HIGH-RESOLUTION RESONANCE PHOTOEMISSION STUDY OF CeNi*

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We have performed the high-resolution Ce $3d$–$4f$ resonance photoemission study of a considerably hybridized CeNi with the Kondo temperature of ~ 150 K. The tail of the Kondo-resonance peak is predominantly observed in the bulk Ce $4f$ photoemission spectra, where its spin–orbit partner is suppressed compared with the so far reported surface-sensitive Ce $4d$–$4f$ resonance spectrum. Our results show that the bulk $4f$ electronic states are essentially understood by the single impurity Anderson model.

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1. Introduction

Owing to the bulk-sensitive high-resolution Ce $3d$–$4f$ resonance photoemission spectroscopy (RPES) which has recently become a reality [1, 2], it has been revealed that the bulk Ce $4f$ electronic states in low-T_K (≤ 20 K) compounds such as $CeRu_2Si_2$ are essentially understood within a framework of the single impurity Anderson model (SIAM), which is no longer applicable to a very high-T_K ($\gg 1000$ K) $CeRu_2$ [1,3–5]. In the present stage, however, it is not clear whether the SIAM is applicable to "intermediate-" or high-T_K (> 20 K) systems. In order to settle the above question, we have measured the bulk-sensitive high-resolution Ce $3d$–$4f$ RPES spectra of single crystals of an intermediate-T_K (~ 150 K) system CeNi [6].

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2. Results and discussions

The high-resolution Ce $3d$–$4f$ RPES were performed at the twin-helical undulator beam line BL25SU of SPring-8 [2]. The overall energy resolution was set to 90 meV at $h\nu \sim 880$ eV. In order to obtain clean surfaces, the samples were cleaved *in situ*. The sample temperature was set to about 20 K, which is well below $T_{\rm K} \sim 150$ K. The Ce $4f$ contribution is remarkably enhanced in the Ce $3d$–$4f$ RPES spectra at the photon energies up to 882.6 eV (resonance-maximum) compared with the off-resonance spectrum ($h\nu = 866.1$ eV: inset) as shown in Fig. 1. The overall intensity of the spectrum taken at $h\nu = 883.3$ eV, which is beyond the resonance-maximum, decreases again compared with that of the resonance-maximum spectrum. The spectral line shapes in the on-resonance region ($881.4 \leq h\nu \leq 883.3$ eV) are completely different from that of the off-resonance spectrum. The Ni $3d$ contribution is almost negligible in the spectra measured at $h\nu = 881.7$ and 882.6 eV due to such a prominent resonance enhancement. There are a sharp and prominent peak near the Fermi level ($E_{\rm F}$) and a broad and weak peak centered at ~ 2.8 eV in the on-resonance spectra. The former originates from the $4f^1$ final states whereas the latter is ascribed to the $4f^0$ final state. The Auger emission is also seen in the spectra measured at $h\nu = 882.6$ and 883.3 eV as indicated by vertical bars in Fig. 1. In the off-resonance

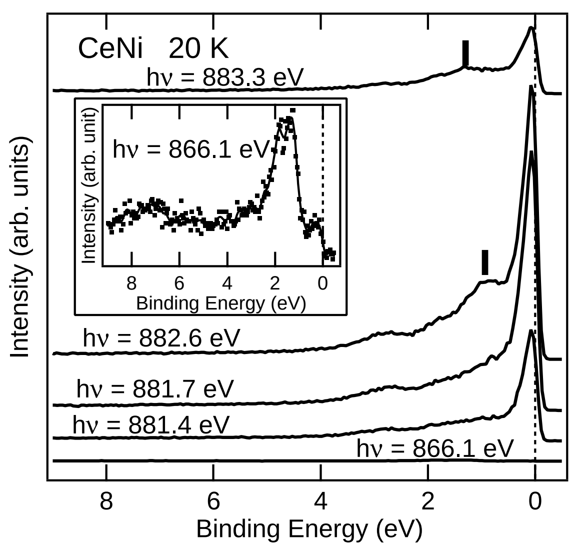

Fig. 1. Ce $3d$–$4f$ RPES spectra of CeNi measured at several photon energies. The inset shows the off-resonance spectra measured at $h\nu = 866.1$ eV.

spectrum in which the Ni $3d$ spectral weight is predominant, there are two peaks centered at 1.5 and 7 eV. The broad peak at 7 eV is ascribed to the so-called two-hole-bound state.

