MAGNETIC BEHAVIOUR OF Co IN $YCo_{4-x}Cu_xB$ COMPOUNDS

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The $YCo_{4-x}Cu_xB$ series form solid solutions in the composition range $x \leq 1$.

The RCo_4B compounds, where R is a rare-earth or yttrium crystallize in a hexagonal structure of $CeCo_4B$-type. In this lattice, the R atoms are located in 1a and 1b sites, Co in 2c and 6i sites and B in 2d positions.

The mean cobalt moments, M_{Co}, were shown to be sensitive to R partner, exchange interactions respectively.

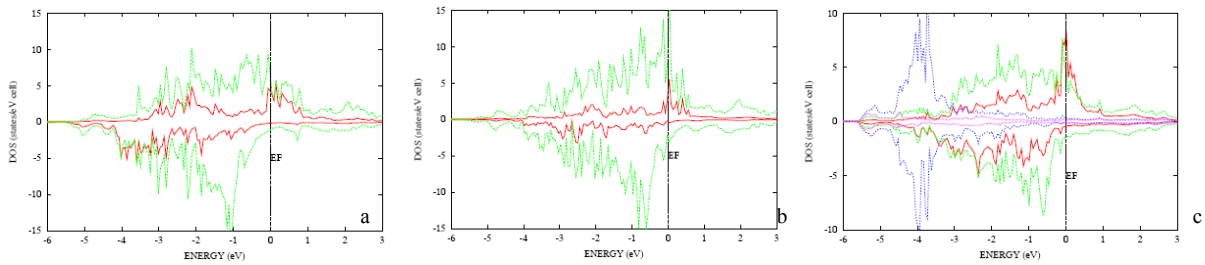
The exchange interactions may be also modified by substituting, in the above compounds, cobalt by a nonmagnetic element. In this way, additional information on cobalt magnetic behaviour can be obtained.

The $YCo_{4-x}Cu_xB$ compounds are ferromagnetically ordered.

Band structure calculations show a parallel diminution of cobalt moments, at 2c and 6i sites, when increasing cooper content, with the same slope of 0.32 ± 0.02 μ_B per one copper substituted atom (table 1 and figure 1).

Table 1. Band structure calculations

Compound	Band structure						Experimental	
	Magnetic moment (μ_B/atom)					M_s	M_s	M_{eff}(Co)
	Y(1b)	Y(1a)	Co(2c)	Co(6i)	B	μ_B/f.u	μ_B/f.u.	μ_B/atom
YCo_4B	-0.22	-0.13	1.44	0.61	-0.03	3.01	2.70	2.27
$YCo_{3.5}Cu_{0.5}B$	-0.15	-0.10	1.25	0.44	-0.03	1.80	1.70	1.98
YCo_3CuB	-0.12	-0.07	1.11	0.32	-0.02	1.20	0.95	1.83
$YCo_{2.5}Cu_{1.5}B$							0.35	



YCo_4B $YCo_{3.5}Cu_{0.5}B$ YCo_3CuB

Fig. 1. The results obtained for YCo_4B, $YCo_{3.5}Cu_{0.5}B$ and YCo_3CuB

The Y4d bands are polarized. The induced Y4d bands polarizations are antiparallely oriented to cobalt moments and dependent on Y4d-Co3d short range exchange interactions.

The 4d-3d short range exchange interactions may be described by the Hamiltonian

$$H = -2\sum_{i,j} J_{3d_i - 4d_j} S_{4d_j} \sum_i S_{3d_i} \qquad (1)$$

The 4d-3d exchange interactions act as an internal field, H_{exch}, on the 4d band and a polarization of this band is induced. The Hamiltonian was analysed in molecular field

approximation assuming that $J_{4d_j-3d_i}$ exchange interactions are not dependent on the lattice sites. In this case the Y4d band polarizations can be described by the next relation:

$$M4d_j \propto \sum_i n_i M_{Co_i} \quad (2)$$

A linear variation of Y4d band polarizations, M_{4d}, as function of $\sum n_i M_{Co_i}$ was obtained with a slope $\alpha \cong 1.2 \cdot 10^{-2}$ similar to that obtained for other rare-earth-transition metal compounds (figure 2).

