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Section 2. Intermetallic compounds, alloys and glasses

Magnetic properties and electronic structures of $YCo_{3-x}Ni_xB_2$ compounds

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The $YCo_{3-x}Ni_xB_2$ compounds for $x \leq 2$ are paramagnetic in all the temperature range. The magnetic susceptibilities increase up to a temperature T_m and above a characteristic value T* a Curie-Weiss behavior was shown. The T_m values decrease from $\cong$ 150 K (x=0) to $\cong$ 25 K (x=2). The effective cobalt magnetic moment in YCo_3B_2 compound is 1.34 μ_B. The band structure calculations show that the Fermi level in YCo_3B_2 is situated near a maximum in the density of states. When increasing Ni content the Fermi level shift gradually to a region with lower DOS. The magnetic behavior of the above system is analyzed in the spin fluctuation model.

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1. Introduction

The RCo_3B_2 compounds ($x \leq 2$), where R is a rare-earth or yttrium crystallize in a hexagonal structure having P6/mmm space group [1]. This structure is derived from the $CaCu_5$ one, in which the RCo_5 compounds crystallize. Cobalt occupies in RCo_3B_2 lattice, (3g) site, while boron atoms are located on (2c) sites.

Previously, it was suggested that cobalt atoms in RCo_3B_2 compounds have not a spontaneous magnetic moment [2,3]. A slight polarization of cobalt atoms antiparallelly oriented to gadolinium moment was shown in $Gd_xY_{1-x}Co_3B_2$ [4-6]. Band structure calculations were performed on YCo_3B_2 [7]. The magnetic properties of $SmCo_{3-x}Ni_xB_2$ with $x \leq 0.9$ were also reported [8]. In order to obtain information on the magnetic behavior of transition metals in yttrium compounds we studied the $YCo_{3-x}Ni_xB_2$ system.

2. Experimental

The $YCo_{3-x}Ni_xB_2$ compounds ($x \leq 2$) were prepared by levitation method in purified argon atmosphere. All samples were thermally treated in vacuum, at 900 ^oC, for ten days. The X-ray analyses show the presence of only one phase for $x \leq 1.5$. In case of $YCoNi_2B_2$ a small amount of other phase was observed.

Magnetic measurements were performed in the temperature range 4.2(2) K – 700(300) K and magnetic fields up to 10 T. The magnetic susceptibilities, χ, were determined from their field dependences, according to the relation $\chi_m=\chi+cM_sH^{-1}$, by extrapolation of the measured values χ_m to $H^{-1}\rightarrow 0$. By c is denoted a presumed impurity content and M_s is their saturation magnetization. By this method any possible alteration of magnetic susceptibility, as result of small quantity of magnetic ordered phase, is avoided. For all compounds, the estimated impurity content, if exists, is smaller than 0.2 %.

Band structure calculations were carried out by using the ab initio tight-binding linear muffin tin orbital method in the atomic sphere approximation (TB-LMTO-ASA). The detailed procedure of the calculations was described elsewhere [9-11]. In the framework of the local density approximation (LDA) the total electronic potential is the sum of external, Coulomb and exchange-correlation potentials [12]. The functional form of the exchange correlation energy used in the present work was the free-electron gas parameterization of von Barth and Hedin [13]. Relativistic corrections were included.

3. Experimental results and band structures

The thermal variations of magnetic susceptibilities are plotted in Fig. 1. The compounds are paramagnetic in all the studied composition range. The magnetic susceptibilities increase up to a temperature T_m. The T_m values decrease gradually, from 150 K (x=0) to 25 K (x=2). The YCo_3B_2, at 2 K, has an exchange enhanced magnetic susceptibility of 2.34×10^{-3} (emu/f.u.), close to that evidenced in YCo_2 [14]. The magnetic susceptibilities at 4.2(2) K decrease very rapidly as the cobalt is replaced by nickel – Fig. 2. This feature can be attributed to the decrease of electron correlations as effect of cobalt substitution by nickel.

