. Thus, two structures (split by the spin–orbit interaction) are assumed for the surface and subsurface components in order to extract the intrinsic contribution of the bulk Yb$^{2+}$ 4f components.

From the numerical fitting, the integrated intensity ratio for the bulk, subsurface and surface Yb$^{2+}$ 4f components is estimated as $I_b : I_{ss} : I_s = 0.77 : 0.07 : 0.16$. The thicknesses of the surface ($d_s$) and subsurface ($d_{ss}$) layers are given by $d_s = -\lambda \ln(1 - I_s)$, $d_{ss} = -\lambda \ln I_b - d_s$, where $\lambda$ is the mean free path of the photoelectrons ($\lambda \sim 15.8$ Å at $h\nu = 700$ eV) [26]. Then, $d_s \sim 2.8$ Å and $d_{ss} \sim 1.3$ Å are roughly evaluated as the thicknesses of the surface and subsurface layers. $d_s + d_{ss} \sim 4.1$ Å is comparable to the lattice constant of Yb$_{0.6}$Lu$_{0.4}$Al$_3$ ($\sim 4.20$ Å) [11]. 

The Yb$^{3+}$ 4f multiplet structures in the SXPES spectra are fitted as mentioned before [16]. The Lu$^{3+}$ 4f spin–orbit split components are subtracted from the Yb$^{3+}$ 4f components. The temperature independent Mahan’s asymmetry parameters [27] are assumed as $\alpha = 0.12$ and 0.18 for the bulk Yb$^{2+}$ and Yb$^{3+}$ components, respectively. As an example, the fitting result of
the experimental spectrum at 200 K is shown in figure 3(a). The spectrum is well reproduced by this numerical fitting. It is then evaluated that the Yb valence decreases gradually from 2.65 to 2.58 with decreasing the temperature from 200 to 20 K as shown in figure 3(b) in Yb$_{0.6}$Lu$_{0.4}$Al$_3$. For comparison, the Yb valences estimated from the analysis of the Yb $L_{III}$ (2p$_{3/2}$) edge x-ray absorption spectroscopy (XAS) measurements for Yb$_{0.7}$Lu$_{0.3}$Al$_3$ and Yb$_{0.5}$Lu$_{0.5}$Al$_3$ [11] are added in figure 3(b). The Yb valences estimated from the Yb $L_{III}$ XAS spectra for Yb$_{0.7}$Lu$_{0.3}$Al$_3$ and Yb$_{0.5}$Lu$_{0.5}$Al$_3$ are larger than those estimated by the SXPES spectra for Yb$_{0.6}$Lu$_{0.4}$Al$_3$. In the case of the Yb $L_{III}$ XAS, the Yb$^{2+}$ and Yb$^{3+}$ components strongly overlap and the separation of the XAS spectrum into the two components has some ambiguities. Thus, the accuracy of the valence evaluation from the Yb $L_{III}$ XAS spectra is rather limited. In the SXPES, on the other hand, the Yb 4f spectra can be clearly separated into the Yb$^{2+}$ and Yb$^{3+}$ components, facilitating accurate estimation of the Yb valence. Figures 3(c) and (d) show the temperature dependence of the bulk Yb$^{2+}$ 4f$_{7/2}$ peak position and the center of gravity (COG) of the Yb$^{3+}$ 4f multiplet structures, respectively. In Yb$_{0.6}$Lu$_{0.4}$Al$_3$, the peak positions of the bulk Yb$^{2+}$ 4f$_{7/2}$ spectra stay at 57–55 meV below 200 K. In contrast, the whole peaks of the
Figure 3. (a) Numerical fitting to the valence-band spectrum of Yb$_{0.6}$Lu$_{0.4}$Al$_3$ measured at 200 K. For the Yb$^{3+}$ 4f components, B, SS and S represent the bulk, subsurface and surface components, respectively. For Lu$^{3+}$ 4f states only the surface states S are separated beside the B + SS components. (b) Comparison of the Yb valence as a function of temperature. Triangle and diamond symbols indicate the values determined from the analysis of the Yb $L_{III}$ XAS spectra for Yb$_{0.7}$Lu$_{0.3}$Al$_3$ and Yb$_{0.5}$Lu$_{0.5}$Al$_3$, respectively [11]. Square and closed-circle symbols are the results estimated by the SXPES for YbAl$_3$ and Yb$_{0.6}$Lu$_{0.4}$Al$_3$, respectively. Open circles are the best-fit NCA calculation results for Yb$_{0.6}$Lu$_{0.4}$Al$_3$ as discussed in the text. (c) Temperature dependence of the bulk Yb$^{3+}$4f$^{7/2}$ peak position and (d) COG of the Yb$^{3+}$ 4f multiplet structures evaluated by the SXPES for Yb$_{0.6}$Lu$_{0.4}$Al$_3$ and YbAl$_3$. Open circles in (c) and (d) show the peak positions estimated from the best-fit NCA spectra for Yb$_{0.6}$Lu$_{0.4}$Al$_3$. 
Yb$^{3+}$4f multiplet structures are found to shift by ~20 meV toward higher $E_B$ with decreasing the temperature from 200 to 20 K. Namely, the COG of the Yb$^{3+}$4f multiplet structures shifts from ~7.035 eV at 200 K to ~7.056 eV at 20 K. In strong contrast to these results for Yb$_{0.6}$Lu$_{0.4}$Al$_3$, the peak position of the bulk Yb$^{2+}$4f$_{7/2}$ spectra is found to shift by ~16 meV toward lower $E_B$ from 200 to 20 K whereas the COG’s of the Yb$^{3+}$4f multiplet structures stay at 6.995 ± 0.005 eV at all measuring temperatures for YbAl$_3$.

