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2003 J. Phys.: Condens. Matter 15 S2183

(http://iopscience.iop.org/0953-8984/15/28/348)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **15** (2003) S2183–S2186 PII: S0953-8984(03)62551-8

Magnetic Compton scattering study of $CeRh_3B_2$

Y Sakurai[1], M Itou[1], J Tamura[2], S Nanao[2], A Thamizhavel[3], Y Inada[3], A Galatanu[4], E Yamamoto[4] and Y Ōnuki[3,4]

[1] Japan Synchrotron Radiation Research Institute (JASRI), SPring-8, 1-1-1 Kouto, Mikazuki, Sayo, Hyogo 679-5198, Japan
[2] Institute for Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro, Tokyo 153-8505, Japan
[3] Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan
[4] Advanced Science Research Centre, Japan Atomic Energy Research Institute (JAERI), Tokai, Ibaraki 319-1195, Japan

E-mail: sakurai@spring8.or.jp

Received 12 November 2002
Published 4 July 2003

Abstract

The spin-polarized electron momentum distribution (magnetic Compton profile: MCP) of ferromagnetic $CeRh_3B_2$ has been measured using the magnetic Compton scattering technique at 10 K for the $[11\bar{2}0]$ direction. In this compound, the orbital moment dominates the magnetization. An analysis of the MCP reveals that the Ce 4f and Ce 5d spin moments are aligned parallel with a value of -0.68 ± 0.08 and 0.41 ± 0.04 μ_B, respectively, while Rh 4d electrons do not carry any significant spin moment. The ratio of orbital to spin moments for Ce 4f electrons, which has been determined from comparison of the present data with recent polarized neutron diffraction data, is rather smaller than that for Ce^{3+} ions. This result implies strong hybridization of the Ce 4f orbital with the orbitals on the surrounding ions.

1. Introduction

$CeRh_3B_2$ has drawn much attention due to its unusual magnetic properties. This compound orders magnetically with an unusually high Curie temperature of 115 K, despite its small saturated magnetic moment of 0.4 μ_B [1]. Itinerant ferromagnetism associated with Rh 4d or Ce 4f bands has been ruled out experimentally, and currently it is accepted that localized or nearly localized Ce 4f electrons are responsible for the ferromagnetism [2–6]. The strong couplings between the localized moments are, however, not explained by the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction [7, 8]. At present it is conceivable that the strong inter-atomic Ce 4f–5d hybridization and the intra-atomic Ce 4f–5d exchange interaction play important roles in the coupling between the Ce 4f moments [9–11]. In order to examine this scenario, experimental determination of the spin moment on each electronic state is essential.

0953-8984/03/282183+04$30.00

Magnetic Compton scattering (MCS) probes uniquely the spin component of the magnetization in a sample [12, 13]. When the incident x-rays are circularly polarized, the scattering cross-section contains a spin-dependent term. The experimental extraction of the spin dependence results in a magnetic Compton profile (MCP), $J_{mag}(p_z)$, that is defined as the one-dimensional projection of the spin-polarized electron momentum distribution:

$$J_{mag}(p_z) = \int\int [n^{\uparrow}(\boldsymbol{p}) - n^{\downarrow}(\boldsymbol{p})]\, \mathrm{d}p_x\, \mathrm{d}p_y, \tag{1}$$

where $n^{\uparrow}(\boldsymbol{p})$ and $n^{\downarrow}(\boldsymbol{p})$ are the momentum densities of the majority and minority spin bands, respectively. The area under the MCP is equal to the total spin moment (μ_{spin}) per formula unit (FU):

$$\int_{-\infty}^{+\infty} J_{mag}(p_z)\, \mathrm{d}p_z = \mu_{spin}. \tag{2}$$

When the MCP can be decomposed into a few partial profiles with the characteristic shape of a specific electronic state, the area under the partial profile gives the partial spin moment associated with that state. In this paper we report a MCS study on a well-characterized single crystal of $\mathrm{CeRh_3B_2}$.

2. Experiment

An ingot of $\mathrm{CeRh_3B_2}$ was grown by the Czochralski pulling method in a tetra-arc furnace, and a single crystal was cut from the ingot in a rectangular shape with a size of $2.1 \times 2.3 \times 3.5$ mm^3. The MCS experiments were carried out on the high-energy inelastic scattering beamline (BL08W) at SPring-8 [14]. The spectrometer consists of a superconducting magnet and a 10-element Ge solid-state detector. The incident x-ray energy was 175 keV. The scattering angle was 178.5°. The sample's magnetization was reversed with a magnetic field of ±2.5 T, and a MCP was measured at 10 K along the $[11\bar{2}0]$ direction. The overall momentum resolution was 0.45 atomic units (au).

