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ROLE OF BORON IN $Nd(Co_{1-x}B_x)_5$ SYSTEM

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The influence of boron atoms on the magnetic properties of $Nd(Co_{1-x}B_x)_5$ (i.e. $NdCo_5$, $NdCo_4B$, $Nd_3Co_{11}B_4$ and $Nd_2Co_7B_3$) compounds has been studied. These structures are based on the well-known $CaCu_5$ structure. They all have the hexagonal symmetry and belong to the space group of $P6/mmm$. The experimental values of the Curie temperatures (T_C) of $Nd(Co_{1-x}B_x)_5$ are used to calculate the effective intersublattice exchange interactions (J_{NdCo}) between Nd and Co sublattices. As the B content increases, a tendency to decrease in J_{NdCo} and T_C is found. This variation is compared with that observed for the Co magnetic moment.

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1. Introduction

The study of magnetic behavior of the rare earth (R)-transition metal (T) compounds has been a subject of great interest from both the theoretical and practical point of view. In the rare earth-transition metal compounds, it is generally accepted that three types of interactions exist: the R–R, R–T and T–T exchange interactions. Two different microscopic models for the exchange coupling have been proposed in literature. Campbell [1] postulated a $4f-5d-3d$ interaction model, based on the idea that due to the localized nature of the $4f$ states their interaction with itinerant spins can only be mediated through the local exchange interaction (mainly J_{4f-5d}) at the rare earth atom, with a subsequent $5d-3d$ interaction (J_{5d-3d}). In contrast, Brooks et al. [2] have outlined that the intersublattice coupling arises from combination of local $4f-5d$ exchange and $5d-3d$ hybridization, and the value of the intersublattice molecular-field coefficient n_{RT} is essentially determined by J_{4f-5d}, and there is no major contribution of an effective J_{5d-3d}. The crystal structures of the $R_{n+1}Co_{3n+5}B_{2n}$ (or $Nd(Co_{1-x}B_x)_5$) compounds, where R is a rare earth or yttrium and $n = 0$ (RCo_5), $n = 1$ (RCo_4B), $n = 2$ ($R_3Co_{11}B_4$), $n = 3$ ($R_2Co_7B_3$) and $n \to \infty$ (RCo_3B_2), can be imagined as being built up by ordered substitutions of boron atoms into the cobalt sites in an RCo_5-type structure [3]. The unit cells of these compounds are formed by alternative stacking of one layer of RCo_5 and n layers of RCo_3B_2 unit cells.

In this paper we will present the influence of B atoms on the magnetic properties of $Nd(Co_{1-x}B_x)_5$ system.

2. Evaluation of the Nd–Co exchange coupling parameter

The R–T exchange interaction is a very important parameter in the description of magnetic properties of rare earth-transition metal compounds. Although its strength is modest compared with the T–T interaction which primarily determines the Curie temperatures, the R–T interaction has considerable influence on magnetocrystalline anisotropy and its temperature dependence since it couples the strongly anisotropic R-sublattice magnetization to the much less anisotropic T-sublattice magnetization. In order to derive information regarding the coupling constant J_{RCo} between rare earth and cobalt moments in $Nd(Co_{1-x}B_x)_5$ compounds, we have performed a standard mean-field analysis of the observed Curie temperatures T_C. In this method J_{RCo} can be expressed as [4]

$$J_{RCo}^2 = 9k_B{}^2T_C(T_C - T_T)/4Z_{RT}Z_{TR}G_RG_T, \tag{1}$$

where T_C and T_T represent the Curie temperatures of $R(Co_{1-x}B_x)_5$ compounds in which R is magnetic (Nd) or R is nonmagnetic (Y), respectively. G_R is the de Gennes factor $(g-1)^2J(J+1)$ for the rare earth atom and G_T is the corresponding de Gennes factor for the transition metal, $G_T = S_T(S_T+1) = p_{eff}^2/4$. p_{eff} is the Co effective paramagnetic moment, given in Ref. [5]. Z_{RT} is the average number of T nearest neighbors to one R atom and Z_{TR} is the average number of R nearest neighbors to one T atom. Representative Z_{RT}, Z_{TR}, T_C, T_T and p_{eff} values for the Nd–Co–B compounds are listed in Table. The values of T_C and M_{Co} for $NdCo_5$, $NdCo_4B$, $Nd_3Co_{11}B_4$ and $Nd_2Co_7B_3$ are taken from [6, 7] (Table).