In order to discuss the temperature dependence of the bulk Yb 4f spectra for Yb$_{0.6}$Lu$_{0.4}$Al$_3$, we have carried out the NCA calculation based on the SIAM. In this calculation, the 4f at all measuring temperatures for YbAl$_3$ from 200 to 20 K whereas the COG’s of the Yb$^{3+}$4f multiplet structures stay at 6.995 ± 0.005 eV at all measuring temperatures for YbAl$_3$.

Table 1. Estimated NCA parameters (bare 4f energy level ($\varepsilon_f$), Coulomb repulsive energy ($U_R$) and averaged hybridization strength ($\Delta$)) to reproduce the temperature dependence of the bulk Yb 4f spectra for Yb$_{0.6}$Lu$_{0.4}$Al$_3$. The parameter sets (A), (B) and (C) are used to calculate the 4f spectra in figures 4(a), (b) and (c), respectively. The parameter set (C) reproduces best the experimental results. Estimated $T_K$′s are also given.

| $\varepsilon_f$ (eV) | $U_R$ (eV) | $\Delta$ (meV) | $T_K$ (K) |
|---------------------|-----------|---------------|--------|
| (A) -0.20           | 7.1       | 20.2          | ~810   |
| (B) -0.40           | 7.2       | 34.6          | ~790   |
| (C) -0.27           | 7.1       | 25.9          | ~840   |

Figures 4(a) and (b) show the calculated spectra at 200 and 20 K with the NCA parameter sets (A) and (B) listed in table 1, where 4f$^{12}$ multiplet structures are represented by a single component (the intensity and the peak position correspond to the integrated intensity of the whole multiplet structures and the COG, respectively). In both NCA calculations, it is predicted that while the 4f$^{13}_{7/2}$ and 4f$^{13}_{5/2}$ peak positions do not change much with temperature, the COG of the 4f$^{12}$ multiplet structures shifts by ~20 meV toward higher $E_B$ with decreasing the temperature from 200 to 20 K if the energy scale is expanded as in the case of (c). Thus the temperature dependence of the Yb 4f peak positions for Yb$_{0.6}$Lu$_{0.4}$Al$_3$ is roughly reproduced. However, the Yb valence calculated with these parameter sets at 200 K (20 K) becomes 2.64 (2.54) for (A) and 2.73 (2.67) for (B). These Yb valences are somewhat deviated from the experimental values of 2.65 (2.58) for Yb$_{0.6}$Lu$_{0.4}$Al$_3$ (figure 3(b)).
Figure 4. Results of NCA calculation (based on the SIAM). (a) and (b) at 20 and 200 K for parameters in table 1 (A) and (B). All calculated spectra have been normalized by the 4f^{12} peak intensity and convoluted with the Fermi–Dirac function and the Gaussian function (65 meV FWHM). (c) shows the best-fit spectra explaining the results of Yb_{0.6}Lu_{0.4}Al_{3} in figure 2(a).