Above a characteristic temperature T*, a Curie-Weiss type behavior is evidenced. The T* values decrease when increasing nickel content. The Curie constants are given also in Fig. 2. The effective cobalt moment determined from the Curie constant in YCo_3B_2 compound is $\mu_{eff}(Co)=1.34\ \mu_B$.

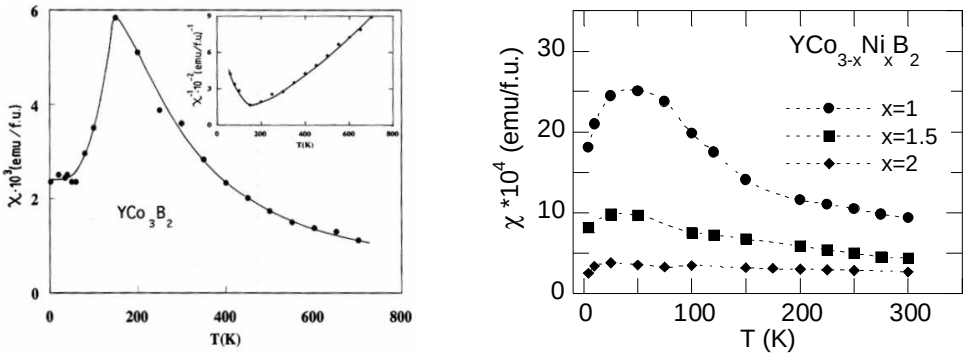

Fig. 1. Thermal variations of magnetic susceptibilities for $YCo_{3-x}Ni_xB_2$ compounds.

The band structures of some representative compounds are plotted in Fig. 3. The Fermi level in YCo_3B_2 is situated near a maximum in the density of states. There is a strong hybridization between 3d-states of cobalt and 2p-states of B. When substituting gradually cobalt by nickel the Fermi level shifts to a region having lower state density.

The susceptibilities determined from band structure calculations describe reasonable the experimentally determined values, at low temperatures – Fig. 2.

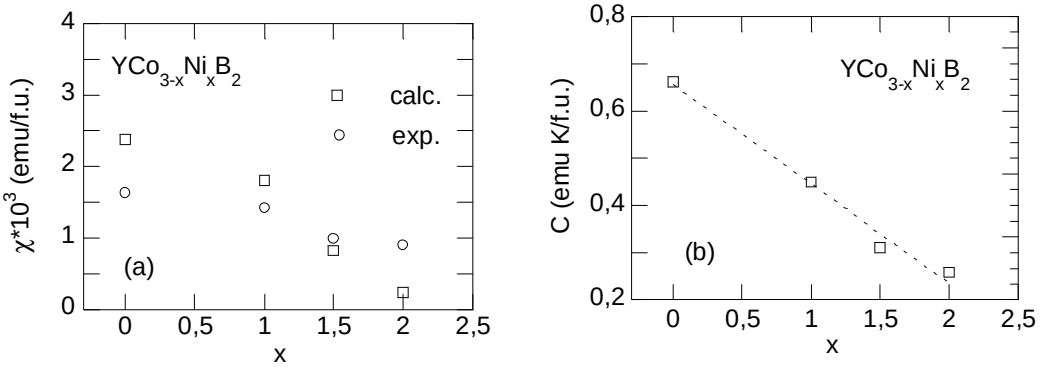

Fig. 2. Composition dependencies of the magnetic susceptibilities at 4.2(2) K experimentally determined and obtained from band structure calculations (a), and of the Curie constants (b) in $YCo_{3-x}Ni_xB_2$ compounds.

4. Discussion

For YCo_3B_2 compound there is no self consistent solution for the ferromagnetic state [7]. The cobalt atoms at (3g) site are situated between the B atom layers and the cobalt d-band is almost filled due to 3d-2p hybridization. The magnetic susceptibilities at 4.2(2) K decrease strongly when cobalt is gradually replaced by nickel. Since both cobalt and nickel are isoelectronic in pseudoternary compounds, the observed trend of the χ values may be attributed only to the diminution of the electron correlation in d-bands. Thus, the exchange enhancement factor of the magnetic susceptibilities decreases.

