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Magnetic properties of the $Pr_{1-x}Gd_xCo_4B$ compounds

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ABSTRACT

In this work, we have investigated the effect of the substitution of Gd for Pr on the crystal structure and magnetic properties of the $Pr_{1-x}Gd_xCo_4B$ compounds for $0 \leqslant x \leqslant 1$ using X-ray powder diffraction, magnetic measurements, and differential scanning calorimetry (DSC). These compounds have hexagonal $CeCo_4B$-type structure with the space group P6/mmm. The substitution of Gd for Pr leads to a decrease of the unit-cell parameters a and the unit-cell volume V, while the unit-cell parameter c increases slightly. Magnetic measurements indicate that all samples are ordered magnetically below room temperature. The Curie temperatures determined by DSC technique increase as Pr is substituted by Gd. The saturation magnetization at 5 K decreases upon Gd substitution up to $x = 0.6$, and then increases again.

1. Introduction

During the past years, the intermetallic compounds with general formula RT_5 (R = rare-earth and T = transition element) and their substitutional derivatives have been extensively studied because of a variety of interesting properties they exhibit, such as high coercivity, crystal field effects, magnetocaloric effect, spin fluctuation, magnetic anisotropy, etc. Rare-earth (R) metals have strongly localized 4f electrons which may interact with 3d electrons of transition metals. Therefore, there is interplay between the localized and itinerant magnetism, yielding a variety of interesting physical properties [1–6]. The RCo_4B compounds are attracting a great deal of interest, not only because of their possible applications as permanent magnetic materials but also because of the opportunities they offer for investigating the magnetic properties of the 4f and 3d elements [7–11]. The RCo_4B phases, belonging to the $R_{n+1}Co_{3n+5}B_{2n}$ ($n = 0, 1, 2, 3, \infty$) family of compounds with $n = 1$, crystallize in the hexagonal (P6/mmm) $CeCo_4B$-type structure which is obtained by an ordered substitution of boron for cobalt in every second layer of the $CaCu_5$-type structure. In the $CeCo_4B$-type structure, the R atoms occupy the 1a and 1b sites, the Co atoms are in the 2c and 6i sites, and the B atoms reside in the 2d sites [12,13]. As can be seen in Fig. 1, the cobalt atoms occupy distinct sites having different types and numbers of neighbouring atoms. Consequently, their magnetic contributions are expected to be different. By magnetic measurements only the mean values of cobalt moments may be obtained.

Previous investigations on RCo_4B compounds have shown that $PrCo_4B$ is ferromagnetically ordered, while in the case of $GdCo_4B$ a ferrimagnetic-type ordering was shown [14–20]. The Curie temperature T_C and the saturation magnetization at 5 K are 459 K and 5.4 μ_B/f.u. for $PrCo_4B$, and 503 K and 3.2 μ_B/f.u. for $GdCo_4B$, respectively [17]. The compound $GdCo_4B$ has also the compensation point T_{Comp} at 421 K [15]. In the case of $PrCo_4B$, the planar anisotropy of the Pr sublattice is enhanced below T_C [17], while the $GdCo_4B$ is axial below T_{Comp} and planar between T_{Comp} and T_C [15]. This study deals with the crystal structure and the magnetic properties of the $Pr_{1-x}Gd_xCo_4B$ compounds.

2. Experimental

Polycrystalline $Pr_{1-x}Gd_xCo_4B$ compounds with $x = 0.0$, 0.2, 0.4, 0.6, 0.8, and 1.0 were prepared by arc melting under argon atmosphere with appropriate amounts of Pr (99.9%), Gd (99.9%), Co (99.5%), and B (99.7%) in a water-cooled copper boat. The ingots were inverted and remelted several times to ensure homogeneity. X-ray diffraction (XRD) studies were carried out

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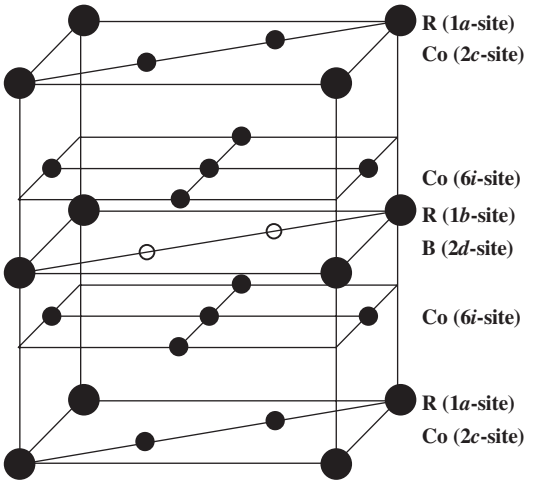

Fig. 1. The unit cell of the $CeCo_4B$-type structure.

by using a Brucker D8 Advance diffractometer equipped with CuKα radiation. The characterization of the samples by differential scanning calorimetry (DSC) was performed using DSC 2010 (TA Instruments) in an alumina box under protective nitrogen gas above room temperature. The heating ramp was run at 20 K/min. Magnetic measurements were carried out using a Q-3398 (Cryogenic) magnetometer in the temperature range from 5 to 300 K, with a maximum applied magnetic field of 7 T.