3. Results and discussion

In order to normalize the area under the experimental MCP of the Ce sample to an absolute spin moment, additional experiments were carried out on Fe, Ni, Co at room temperature. The magnetic effect R is defined by the following equation:

$$R = \frac{I^+ - I^-}{I^+ + I^-}, \tag{3}$$

where I^+ and I^- are the integrated intensity of Compton-scattered x-ray spectra when the direction of the magnetic field is parallel (+) and anti-parallel (−) to the scattering vector, respectively. The magnetic effect is also proportional to the value of the spin moment (μ_{spin}) divided by the effective number of electrons (N) in the FU:

$$R = A\left(\frac{\mu_{spin}}{N}\right). \tag{4}$$

The coefficient $A = 0.2037 \pm 0.0238$ was determined by a linear fit to the data for the Fe, Co, and Ni results, where the values of 2.083, 1.523, and 0.518 were used as μ_{spin} [15] for Fe, Co, and Ni, respectively. The magnetic effect R of $\mathrm{CeRh_3B_2}$ was $-0.001\,40 \pm 0.000\,15$. This leads to the spin moment $\mu_{spin} = -1.16 \pm 0.12\ \mu_B$ using equation (4). Comparing with the saturated magnetization of 0.45 μ_B, we obtain the orbital moment of $1.61 \pm 0.12\ \mu_B$.

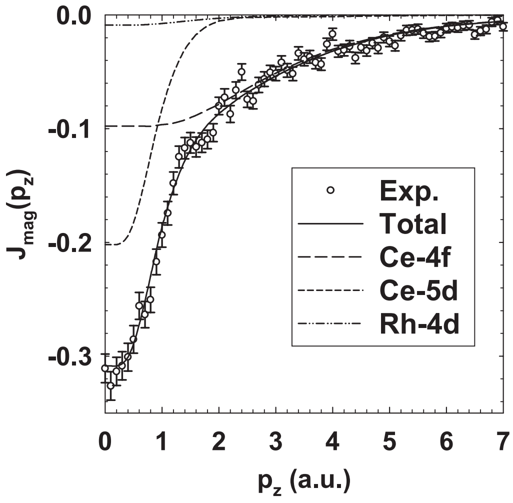

Figure 1. The experimental MCP of $CeRh_3B_2$ and the best fit with atomic profiles to the experimental MCP.

Table 1. Experimental spin and orbital moments on each electronic state. The spin moments are obtained from the MCS experiments. The orbital moments are determined by comparison between the MCS data and the polarized neutron diffraction data [18].

Ce 4f		Ce 5d		Rh 4d		
Spin (μ_B)	Orbital (μ_B)	Spin (μ_B)	Orbital (μ_B)	Spin (μ_B)	Orbital (μ_B)	
−0.69(8)	+1.25(9)	−0.41(4)	+0.23(6)	−0.03(4)	—	Present work
−0.30(4)	+0.86(5)	−0.34(7)	+0.16(7)	−0.05(3)	—	Reference [17]

Figure 1 shows the experimental MCP along the $[11\bar{2}0]$ direction, in which the area under the profile is normalized to the value of $-1.16\ \mu_B$. The MCP is decomposed into partial profiles by fitting with the Ce 4f, Ce 5d, and Rh 4d atomic profiles [16]. The area under each fitted profile is presented in table 1, together with those obtained by Yaouanc *et al* [17]. The difference in Ce 4f spin moment between the present and previous results is probably due to the inadequate fit to the previous data which has fewer data points with poor statistical accuracy. A noticeable point is that the Ce 5d electrons have a significant spin moment which is parallel to the Ce 4f one. This suggests effects of the intra-atomic Ce 4f–5d exchange interaction. Comparing the present results with those obtained from the polarized neutron scattering experiments [18], we have determined the orbital moments on the Ce 4f and Ce 5d states (see table 1). The ratio of orbital to spin moments on the Ce 4f state is $\sim$1.8, which is smaller than the value of 4 expected for the Ce^{3+} ion. This moment reduction can be explained by the strong inter-atomic hybridization of the Ce 4f orbital with the orbitals on the surrounding ions [19].

Consequently, the present study supports the conclusion that both the inter-atomic 4f–5d hybridization and the intra-atomic 4f–5d exchange interaction play important roles in explaining the unusual ferromagnetism of $CeRh_3B_2$.

Acknowledgments

It is a pleasure to acknowledge important discussion with Nozumu Hiraoka, Hiroshi Yamagami and Aniruddha Deb. This work was financially supported by both a Grant-in-Aid for COE Research (10CE2004) from the Ministry of Education, Culture, Sports, Science and Technology of Japan and the SPring-8 Research Promotion Scheme under the auspices of the Japan Science and Technology Corporation.

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