Journal of Alloys and Compounds, 191 (1993) L9–L10
JALCOM 544

Letter

The $GdPt_2Sn$-type crystal structure of $CePd_2In$

B. Xue and F. Hulliger
Laboratorium für Festkörperphysik, ETH Hönggerberg, CH-8093 Zürich (Switzerland)

Ch. Baerlocher and M. Estermann
Institut für Kristallographie und Petrographie, ETH Zentrum, CH-8092 Zürich (Switzerland)

(Received October 7, 1992)

1. Introduction

Ternary compounds with the general composition RPt_2In and RPt_2Sn (R, rare earth) were investigated by Mooij and Buschow [1] and Dwight [2]. The crystal structure of these compounds was found to be of the hexagonal $ZrPt_2Al$ type (space group $P6_3/mmc$), more correctly named the $GdPt_2Sn$ type according to Parthé [3]. As part of an investigation into the crystal structures of cerium compounds of the form CeT_2X (T, transition element; X, B element), the crystal structure of $CePd_2In$ has been determined by the Rietveld powder method.

2. Experimental details

The sample was synthesized by arc melting the constituent elements under purified argon in a water-cooled copper hearth. All elements had a nominal purity of 99.9%. Traces of foreign phases were detectable on the Guinier powder photograph taken with copper K α_1 radiation. Attempts to improve the phase purity by annealing at 580 and 600 °C for 2–4 days had little success. Indexing was verified with the aid of the Lazy-Pulverix programme [4]. Diffraction data were collected on a PADX diffractometer with Cu Kα radiation in steps of 0.02° within the range $18° < 2\theta < 85°$. For the structure refinement we used the X-ray Rietveld system XRS-82 [5]. A total of 22 structural parameters and nine profile parameters were varied during the course of the refinements. After deleting the foreign phases, the refinement finally converged to $R_F = 0.047$, $R_{wp} = 0.169$ and $R_{exp} = 0.047$.

The magnetic susceptibility was measured on the polycrystalline sample between 2 and 300 K in a field of 10 kOe.

3. Results and discussion

The crystallographic data for $CePd_2In$ and the relevant interatomic distances are given in Tables 1 and 2 respectively. The crystal structure is shown in Fig. 1. The weakest and strongest bonds are found between Ce and Pd and between In and Pd atoms respectively. The shortest bond length is In–Pd = 2.764 Å, equivalent to an 8.8% contraction with respect to the element radii [11]. The present bond lengths and angles are comparable with those of YPt_2In, where the shortest bond length is 2.746 Å between Pt and In, corresponding to the largest contraction of 10% [2]. As expected, the $CePd_2In$ unit cell is slightly larger than that of YPt_2In. Similar Ce–Ce, In–In, Ce–In, Pd–Pd and Pd–In bond lengths are also found in related compounds such as Ce_2In [6] and $LaPd_2In$ [7].

The magnetic measurements showed that the Curie–Weiss law is obeyed from about 100 to 300 K

TABLE 1. Crystallographic data for $CePd_2In$ ($T = 295$ K): $GdPt_2Sn$ type, $P6_3/mmc$ (No. 194), $Z = 2$, $a = 4.6272(5)$ Å, $c = 9.1975(5)$ Å, $V = 170.54(9)$ Å^3, $d_x = 9.107$ g cm^{-3}

Element	Site	x	y	z	U_{eq}
Pd	4*f*	$\frac{1}{3}$	$\frac{2}{3}$	0.5775(1)	0.0166(4)
Ce	2*c*	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	0.0171(4)
In	2*a*	0	0	0	0.0160(0)

$R_f = 0.047$, $R_{wp} = 0.169$, $R_{exp} = 0.047$.

TABLE 2. Interatomic distances (Å) for $CePd_2In$

Ce–2Pd	3.010(1)	Pd–3In	2.764(1)
6Pd	3.108(1)	1Ce	3.010(1)
6In	3.525(1)	3Pd	3.026(1)
In–6Pd	2.764(1)	3Ce	3.108(1)
6Ce	3.525(1)	1Pd	3.177(1)

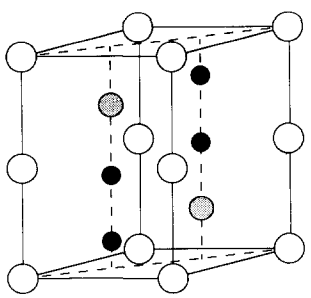

Fig. 1. Schematic representation of the hexagonal unit cell of $GdPt_2Sn$-type $CePd_2In$: ⊛, Ce in 2*c*; ○, In in 2*a*; ●, Pd in 4*f*.

0925-8388/93/$6.00

with an effective Bohr magneton number $n_p = 2.57\ \mu_B$ and a paramagnetic Curie temperature $\Theta_p = -2$ K. The experimental n_p fits well with the theoretical value of 2.54 μ_B. Small deviations from the Curie–Weiss law were observed below 100 K, demonstrating a weak crystal electric field influence on the $^2F_{5/2}$ ground state of the single 4f electron of cerium. No magnetic ordering was observed down to 2 K.

Acknowledgments

We thank Dr. S. Takagi (Tohoku University, Japan), Professor H. U. Nissen and Dr. C. Beeli for stimulating the work. Moreover, we are greatly indebted to Mr. St. Siegrist who prepared the samples, Dr. A. Stahel and Mr. M. Romer (Institute of Mineralogy and Petrography, ETHZ) who kindly helped us in data collection during the primary stage of the structure determination, and Professor H. C. Siegmann for his encouragement and support. Financial support by the Swiss National Science Foundation is also gratefully acknowledged.

References

1 D. B. de Mooij and K. H. J. Buschow, *J. Less-Common Met., 102* (1984) 113.
2 A. E. Dwight, *Mater. Res. Bull., 22* (1987) 201.
3 E. Parthé, personal communication, 1992.
4 K. Yvon, W. Jeitschko and E. Parthé, *J. Appl. Crystallogr., 10* (1977) 73.
5 Ch. Baerlocher, *X-ray Rietveld System XRS-82*, Crystallographic Institute, ETH, Zürich, 1982.
6 A. Palenzona, *J. Less-Common Met., 16* (1968) 379.
7 B. Xue, H. Schwer and F. Hulliger, *Acta Crystallogr., C48* (1992) 2064.