3. Results and discussion

X-ray diffraction patterns at room temperature confirm the existence of a hexagonal main phase having the $CeCo_4B$-type structure with minor amounts of extra phases. The lattice parameters a and c determined using the standard pattern matching method of the FULLPROF [21] program and the unit-cell volume V for the $Pr_{1-x}Gd_xCo_4B$ samples at room temperature are shown in Fig. 2, while the refined unit-cell parameters a and c, c/a and unit-cell volume V are given in Table 1. It can be seen that substitution of Gd for Pr results in a linear decrease in the lattice constant a, while the lattice constant c is only little dependent on composition and increases linearly. The evaluation of the crystal structure and interatomic distances allows us to conclude that the lattice parameter c depends on the Co(2c)–Co(6i) and Co(6i)–B(2d) distances, while the lattice parameter a is determined by the interatomic distances between R(1a)–Co(2c) and R(1b)–B(2d) atoms located in the same (u,v,0) plane. The change in the metallic radius in the rare-earth site during alloying affects significantly the lattice parameter a [17]. Therefore, decreases of the unit-cell constant a may be associated with the smaller metallic radius of Gd atom compared with Pr atom. Similar behavior was also observed by Burzo et al. [20]. The ratio c/a increases linearly with increasing Gd content x. The lattice parameters obtained for $x = 0$ and 1 are in good agreement with previously reported values in the literature [14,17,19].

The temperature dependence of the magnetization of the $Pr_{1-x}Gd_xCo_4B$ compounds in the temperature range 5–300 K in an applied field of 0.1 T is shown in Fig. 3. It can be seen that all samples order magnetically and there is no magnetic phase transition below room temperature. From the M–T plots at 0.1 T, it can be inferred that the Curie temperature of this series of compounds is above room temperature. The magnetization as a function of temperature behaves differently for the different compositions. The magnetization decreases weakly for the

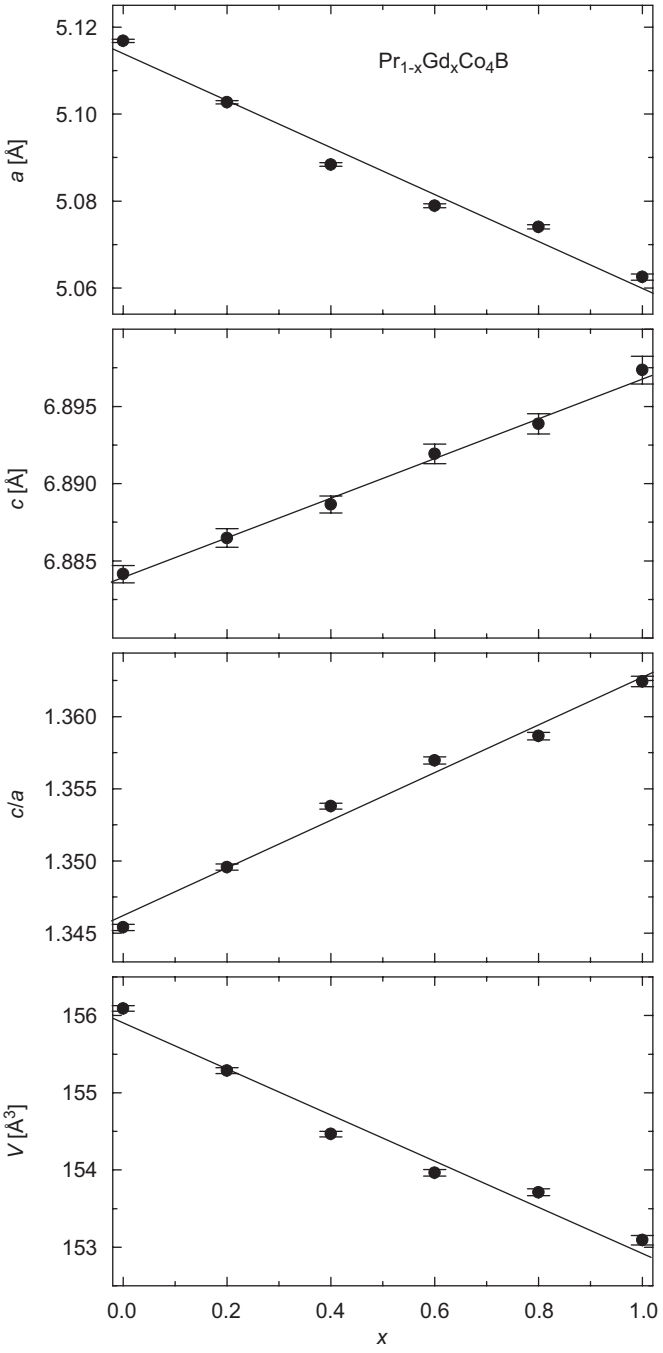

Fig. 2. Variation of the lattice constants a and c, c/a, and the unit-cell volume V with Gd concentration x at room temperature for the $Pr_{1-x}Gd_xCo_4B$ compounds.

Table 1
The lattice constants a and c, c/a, the unit-cell volume V, the saturation magnetization M_S, the magnetic moment of the Co atom M_{Co} and the Curie temperature T_C for the $Pr_{1-x}Gd_xCo_4B$ compounds

x	a (Å)	c (Å)	c/a	V (Å^3)	M_S (μ_B/f.u.)	M_{Co} (μ_B/Co)	T_C (K)
0.0	5.1168(4)	6.8841(6)	1.3454(2)	156.09(4)	6.17	0.74	458±2
0.2	5.1027(4)	6.8865(6)	1.3496(2)	155.29(4)	4.23	0.77	470±4
0.4	5.0884(4)	6.8886(6)	1.3538(2)	154.46(4)	1.70	0.64	480±4
0.6	5.0789(5)	6.8919(6)	1.3570(3)	153.96(4)	0.81	0.93	493±5
0.8	5.0740(5)	6.8939(7)	1.3587(3)	153.71(4)	1.44	0.88	494±4
1.0	5.0625(7)	6.8974(9)	1.3624(4)	153.09(6)	3.42	0.89	505±3