The temperature dependence of the best-fit NCA spectra is shown in figure 4(c) for which the NCA parameter set (C) is given in table 1. In this case, the COG of the 4f^{12} multiplet structures shifts from \sim 7.030 eV at 200 K to \sim 7.055 eV at 20 K. Therefore, the peak shift is predicted to be \sim 25 meV toward higher \EB with decreasing the temperature. On the other hand, the peak position of the 4f^{13}_{7/2} spectra stays at \sim 60 meV even with changing the temperature. The Yb valence predicted by the present NCA calculation decreases gradually from 2.66 at 200 K to 2.57 at 20 K (figure 3(b)). These theoretical results are in good agreement with the temperature dependences evaluated from the bulk Yb 4f spectra of Yb_{0.6}Lu_{0.4}Al_{3}. In addition, we have simulated the magnetic excitation spectrum using this NCA calculation with the same parameter set (C) in order to estimate \TK (\TK for (A) and (B) are given for reference in table 1). \TK is estimated as \sim 840 K from the peak position of the predicted magnetic excitation spectrum. This value is comparable to that of \TK \sim 1000 K estimated from the magnetic susceptibility [10, 11]. Thus the results of Yb_{0.6}Lu_{0.4}Al_{3} are well explained by the SIAM. Our new results for Yb_{0.6}Lu_{0.4}Al_{3} indicate that the lattice periodicity of the Yb ions is responsible for the Kondo lattice effects.
We compare the Yb valence and $T_K$ of Yb$_{0.6}$Lu$_{0.4}$Al$_3$ to those for YbAl$_3$. The Yb valence of Yb$_{0.6}$Lu$_{0.4}$Al$_3$ (decreasing from 2.65 at 200 K to 2.58 at 20 K) is smaller than that of YbAl$_3$ (decreasing from 2.71 at 200 K to 2.65 at 20 K), i.e. the bulk Yb divalent component is larger by $\sim$20% for the Lu concentration of $x = 0.4$. $T_K$ increases also from $\sim$500 K for YbAl$_3$ to $\sim$840 K for Yb$_{0.6}$Lu$_{0.4}$Al$_3$. These differences of the Yb valence and $T_K$ are not due to a simple chemical pressure effect since the lattice parameter decreases by only $\sim$0.3% from YbAl$_3$ to LuAl$_3$ [11]. In Yb$_{1-x}$Lu$_x$Al$_3$, the Lu substitution into YbAl$_3$ is predicted to induce the electron doping due to the addition of the Lu 5d$^1$ electron as conduction electrons. This is related to the decreasing electrical resistivity from YbAl$_3$ to LuAl$_3$ [12]. The electron doping raises $E_F$ and moreover strengthens the effective hybridization $\rho V^2$ between the Yb 4f and conduction electrons near $E_F$, resulting in the decrease of the Yb valence and the increase in $T_K$ [29]. Although $T_K$ is increased by the Lu substitution, the temperature dependences of the bulk Yb 4f spectra in Yb$_{0.6}$Lu$_{0.4}$Al$_3$ are well interpreted within the SIAM. This indicates that the Kondo lattice effects are suppressed due to the random potential by the substituted Lu ions.

4. Conclusions

In conclusion, we have studied the Lu substituted compound Yb$_{1-x}$Lu$_x$Al$_3$ by the soft x-ray photoelectron spectroscopy. In Yb$_{0.6}$Lu$_{0.4}$Al$_3$, it is found that the peak positions of the bulk Yb$^{2+}$ 4f spectra are found to be almost independent of temperatures while the whole peaks of the Yb$^{3+}$ 4f multiplet structures are found to shift by $\sim$20 meV toward higher $E_B$ with decreasing the temperature from 200 to 20 K. The bulk Yb valence decreases gradually from 2.65 at 200 K to 2.58 at 20 K. These thermal behaviors in Yb$_{0.6}$Lu$_{0.4}$Al$_3$ are well understood in the framework of the SIAM whereas $T_K$ is obviously higher than for YbAl$_3$. These results are qualitative different from those for YbAl$_3$, suggesting that the Kondo lattice effects are important for describing the bulk electronic states of YbAl$_3$. Thus, we understand that the lattice periodicity of the Yb ions without randomness besides the strong hybridization is responsible for the Kondo lattice effects. Concrete analyses of YbAl$_3$ within the framework of the periodic Anderson model will be really required in the near future to discuss the temperature dependence of the bulk Yb 4f spectra.

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