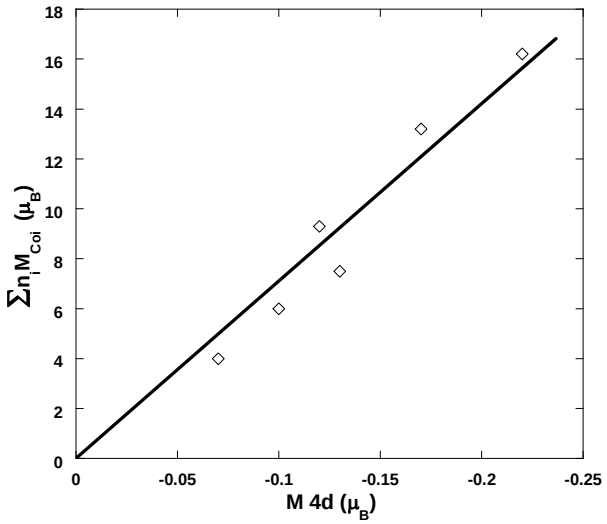


Fig. 2. Linear variation of Y4d band polarizations, M_{4d}, as function of $\sum n_i M_{Co_i}$

There is a hybridization of Co3d band with B2p ones, particularly for atoms located in 6i sites. As a result, a polarization of – 0.03 μ_B is induced on boron sites, antiparallely oriented to cobalt moments.

The compounds $YCo_{4-x}Cu_xB$ are ferromagnetically ordered. For these compounds, the thermal variations of spontaneous magnetization, M_s are presented in the figure 3.

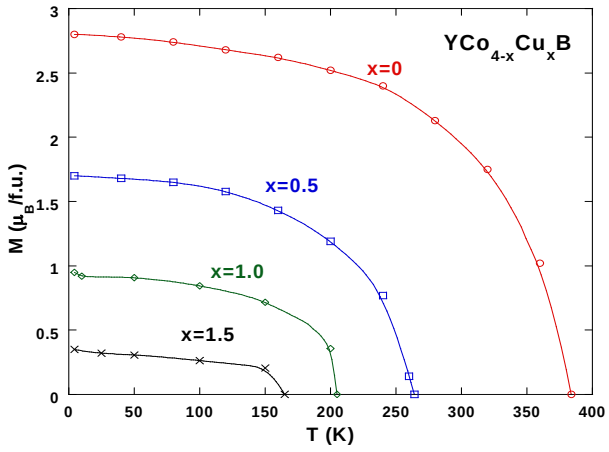


Fig. 3. The thermal variations of spontaneous magnetization for the compounds $YCo_{4-x}Cu_xB$

The saturation magnetizations and Curie temperatures, T_C, decrease when increasing the copper content (figure 4).

Since T_C values are determined by the exchange interactions, the change in the magnetizations can be correlated with the diminution of exchange field acting on cobalt.

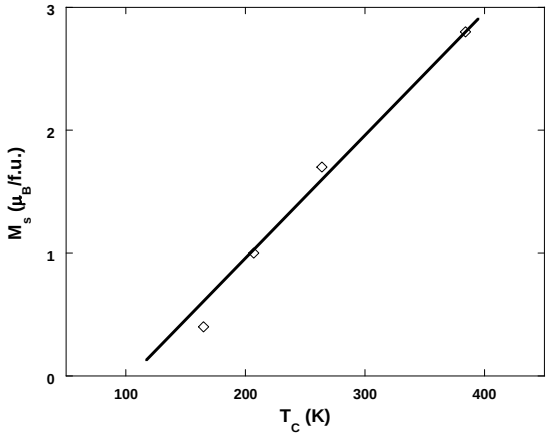


Fig. 4. The saturation magnetizations and Curie temperatures

The variation of cobalt moments in rare earth compounds is linearly dependent on exchange fields. A similar dependence can be obtained in the present system, although the proportionality constant is somewhat lower than $(3\cdot10^6)^{-1}$ μ_B/Oe evidenced in Laves phase structures (figure 5).

