Photoelectron spectroscopy of YbInCu(4): Direct Testing of Correlatec Electron Models

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Photoelectron Spectroscopy of YbInCu₄:
Direct Testing of Correlated Electron Models

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The electronic properties of single crystal YbInCu₄ have been investigated by means of high resolution photoelectron spectroscopy. A first order, isostructural phase transition for YbInCu₄ at Tᵥ=42 K leads to changes in the Kondo temperature (Tₖ), of more than an order of magnitude (27 K vs. 400 K). This phase transition and accompanying Kondo temperature change provide the most direct test of the single impurity model (SIM) to date. Particle-hole symmetry allows the SIM to be used for Yb compounds as well as Ce heavy fermions with the great advantage that the predicted Kondo resonance is found on the occupied side of the spectral weight function for Yb materials and is thus directly observable in photoemission. The photoemission results are incongruous with the single impurity model predictions for temperature dependence, binding energy and 4f occupancy, encouraging a reevaluation of the single impurity model. The experiments were conducted using the PGM undulator and 4 meter NIM beamlines at SRC. The spectra were taken at photon energies of 40 eV and 90 eV and the combined energy resolution of the analyzer and monochromator was 45-85 meV.

We tested directly three of the central predictions of SIM, the temperature dependence of the Kondo Resonance spectral intensity, the 4f hole occupancy, and the energy shift of the Kondo resonance as a function of Tₖ. The divalent 4f related features in the valence band are identified as the bulk 4f₇/₂, surface 4f₇/₂ and the bulk 4f₅/₂ moving away from the Fermi level with binding energies of -0.02 eV, -0.80 eV and -1.3 eV respectively. For the PES data, the change in the integrated spectral intensity for the bulk divalent 4f features of Yb in YbInCu₄ is roughly 25% between 20 and 80 K. The SIM model calculations using the NCA framework for the same material and temperature range show a reduction in the 4f spectral intensity by a factor of 10.

The discrepancies between SIM and experimental data persist with SIM predicting a hole occupancy (n₄) for the low Tₖ phase of YbInCu₄ in the range of 0.9 to 0.95 while PES deter-
mines the $n_f$ to be 0.5, much closer to the values used in a band calculation for YbInCu$_4$. The hole occupancy is defined as $n_f = \frac{I(f^{13})}{I(f^{13}) + \frac{13}{14} I(f^{14})_{\text{bulk}}}$, were $I(f^{13})$ is the integrated intensity of the primary trivalent 4f component and $I(f^{14})_{\text{bulk}}$ is the integrated primary bulk divalent 4f component from the lineshape analysis. A full valence band spectrum for YbInCu$_4$ at $h\nu = 90$ eV is shown in Fig. 1 with the shaded region indicating the inelastic background emission along with the Cu 3d emission. LuInCu$_4$ was used to determine the non-4f contribution to the emission with the top inset showing the fitting of the divalent YbInCu$_4$ region and the bottom inset the trivalent region. The lineshape analysis discussed in Ref. 2 is used to separate the 4f from the non-4f as well as the divalent 4f signal into surface and bulk components. By isolating the primary emissions in this manner, for both the trivalent and bulk divalent 4f signals, we are able to calculate the $n_f$ for the 4f levels. The PES data gives an $n_f=0.50$ for YbInCu$_4$ at $T=80$ K where SIM predicts $n_f>0.90$. Along with the large discrepancy in temperature dependence and the lack of a predicted energy shift moving through the phase transition, this huge discrepancy in $n_f$ between model and data makes the use of SIM for heavy fermions inappropriate.

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