Figure 2(a) shows the bulk-sensitive high-resolution RPES spectra near $E_{\rm F}$ of CeNi measured at $h\nu = 881.7$ and 882.6 eV, where the Ce $4f$ contribution is predominant. These line shapes are mutually similar, suggesting that there is no effect caused by the Auger contribution near $E_{\rm F}$ even at the resonance maximum. A prominent peak is observed in the vicinity of $E_{\rm F}$ while a weak shoulder is seen at 0.2 eV in the RPES spectra. The obtained bulk $4f$ line shape is quite contradictory to that of the surface-sensitive $4d$–$4f$ RPES spectra of CeNi, in which clear doublet peaks ascribable to the tail of the Kondo resonance ($4f^1_{5/2}$ final state) and its spin-orbit partner ($4f^1_{7/2}$ final state) have been observed [7]. We have compared the bulk Ce $4f$ spectrum of CeNi with that of low-$T_{\rm K}$ $CeRu_2Si_2$ ($T_{\rm K} \sim 20$ K) and very high-$T_{\rm K}$ $CeRu_2$ ($T_{\rm K} \gg 1000$ K) as shown in Fig. 2(b). The line shape of CeNi is qualitatively similar to that of $CeRu_2Si_2$ which has been well reproduced by a spectral calculation based on the SIAM [3], but completely different from that of $CeRu_2$ which can be explained by a band-structure calculation [4]. Namely, the bulk RPES spectra of CeNi are essentially understood by the SIAM and therefore the prominent peak in the vicinity of $E_{\rm F}$ and the shoulder at 0.2 eV seen in the high-resolution Ce $3d$–$4f$ RPES spectra originate from the tail of the Kondo resonance and its spin-orbit partner, respectively. The tail of the Kondo resonance of CeNi is relatively stronger than that of $CeRu_2Si_2$, indicating that the hybridization between the Ce $4f$ and other valence-band electrons is stronger for CeNi than for $CeRu_2Si_2$.

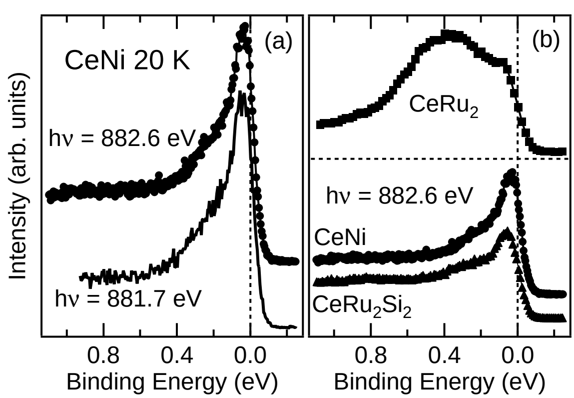

Fig. 2. (a) High-resolution Ce $3d$–$4f$ RPES spectra near $E_{\rm F}$ of CeNi. (b) Comparison of the RPES spectrum of CeNi ($T_{\rm K} \sim 150$ K) with that of $CeRu_2Si_2$ ($T_{\rm K} \sim 20$ K) and $CeRu_2$ ($T_{\rm K} \gg 1000$ K).

3. Conclusion

In conclusion, the prominent peak originating from the tail of the Kondo resonance as well as the weak shoulder ascribable to the spin–orbit partner is clearly seen in the bulk-sensitive high-resolution Ce $3d$–$4f$ RPES spectra of CeNi. It has been revealed that the bulk $4f$ electronic states of CeNi are essentially explained by the SIAM.

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