(PS35)

Band calculation for Ce compounds on the basis of the dynamical mean field theory

O. Sakai[1], Y. Shimizu[2] and Y. Kaneta[3]

[1] Department of Physics, Tokyo Metropolitan University, Hachioji 192-0397

[2] Department of Applied Physics, Tohoku University, Sendai 980-8579

[3] Department of Quantum Engineering and System Science, The University of Tokyo, Tokyo 153-8904

The band calculation scheme for f electron compounds is developed on the basis of the dynamical mean field theory (DMFT) and the LMTO method. The effective impurity problem is solved by a method named as NCAf^2v', which includes the correct exchange process of the $f^1 \to f^2$ fluctuation as the vertex correction to the non-crossing approximation (NCA) for the $f^1 \to f^0$ fluctuation. This method leads correct magnitude of the Kondo temperature, $T_{\rm K}$, and makes it possible to carry out quantitative DMFT calculation including the crystalline field (CF) and the spin-orbit (SO) splittings of the self-energy. The magnetic excitation spectra are also calculated to estimate $T_{\rm K}$. It is applied to Ce metal and CeSb at $T = 300$ K as the first step. In Ce metal, the hybridization intensity (HI) just below the Fermi energy is reduced in DMFT band. The photo-emission spectra (PES) have a conspicuous SO side peak, similar to that of experiments. $T_{\rm K}$ is estimated about 50 K and 320 K, respectively for γ and α Ce. These are comparable magnitude to the CF splitting. In CeSb, the double peaks structure of PES is reproduced. In addition rather higher $T_{\rm K}$, about 80 K is obtained as the hybridization becomes strong just at the Fermi energy in DMFT band.

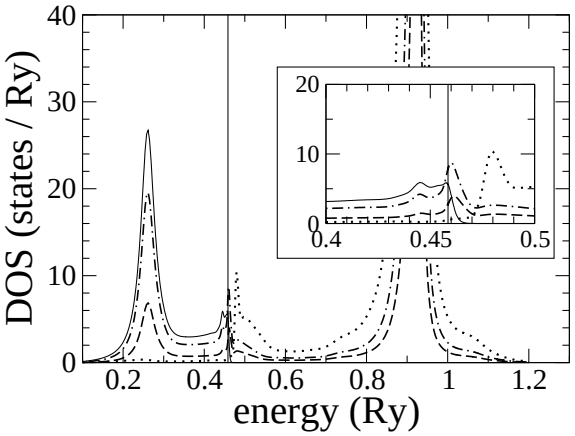

Figure 1: $4f$ spectra for γ Ce at $T = 300$ K. The solid line is the total $4f$ PES spectra. The dashed line is DOS of $(5/2)\Gamma_7$, the dot-dashed line is DOS of $(5/2)\Gamma_8$ and the dotted-line is DOS of $j = 7/2$ components. In set shows the spectra near the Fermi energy.

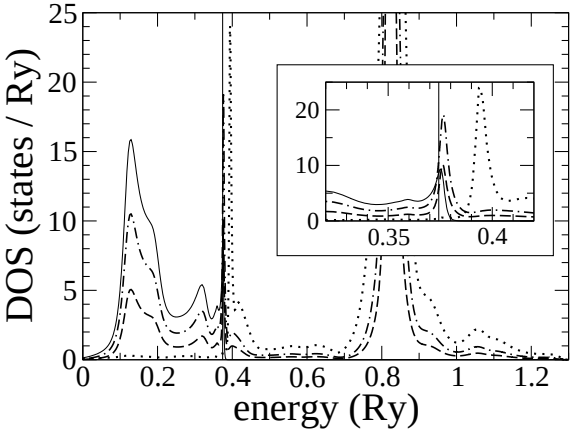

Figure 2: $4f$ spectra for CeSb at $T = 300$ K. Note we have a peak just at the Fermi energy. $T_{\rm K}$ is estimated to be about 80 K from the calculation of the magnetic excitation. This magnitude is rather too high, but will be reduced when the overlapping between the Sb-$5p$ valence and Ce-$5d$ conduction band is reduced.