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DMFT band calculation for Ce compounds

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Non-empirical band calculation for the strongly correlated systems has been extensively developed on the basis of the dynamical mean field theory (DMFT). In 4f electrons of Ce compounds the crystalline field splitting (CFS) and the spin-orbit interaction (SOI) play important roles[1]. A theory, which is named as NCAf^2vc is recently developed to solve the auxiliary impurity Anserson model[2], and it is combined with the LMTO method to carry out the DMFT band calculation. The present calculation can include the CFS and SOI effects and also the correct exchange process of $f^1 \rightarrow f^0, f^2$ valence fluctuation, and it give accurate order of the Kondo temperature. We report the result of the DMFT band calculation for a series of Ce pnictides.

Ce pnictides have a characteristic double peak structure in PES; the shallow-energy one is at about 0.8 eV below $E_{\rm F}$ and the deep-energy one is at about 3 eV below $E_{\rm F}$. The shallow one is ascribed to the $p-f$ bonding state of hole excitation. Its intensity increases gradually as pnictogen becomes light from Bi to P, and CeN shows α Ce like properties. These behaviors have been qualitatively explained by using the hybridization intensity (HI) estimated from the LDA band calculation on the basis of the impurity Anderson model[3]. $T_{\rm K}$ was calculated by using the same HI. It is very low, about 10^{-5} K because of the small density of states near $E_{\rm F}$. However $T_{\rm K}$ higher than 1 K, had been expected from the transport properties.

In the DMFT calculation, the double-peak structure is obtained. At the same time a rather higher $T_{\rm K}$ is obtained, since HI of DMFT has a sharp peak just at $E_{\rm F}$ caused by the hybridization of the bands with the correlated $4f$ bands[1]. In Fig. 1, we show the single particle spectra of CeSb at T=300K. The solid line gives the total 4f PES. The dashed line is the DOS of the $(j=5/2)\Gamma_7$ component and the dot-dashed line is the DOS of the $(j=5/2)\Gamma_8$ component. The two-dotts-dashed line is the DOS of the $j=7/2$ component. The Fermi energy is indicated by the vertical dot-dashed line. The inset shows the spectra near the Fermi energy.

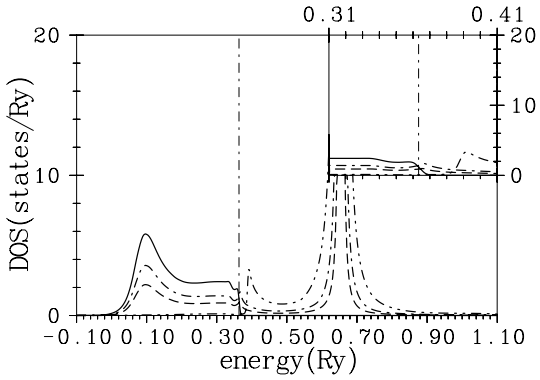

Figure 1: Single particle excitaion spectra of CeSb at T=300K.

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3. M. Takeshige, O. Sakai and T. Kasuya: J. Magn. Magn. Mater **52** (1985) 363.