TABLE

Values of the Co magnetic moment (M_{Co}), effective paramagnetic moment (p_{eff}), the number of nearest neighbors of Nd and Co atoms (Z_{NdCo} and Z_{CoNd}), Curie temperature (T_C) and values of J_{NdCo} in a number of Nd–Co–B compounds. The ordering temperature (T_{Co}) for the corresponding Y(La)–Co–B compounds are also listed.

Compounds	M_{Co} [μ_B/at]	p_{eff} [μ_B/at]	Z_{NdCo}	Z_{CoNd}	T_C [K]	T_{Co} [K]	J_{NdCo} [10^{-22}J]
$NdCo_5$	1.26	2.60	18.0	3.60	930	874	3.33
$NdCo_4B$	0.65	2.35	15.0	3.75	458	382	3.23
$Nd_3Co_{11}B_4$	0.24	2.20	14.0	3.80	392	345	2.58
$Nd_2Co_7B_3$	0.20	2.20	13.5	3.85	332	310	1.64

3. Results and discussion

On the basis of Eq. (1), the Nd–Co exchange coupling parameter was evaluated for all $Nd(Co_{1-x}B_x)_5$ compounds. The results obtained are presented in Table. J_{NdCo} and M_{Co} are plotted as a function of B concentration in Figs. 1 and 2. Both J_{NdCo} and M_{Co} decrease with increasing x in the $Nd(Co_{1-x}B_x)_5$ compounds. Similar results were reported for $Gd_2Fe_{17}N_x$ by Loewenhaupt et al. [8].

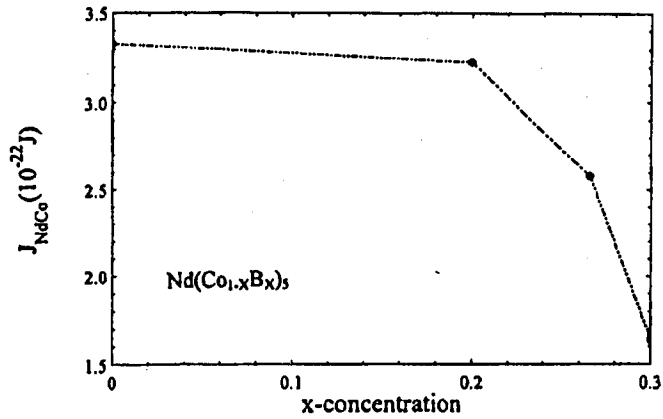

Fig. 1. J_{NdCo} as a function of x in the $Nd(Co_{1-x}B_x)_5$ compounds.

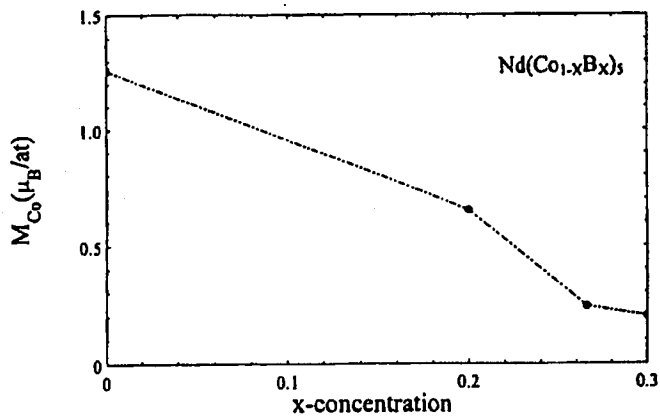

Fig. 2. Experimental Co-magnetic moment as a function of x in the $Nd(Co_{1-x}B_x)_5$ compounds.

