Electron Spectroscopy Studies of $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$

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Introduction

The superconductivity of the isostructural alloy system $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ is quenched with increasing x [1]. The normal state electrical resistivity for $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ shows a transition from metallic to semiconducting behavior, with the monotonic suppression of T_C, for the samples with x>0.6 being non-superconducting. Magnetic, Hall-effect, and structural studies indicate that a valence state for the Pr ion is greater than 3+ [2], and thus the hole-filling mechanism in the Cu-O planes is suggested as an origin for the suppression of superconductivity. On the other hand, high energy spectroscopies yield a Pr valence close to 3+ and signatures of hybridization between Pr 4f and valence band electrons [3], implying the importance of magnetic interaction between the Pr ion and the Cu-O planes [4].

Experimental Details

The synchrotron radiation photoemission (PES), X-ray photoemission (XPS), and BIS (bremsstrahlung isochromat spectroscopy) measurements were performed for the polycrystalline samples of $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ (x=0, 0.2, 0.4, 0.6, 0.8, 1.0). The measured surfaces were obtained by cleaving the samples *in situ* in a vacuum chamber with a base pressure of 7 X 10^{-11} Torr and 3 X 10^{-10} Torr for the PES/XPS and BIS measurements, respectively.

Results and Discussion

The valence band spectra near the Cu 3p absorption edge show a resonance of the emission of the d^8*-like* satellite, located at -12.4eV, for all x. The Pr 4f emission is spread throughout the valence band of Cu 3d and O 2p states. The photon energy dependences of the Pr 4f emissions near the Pr 4d absoprtion edge provide evidence that the Pr valence is close to 3+ for all x. The line shapes of the extracted Pr 4f PES spectra are essentially alike for all x. The top panel of Fig. 1 shows the extracted Pr 4f PES/BIS spectral weight distribution for x=1.0. For comparison, the bottom panel of Fig. 1 shows the analogous Pr 4f spectrum for Pr metal, obtained by combining BIS and PES data of Ref. 5 and 6, respectively. The 7eV BIS feature is assigned as the $4f^2$--->$4f^3$ transition. We interprete the $PrBa_2Cu_3O_{7-\delta}$ 4f spectrum as essentially trivalent, but with the BIS/PES peaks near E_F signaling much larger hybridization effects than for the Pr metal. We have attempted to fit the Pr 4f spectrum using the impurity Anderson Hamiltonian to measure the Pr valence and hybridization strength (Δ_{sv}). The calculated ground state parameters are n_f=2.02 (n_f : Pr 4f occupancy), Δ_{sv}=0.16eV, and T_K=125K (T_K : Kondo temperature). It is suggestive that the obtained value of T_K (125K) is the same order of magnitude as T_C (90K), which is the condition for maximum suppression of T_C by a magneitc impurity in a BCS superconductor.

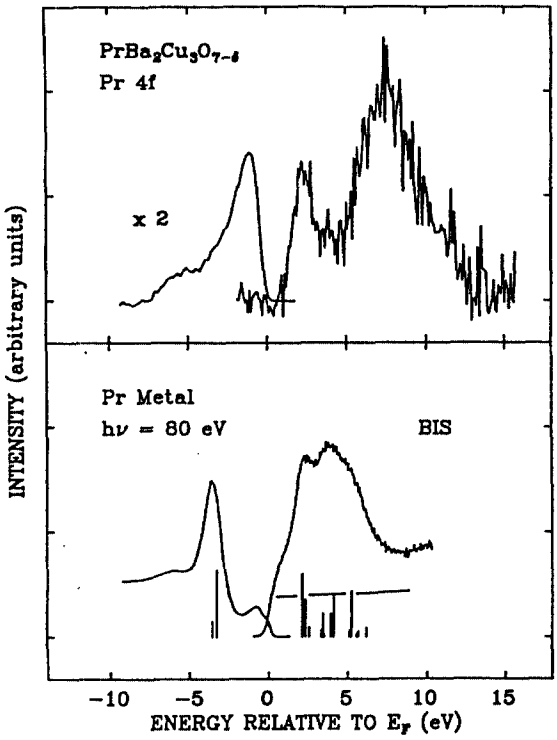

Fig. 1. The Pr 4f spectrum for $PrBa_2Cu_3O_{7-\delta}$ (top) and for Pr metal (bottom).

Conclusions

We have found that the Pr valence is close to 3+ in $Y_{1-x}Pr_xBa_2Cu_3O_{7-\delta}$ for all x and that there is extensive Pr 4f hybridization with the Cu 3d and O 2p valence states. From these findings we speculate that Pr 4f hybridization with other valence electrons has enabled Pr spin fluctuations to cause the T_C-suppression. However, the experimental uncertainties concerning the gap around E_F should be resolved more carefully.

Acknowledgments

I am deeply indebted to J.W. Allen and M.B. Maple for this work. I also thank O. Gunnarsson, Bowha Lee, Z.-X. Shen, J.J. Yeh, W.P. Ellis, W.E. Spicer, and I. Lindau for their collaboration.

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