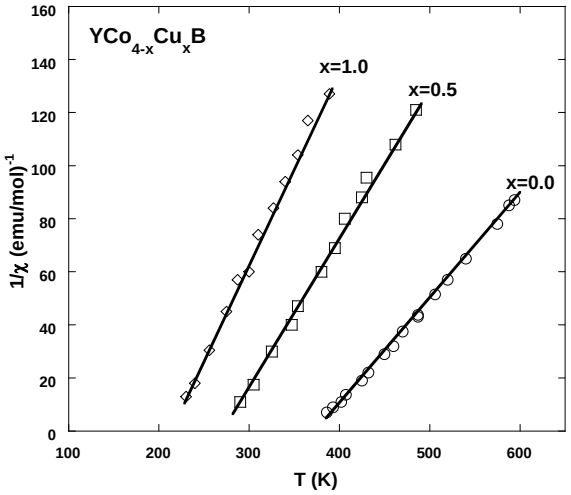


Fig. 5. The variation of cobalt moments in rare earth compounds

The temperature dependences of reciprocal susceptibilities follow Curie-Weiss type behavior:

$$\chi = C(T-\theta)^{-1} \qquad (3)$$

The mean effective cobalt moments decrease from 2.20 μ_B/atom for x = 0 up to 1.80 μ_B/atom for x = 1.0.

Neglecting the Y4d band polarizations, the M_{Co} values decrease from 0.67 μ_B (x=0) to 0.486 μ_B (x=0.5) and finally to 0.32 μ_B (x=1).

Information on the degree of itinerancy of cobalt atoms can be obtained from the ratio r = S_p/S_o, between the mean number of spins determined from Curie constants, S_p, and those obtained from saturation measurements, S_o.

The r ratio increases from r=2.9 (x=0) to r ≅3.8 (x=1.0) showing an increase of the degree of itinerancy.

Conclusions

The cobalt in the present system can be characterized as a weak ferromagnet, as showed by the sensitivity to the exchange interactions as well as by the rather high difference between the number of spins determined from Curie constants and saturation measurements.

References

[1] Burzo, E., Plugaru, N., I. Creanga, I., Ursu, I., *J. less Common Met*. 155, 281, 1989.
[2] Anderson, O.K., Jepsen, O., *Phys. Rev*. B12, 3060, 1975.
[3] Anderson, O.K., Jepsen, O., Gözel, D. in F. Bessani, F. Fumi, and M.P. Tosi (Eds.), *Highlights of Condensed Theory*, North Holland, Amsterdam, 1995.
[4] Jones, R.O., Gunnarson, *Rev. Mod. Phys*. 61, 689, 1989
[5] Von Barth, U., Hedin, L*., J. Phys. C.: Solid State* 5, 1629, 1972.
[6] Burzo, E., Chelkovski, A., Krichmayr, H.R., *Landold Börnstein Handbook*, Springer, Berlin, vol. 19d2, 1990.
[7] Burzo, E., Chioncel, L., Costina, I., Chiuzbaian, S.G., *J. Phys.: Condens. Matter* 18, 4861 2006.
[8] Burzo, E., *Mol. Cryst. Liq. Cryst*. 417, 491, 2004.
[9] Burzo, E., *J. Solid State Chem*. 16, 257 (1976); *J. less Common Met*. 77, 251, 1981.
[10] Georges, A., Kothar, G., Krauth W., Rosenberg, M.J., *Rev, Mod. Phys*. 68, 13, 1996.