The $3d$–$4f$ exchange interaction in R–T compounds is mediated by the interatomic $3d$–$5d$ interaction and the intraatomic $4f$–$5d$ interaction. For the given series of R–T compounds, the absolute value of J_{RT} usually decreases monotonically with increasing atomic number of the R component [9]. This has been experimentally observed in most of the studied series [2] and has been theoretically explained as being due to an increasing spatial separation between $4f$ and $5d$ shells in the R atoms [10]. An increasing $5d$ concentration usually results in an increase in J_{RT} as found for the R–Co and R–Fe systems [11], whereas, here, $2p$ (B) electrons cause J_{RCo} to reduce in Nd–Co–B system. For the strong ferromagnetic compounds, a decrease in Co magnetic moment is usually associated with the enhancement of

the induced $5d$ magnetic moment due to the $3d$–$5d$ hybridization. This gives rise to the increase of $4f$–$3d$ exchange interaction [2]. The entrance of the $2p$ electrons, on the contrary, reduces not only the $3d$–$5d$ hybridization, but also the $3d$ band splitting, since the density of $3d$ states at the Fermi level is lowered [12]. As a consequence, it reduces the $5d$ magnetic moment and then the strength of Nd–Co interactions in $Nd(Co_{1-x}B_x)_5$ compounds. T_C decreases on replacing Co atoms in $Nd(Co_{1-x}B_x)_5$ by B atoms (Table). This reduction in T_C presumably results from weakened Co–Co exchange interactions due to the replacement of Co by B at the $2c$ sites. The decrease in T_C is also observed in $Y(Co_{1-x}B_x)_5$ [13]. In conclusion, the partial replacement of the Co atoms by boron in $Nd(Co_{1-x}B_x)_5$ system causes the decreasing of the T_C and M_{Co}, and also the lowering of th intersublattice exchange interaction J_{NdCo}.

References

[1] I.A. Campbell, *J. Phys. F, Metal Phys.* **2**, L47 (1972).

[2] M.S.S. Brooks, B. Johansson, in: *Ferromagnetic Materials*, Ed. K.H.J. Buschow, Vol. 7, North-Holland, Amsterdam 1993, p. 139.

[3] N.B. Kuz'ma, N.S. Bilonizhko, *Kristallografiya* **18**, 710 (1973).

[4] X.P. Zhong, F.R de Boer, T.H. Jacobs, K.H.J. Buschow, *J. Magn. Magn. Mater.* **92**, 46 (1990).

[5] E. Burzo, V. Pop, C.C. Borodi, R. Ballou, *IEEE Trans. Magn.* **30**, 628 (1994); R. Ballou, E. Burzo, V. Pop, *J. Appl. Phys.* **73**, 5695 (1993).

[6] A. Kowalczyk, L. Smardz, U. Köbler, in preparation.

[7] E. Burzo, A. Chełkowski, H.R. Kirchmayr, in: *Landolt-Börnstein, New Series Group III*, Ed. H.P.J. Wijn, Vol. 19d, Springer-Verlag, Berlin 1990.

[8] M. Loewenhaupt, P. Tils, D.P. Middleton, K.H.J. Buschow, R. Eccleston, *J. Magn. Magn. Mater.* **129**, 151 (1994).

[9] A. Kowalczyk, *J. Magn. Magn. Mater.* **136**, 70 (1994).

[10] E. Belorizky, M.E. Fremy, J.P. Gavigan, D. Givord, H.S. Li, *J. Appl. Phys.* **61**, 3971 (1987).

[11] N.H. Duc, T.D. Hien, D. Givord, J.M.M. Franse, F.R. De Boer, *J. Magn. Magn. Mater.* **124**, 305 (1993).

[12] M. Aoki, H. Yamada, *Physica B* **177**, 259 (1992).

[13] A. Kowalczyk, P. Stefański, *IEEE Trans. Magn.* **30**, 648 (1994).