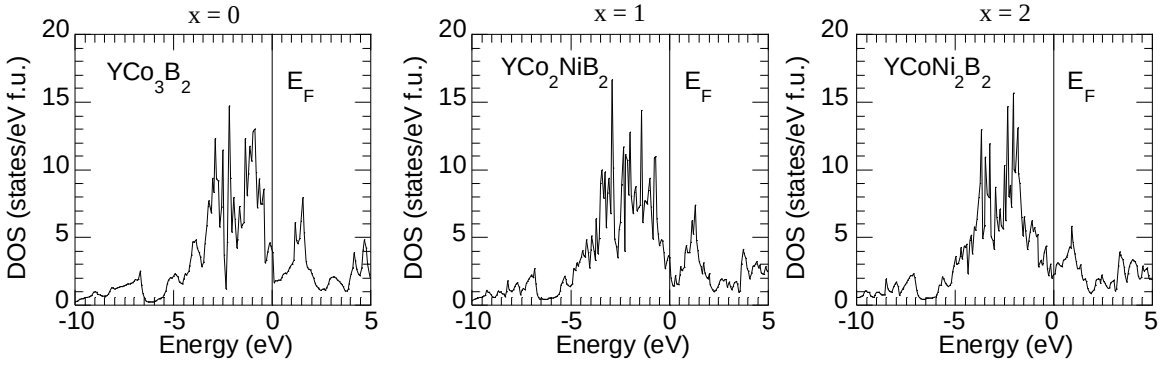

Fig. 3. DOS for $YCo_{3-x}Ni_xB_2$ compounds with x=0, 1 and 2.

The magnetic susceptibilities of $YCo_{3-x}Ni_xB_2$ ($x \leq 2$) increase up to a temperature T_m. Above some characteristic temperatures T*, a Curie-Weiss behavior is shown. The effective cobalt moment in YCo_3B_2 is 1.34 μ_B. This suggest an electronic cobalt configuration (in atomic notation) $3d^{9.4}$. It is difficult matter to analyze the distinct contributions of cobalt and nickel to the Curie constants. We expect that the nickel contributions are rather small and the cobalt ones dominate. The effective moments per transition metal atom decrease from 1.34 μ_B (x=0) to 1.10 μ_B (x=1.0) and 0.80 μ_B (x=2). The magnetic behavior of $YCo_{3-x}Ni_xB_2$ compounds may be analyzed in models what take into account the electron correlation effects in d-band, as spin fluctuation model [17] or dynamical mean field theory [18]. These models reconcile the dual character of electron, which as particle require a real space description and as a wave, a momentum space description. The spin fluctuation model considers the balance between the frequencies of longitudinal spin fluctuations, which are determined by their lifetime and of transverse fluctuations, which are of thermal origin. These effects lead to the concept of temperature-induced magnetic moment. For an exchange enhanced paramagnet, the wave number dependent susceptibility, χ_q, has a large enhancement due to electron-electron interactions, for small q values. The χ_q shows significant temperature dependence only for q values close to zero. The average amplitude of spin fluctuations $\langle S_{loc}^2 \rangle = 3k_B T \sum \chi_q$ increases with temperature and reaches an upper limit at a temperature T*. For T > T* a Curie-Weiss type behavior is predicted similar as in systems having local moments. The moments are localized in q space. The effective cobalt moments decrease when increasing nickel content. The exchange enhancement factor diminishes when Co is replaced by Ni and as a result the spin fluctuations are not saturated. The magnetic behavior of transition metals in $YCo_{3-x}Ni_xB_2$ may be also analysed in dynamical mean field theory (DMFT) [17] combined with the standard LDA band calculations (LDA+DMFT) [18]. In a strongly correlated system, leading Curie-Weiss behavior, at high temperatures is predicted. For an itinerant system, the time dependence of the correlation function, results in a temperature dependence of $\langle S_{loc}^2 \rangle$. Fluctuating moments and atomic like configurations are large at short time. The moments are reduced at larger time scales, corresponding to a more band like and less correlated electronic structure near Fermi level.

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