High-resolution resonant photoemission spectroscopy study of CeSi

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Introduction

Antiferromagnetic-Ce-compound CeSi with the Néel temperature of 5.9 K has interesting magnetic and electrical properties [1–3]. Such phenomena are derived from a hybridization between the Ce 4*f* state and the conduction-band states. In this study we investigate the Ce 4*f* state in CeSi from the valence-band spectra by means of the high-resolution Ce 4*d*-4*f* resonant photoemission spectroscopy (RPES).

Experiment

Ce 4*d*-4*f* RPES spectra were measured at BL-11D. The overall energy resolution around the Ce 4*d*-4*f* threshold was estimated to be about 80 meV. A single-crystalline sample was grown by the Czochralski pulling method. The sample was checked by x-ray diffraction and electron-microprobe analysis.

Results and Discussion

Figure 1(a) shows the Ce 4*f* spectrum of CeSi. The Ce 4*f* spectrum was obtained by subtracting the resonance-minimum spectrum taken at $h\nu$ = 114.3 eV from the resonance-maximum one at $h\nu$ = 122.3 eV. The spectrum exhibits three peaks at 0.3, 1 and 2.5 eV and a shoulder near the Fermi level (E_F). According to the single impurity Anderson model (SIAM) [4], the peak at 0.3 eV and the shoulder near E_F are ascribed to the Ce $4f^1$ final states while the peak at 2.5 eV the Ce $4f^0$ final state. The peak at 1 eV, however, has not been observed in the Ce 4*f* spectra of conventional Ce compounds. The origin of this peak is discussed later. The spectrum does not show such a sharp peak at E_F as observed in the He II spectra of conventional Kondo compounds $CeSi_x$ ($1.6 \le x \le 2$) [5]. This indicates that no Kondo effect is apparent or that the Kondo temperature is very low (< 1 K) for CeSi, in accordance with the results of the electrical and magnetic measurements [1–3].

In order to discuss on the Ce 4*f* electronic structure of CeSi, we analyzed the Ce 4*f* spectral function using the non-crossing approximation (NCA) calculation [6] based on the SIAM [4]. We directly divided the Ce 4*f* spectrum obtained experimentally into the bulk and surface components. By calculating the electron mean-free path as a function of the kinetic energy, we obtained the surface-to-bulk emission ratio of ~1.77. The bare 4*f* levels were set to 1.6 and 2.2 eV for the bulk and surface components, respectively. The energy dependence of the hybridization strength $\rho v^2(E)$ was first assumed to be proportional to the resonance-minimum spectrum, and finally determined to well fit to the experimental spectrum. The calculated 4*f* spectrum is shown in Fig. 1(b), together with the bulk and surface components. As shown in Fig. 1, the calculated 4*f* spectrum semi-quantitatively reproduces the experimental one including the peak at 1 eV. The obtained average hybridization strength δ calculated by using $\rho v^2(E)$ was 37.8 meV for the bulk component, indicating that CeSi is a fairly localized compound. In comparison of the line shape of $\rho v^2(E)$ with the resonance-minimum spectrum, the peak at 1 eV in the Ce 4*f* spectrum is ascribed to the Ce $4f^1$ final state taken place by the hybridization of the Ce 4*f* state with the Si 3*p* states centered at 1.5 eV.

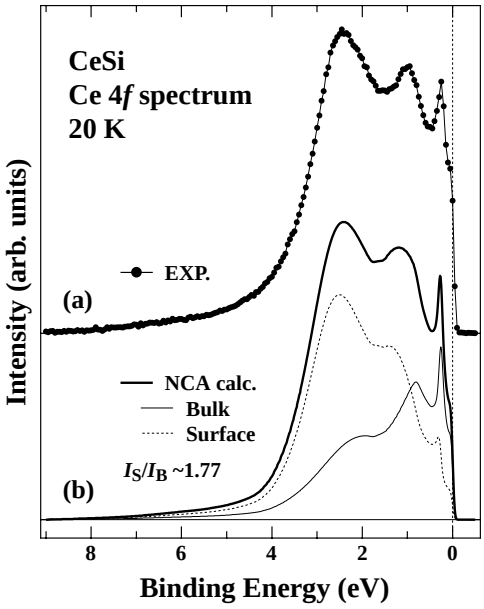

Fig. 1. (a) Ce 4*f* spectrum of CeSi. (b) Ce 4*f* spectral function calculated by the NCA method (thick-solid line). Thin solid- and thin-broken lines indicate the bulk and surface components, respectively.

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