

05.2-9 CRYSTAL AND MAGNETIC STRUCTURE OF PERMANENT MAGNET MATERIALS  $\text{Nd}_2\text{Fe}_{14-x}\text{Co}_x\text{B}$ . By K. Girgis, M. Kraft and U. Weis, Institut für Kristallographie und Petrographie, ETHZ, Switzerland, P. Fischer, Labor für Neutronenstreuung, ETH, Switzerland, and M. Sostarich, Ruhr Universität, PB 102148, 4630 Bochum, FRG.

### 1. Introduction:

A promising group of permanent magnet materials:  $\text{R}_2\text{Fe}_{14}\text{B}$  (R=rare earth metal) was discovered. The main limitation of these compounds is their relatively low Curie temperature (e.g. 585 K for  $\text{Nd}_2\text{Fe}_{14}\text{B}$ ).

### 2. The aim of this work is:

1. try to raise the Curie temperature,
2. study the correlation between the structure and magnetic properties of these materials.

### 3. Experimental procedures:

The samples were prepared, annealed and studied metallographically, by microprobe, X-rays and neutron diffraction methods.

### 4. Lattice constants:

The  $\text{Nd}_2\text{Fe}_{14-x}\text{Co}_x\text{B}$  series crystallizes in the tetragonal space group  $\text{P4}_2/\text{mmm}$  (136) with 68 atoms per unit cell. The tetragonal phase exists over the whole range of composition. The lattice constants decrease with increase of Co-content.

### 5. Curie temperature:

The Curie temperature has been determined from thermal demagnetisation curves at a constant field strength of 6 KOe. The measured values are higher than those measured by (Matsuura, Y. et al., Appl. Lett., 1985, 46, 308; Buschow, K.H.J., et al., J. Less-Common Met., 1985, 109, 79; Fuerst, C.D., et al., J. Magn. Magn. Mater., 1986, 54-57, 567).

### 6. Magnetic structures:

$\text{Nd}_2\text{Fe}_{14-x}\text{Co}_x\text{B}$  compounds with  $x = 1, 4$  and  $8$  respectively have been studied. Iron and cobalt are statistically distributed except for the site  $\text{Fe}_4(8j_2)$  which is preferred by iron where the highest magnetic moments are possible. The atomic parameters agree well with (Herbst, J.F., et al., Phys. Rev., 1984, 29B, 4176), see Fig. 1. All magnetic moments are //c and do not show any tendency for reorientation with temperature. Further investigations are in progress.

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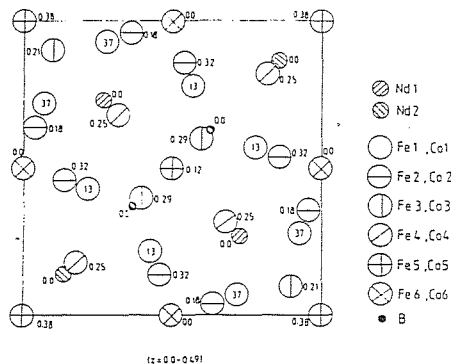


Fig.1. Projection of the structure of  $\text{Nd}_2\text{Fe}_{10}\text{Co}_4\text{B}$  on the x-y-plane (the lower half of the unit cell).

05.2-10 THE MAGNETIC STRUCTURE OF TRANSITION METAL TETRAMETAPHOSPHATES. By W. Gunsser, K. Rohwer, Institut für Physikalische Chemie der Universität Hamburg, FRG, and A. Wiedenmann, Hahn-Meitner-Institut für Kernforschung, D-1000 Berlin (West).

The tetrametaphosphates  $\text{M}_2\text{P}_4\text{O}_{12}$  (M = divalent metal ion) crystallize in the monoclinic space group  $\text{C2}/c$ . The metal ions occupy two non-equivalent sites  $\text{M}_I$  and  $\text{M}_{II}$  within oxygen octahedra forming zigzag chains in  $[101]$  direction. We investigated powder samples of  $\text{M}_2\text{P}_4\text{O}_{12}$  with  $\text{M} = \text{Mn, Ni, Co}$  and  $\text{Cu}$ . Susceptibility measurements between 2 K and 400 K yielded deviations from Curie-Weiss behavior even far above the critical temperatures  $T_C$  (Mn: 3.3 K; Ni: 13.5 K; Co: 8.1 K; Cu: 7.9 K). In the cases of the Mn and Cu compound the magnetic moments increased below  $T_C$ , but did not reach ferromagnetic saturation.  $\text{Cu}_2\text{P}_4\text{O}_{12}$  shows a large temperature-independent contribution (at high temperatures) and hysteresis and thermo-remanent behavior (below  $T_C$ ) at low fields (500 G).

By neutron diffraction between 2 K and 100 K we could show that  $\text{Ni}_2\text{P}_4\text{O}_{12}$ ,  $\text{Mn}_2\text{P}_4\text{O}_{12}$  and  $\text{Co}_2\text{P}_4\text{O}_{12}$  order antiferromagnetically. The spin structures are not quite collinear, but slightly canted. Moments on  $\text{M}_I$  and  $\text{M}_{II}$  have different absolute values, at least in the cases of the Co compound. Within one chain the moments are approximately parallel, while they are nearly antiparallel in the Mn compound. Since no additional reflections occurred below the critical temperature, the Cu compound cannot be antiferromagnetic, but also a ferromagnetic long range order could not be determined.

05.2-11 MAGNETOSTRICTION IN  $\text{Zn}_{1-x}\text{Cu}_x\text{Cr}_2\text{Se}_4$ , WHERE  $0.2 \leq x \leq 1.0$ . By J. Kusz, S. Juszczyk and J. Warczewski, Silesian University, Institute of Physics, ul. Uniwersytecka 4, PL-40-007, Katowice, Poland.

The temperature dependence of the lattice parameter  $a$  of the mixed spinels  $\text{Zn}_{1-x}\text{Cu}_x\text{Cr}_2\text{Se}_4$  was measured in the temperature range 100K-570K by X-ray powder diffraction technique. For  $x = 1.0, 0.9, 0.8, 0.3$  and  $0.2$  the spontaneous magnetostriction  $\omega$ , the bulk modulus  $K$ , the Born index  $n$  of the repulsive energy, and the lattice energy  $U$  were determined. The distances between the cations (in both tetrahedral and octahedral positions) and the anions are also presented. It turns out that: (1) between anions and cations in tetrahedral positions, the covalent bond dominates although there is a small ionic bond contribution in the cases of  $x = 0.3$  and  $0.2$ ; and (2) between anions and cations in octahedral positions, the ionic bond dominates but there is a significant covalent bond contribution. Based on the molecular field theory, the pressure coefficients of the Curie temperature  $dT_C/dp$  as well as the dependences of the Curie temperature  $T_C$  on both the lattice parameter  $a$  and the copper concentration  $x$  were estimated (J. Kusz, S. Juszczyk and J. Warczewski, Phys. Rev. B, submitted).

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