Photon Factory Activity Report 2002 #20 Part B (2003)

11D/2002G020

Resonant Photoemission Spectroscopy of $PrFe_4P_{12}$ and Related Pr compounds

Hiroyoshi ISHII*, Tsuneaki MIYAHARA, Yasuhiro TAKAYAMA,
Hidetsugu SHIOZAWA, Kenji OBU, Hideo OTSUBO, Hideo KIHARA,
Tatsuma D. MATSUDA, Yuji AOKI, Hitoshi SUGAWARA and Hideyuki SATO
Tokyo Metropolitan University, Hachioji-shi, Tokyo 192-0397, Japan

Introduction

Ternary intermetallic compounds RT_4X_{12} (R= rare earth element, T= Fe, Ru, Os and X= P, Sb) with the filled skutterudite structure have attracted much attention because of various interesting properties [1]. In this study, we investigated Pr 4*f* electronic states in $PrFe_4P_{12}$ and related Pr compounds by Pr 4*d*-4*f* resonant photoemission spectroscopy.

Experimental

The photoemission experiments were performed using synchrotron radiation at the beam line BL-11D of the Photon Factory, High Energy Accelerator Research Organization (KEK). The instrumental resolution was 65 meV.

Results and Discussion

The Pr 4*f* spectra of $PrFe_4P_{12}$ and related Pr compounds are shown in the inset of Fig. 1. These spectra were obtained by subtracting the resonance minimum spectra ($h\nu$= 115 eV) from the resonance maximum spectra ($h\nu$= 124 eV). In the 4*f* spectra, the peaks located at ~4.5 eV and ~0.5 eV correspond to the f^1 and f^2 peaks, respectively. For PrT_4X_{12}, the f^1 peak positions are remarkably deep [2]. In Fig. 1, we displayed the f^1 positions as a function of Pr-Pr distance. The difference in position can be considered to be mainly due to the 4*f* level. We discuss the behavior of the f^1 position on the basis of the band narrowing model [3]. With increasing Pr-Pr distance, the width of the Pr 5*d* band becomes narrower. If the number of Pr 5*d* electrons does not change and the energy separation between the Pr 4*f* and 5*d* levels stays rigid, the Pr 4*f* level is shifted toward a higher binding energy with increasing Pr-Pr distance. Figure 1 shows that the trend of the shift is consistent with that of the shift due to the band narrowing model.

For $PrFe_4P_{12}$, the intensity of the f^2 peak in the 4*f* spectrum is stronger than those for the related materials [2]. The intensity indicates the magnitude of the hybridization between the Pr 4*f* and the valence band states mainly. To see the relation between the f^2 intensity and the Pr-X (X= ligand atom) distance, we estimated the weights of the f^2 peaks in the Pr 4*f* spectra by assuming that the f^1 peak is approximately fitted by a Lorentzian curve, as shown in the inset of Fig. 2. The f^2 weights are summarized as a function of the Pr-X distance in Fig. 2. The figure shows that the strong hybridization for $PrFe_4P_{12}$ is due to the short Pr-P distance.

References

[1] H. Sato *et al.*, Phys. Rev. B 62 (2000) 15125.
[2] H. Ishii *et al.*, J. Phys. Soc. Jpn. 71 (2002) 156.
[3] S. Hüfner, *Photoemission Spectroscopy* (Springer-verlag, Berlin, 1995) p. 393.

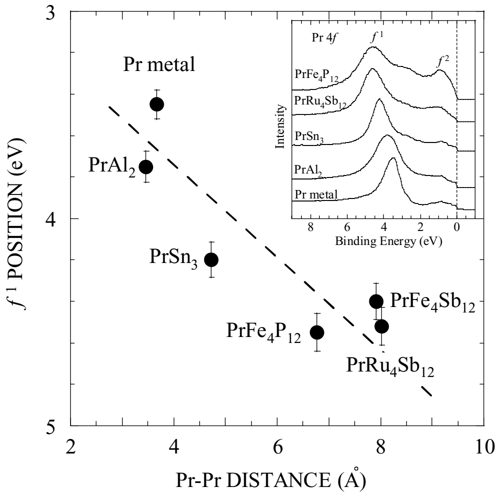

Figure 1: Pr f^1 peak positions as a function of Pr-Pr distance. The inset shows the Pr 4*f* photoemission spectra.

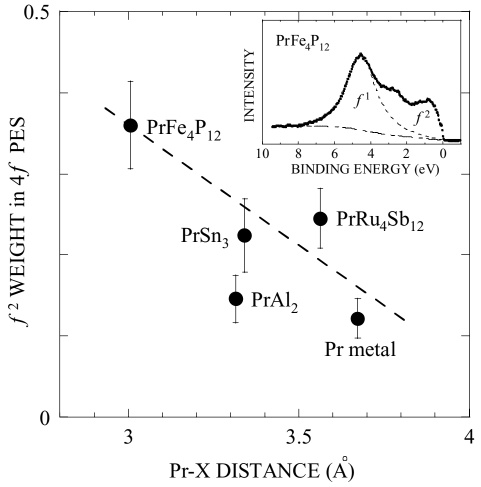

Figure 2: Relation between the weights of the f^2 peaks in the 4*f* spectra and the Pr-X distances. The inset shows the Pr 4*f* spectrum of $PrFe_4P_{12}$.

* ishii@comp.metro-u.ac.jp