The Electronic Properties of Yb in YbB₁₂

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Introduction

Correlated electron systems, such as Kondo and heavy electron systems, high-Tc superconductors and CMR materials, have attracted strong interests, not only because of their interesting ground-state and excited-state properties but also because of their intermediate nature between the localized and itinerant character. These materials require more sophisticated concepts to describe the physical behavior.

Kondo insulators, a class of f-electron systems, have attracted considerable interest in recent year.¹ They are nonmagnetic insulators at low temperatures and behave as local moment (and are often metallic) at room temperature. It has been proposed that the insulating gaps in the electronic states at the Fermi surface are due to hybridization renormalizing the electronic bands² or due to the Kondo interaction.³ In the former case, an itinerant or band theory would provide a meaningful base for an understanding of the system. In the latter case, a local description of the electron structure would be more appropriate.

YbB₁₂ is still believed to be the only Yb-containing Kondo insulator. Recently, a resonant photoemission study⁴ has found a valence of Yb in the intermediate regime between the magnetic, trivalent and nonmagnetic, divalent state, namely n=2.86±0.06.

Results and Discussion

We have performed temperature-dependent x-ray absorption experiments, x-ray diffraction, (inelastic neutron scattering not discussed here) and susceptibility measurements on YbB₁₂.⁵ The Yb L₃-edge XANES is shown in Fig. 1. A single resonance is

observed at the energy expected for purely trivalent Yb-and no indication of a second contribution 7 eV lower in energy expected for the contribution of the divalent Yb. In addition, no indication of a second resonance is observed in the second derivative. Both sets of data can be consistently described with purely trivalent Yb at 10K. We estimate from our data the maximal contribution of divalent Yb to be 5%. Therefore, it is likely that the resonant photoemission study has overestimated the divalent contri-



FIG. 1. X-ray absorption spectra of the Yb L_3 edge of YbB₁₂ taken at 10K. The solid line corresponds to a fit with purely trivalent Yb, whereas the dotted line corresponds to a Yb valence of v=2.85.

bution because their "bulk" contribution may still be influenced by the surface, whereas the hard x-ray absorption experiment probes deep bulk (microns). This interpretation is supported by the second derivative of the Yb L₃ edge, as the derivative is very sensitive to additional contributions to the absorption edge (see Fig. 2). The quantitative information on the valence is required for theories describing the properties of the Kondo insulator.



FIG. 2. Second derivative of the x-ray absorption spectra of the Yb L_3 edge of YbB₁₂ taken at 10K. The solid line corresponds to a fit with purely trivalent Yb, whereas the dotted line corresponds to a *Yb* valence of v=2.85.

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References

¹G. Aeppli and Z. Fisk, Comments Condens. Matter Phys. 16, 155 (1992).

² N.F. Mott, Philos. Mag. 30, 403 (1974).

³ B. Bucher, Z. Schleisinger, P.C. Canfield and Z. Fisk, Phys. Rev. Lett. 72, 522 (1992).

⁴ T. Susaki, A. Sekiyama, K. Kobayashi, T. Mizokawa, A. Fujimori, M. Tsunekawa, T. Muro, T. Matsushita, S. Suga, H. Ishii, T. Hanyu, A. Kimura, H. Namatame, M. Taniguchi, T. Miyahara, F. Iga and M. Kasaya, Phys. Rev. Lett. 77, 4269 (1996).

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