

ELECTRONIC AND MAGNETIC PROPERTIES OF CUBIC LAVE PHASE COMPOUNDS

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Abstract

Band structure calculations and magnetic measurements were performed on RM_2 -based compounds, where R is a rare-earth or yttrium and M = Fe, Co or Ni. The exchange enhanced paramagnets as $Y(Co_xNi_{1-x})_2$, at $T \leq 10$ K, show a T^2 type dependence of magnetic susceptibilities. Above a characteristic temperature, T^* , a Curie-Weiss behaviour was evidenced. The computed mean square amplitude of spin fluctuations, at high temperatures, describes well the experimentally determined effective moments. The transition of cobalt atoms from nonmagnetic to magnetic state was analysed. A small nickel moment is induced in RNi_2 compounds with magnetic rare-earths. The exchange interactions influence little iron moments. The different contributions to the R5d bands polarizations are also analyzed.

1. Introduction

The RM_2 (M=Fe,Co,Ni) compounds crystallize in a cubic $MgCu_2$ -type structure. In this structure the M atoms occupy $\bar{3}m$ sites and R atoms are located in $\bar{4}3m$ positions. Due to their simple structure these systems were intensively investigated, particularly concerning the magnetic behaviour of M atoms [1]. The YCo_2 and $LuCo_2$, at low temperatures, are paramagnetic. A magnetic moment is induced on Co atoms when nonmagnetic Y or Lu are replaced by a magnetic rare-earth [2]. In RNi_2 system it was generally accepted that nickel is nonmagnetic. The RFe_2 compounds have technical applications in magnetostrictive devices [3]. On the support of R-Fe exchange interactions the high magnetostrictions characteristic of rare-earth, at 4.2 K, are translated at room temperature. In addition, the Fe atoms show a rather localized magnetic behaviour.

The magnetic moments of light rare-earths and transition metals are parallel aligned while in case of heavy rare-earths an antiparallel orientation was shown. In earlier publications [1,4], the exchange interactions between R and M atoms were considered to be of RKKY type [5]. Some researches have been done in order to reverse the antiparallel coupling of R and M elements by changing the electron concentration and distances between magnetic atoms [6]. No results have been obtained. The magnetic coupling between R and M atoms can be well described by the Campbell model [7]. The model suggests that the R-M exchange interactions are mediated by R5d band polarization.

In this paper we analyse the magnetic behaviour of RM_2 -based compounds. We discuss, at the beginning, the exchange enhanced paramagnets as $LuCo_2$ or $Y(Co_xNi_{1-x})_2$. Then, the transition from nonmagnetic to magnetic state of cobalt atoms is analysed. The effect of exchange interactions on R5d band polarizations is correlated with the number and magnetic moments of neighbouring transition metal atoms to a R atom as well the R4f moment.

2. Experimental and computing methods

The samples were prepared by melting the constituent elements in an arc furnace. The compounds were thermally treated at $\approx 900^\circ\text{C}$ for one week. The X-ray analyses show the presence of the MgCu_2 type structure. No other phases were evidenced, in limit of experimental errors of 1 %.

Magnetic measurements were performed in the temperature range 1.7 – 1000 K and fields up to 9 T. The saturation magnetizations were determined from magnetization isotherms, according to approach to saturation law, $M = M_s (1-a/H) + \chi_o H$. By χ_o we denoted a field independent susceptibility and a is the coefficient of magnetic hardness. In the paramagnetic range, the magnetic susceptibilities, χ , were determined from their field dependences, according to the relation $\chi_m = \chi + cM_s'/H$, by extrapolation of measured values, χ_m , to $H^{-1} \rightarrow 0$. By c a presumed impurity content is denoted and M_s' is their saturation magnetization. By this method any possible alteration of the magnetic susceptibilities, as a result of the presence of small quantities of magnetic ordered phase is avoided. For all compounds, the estimated impurity content, if it exists, is smaller than 0.1 %.

Band structure calculations were carried out by using the ab initio tight binding linear muffin tin orbitals method (TB-LMTO) [8-10] both in LDA and LDA+U approaches. In the framework of the local density approximation (LDA), the total electric potential is the sum of the external, Coulomb and exchange correlation potentials [4]. The frozen core approximation was employed in the generation of the potential and parametrization of the Von Barth and Hedin [12] was used for the exchange correlation part of the effective one electron potential, obtained within the local spin density approximation of the density functional theory. The LDA+U scheme [13] is based on the Anderson impurity model in mean field approximation that analyses the s and p electrons as non-correlated, described by an orbital independent potential and d electrons as described by an orbital dependent potential [14].

3. Magnetic behaviour of RCo_2 with $\text{R}=\text{Lu}, \text{Y}$ and $\text{Y}(\text{Co}_x\text{Ni}_{1-x})_2$ compounds

The thermal variations of magnetic susceptibilities for RCo_2 ($\text{R} = \text{Lu}, \text{Y}$) compounds are plotted in Fig. 1. The magnetic susceptibilities increase up to a temperature T_{max} and then decrease continuously. Above a temperature T^* , a Curie-Weiss type behaviour was evidenced. In the low temperature range ($T \leq 10$ K), a T^2 dependence of the magnetic susceptibilities can be shown – Fig.2.

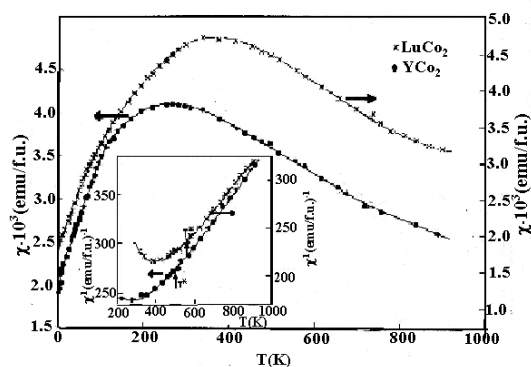


Fig. 1 Thermal variations of magnetic susceptibilities for YCo_2 and LuCo_2 compounds.

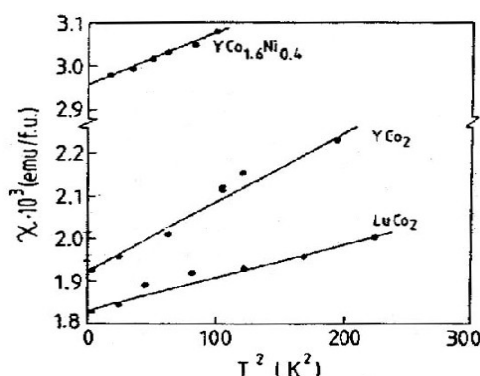


Fig. 2 Thermal variations of magnetic susceptibilities at $T \leq 10$ K for $\text{Y}(\text{Co}_x\text{Ni}_{1-x})_2$ with $x = 1.0$ and 0.8 and LuCo_2

The same behaviour can be evidenced in $Y(Co_xNi_{1-x})_2$ system - Fig.3. The temperatures at which maxima in susceptibilities are shown, decrease when increasing nickel content, from $T_{max} \cong 240$ K ($x = 1.0$) up to $\cong 20$ K ($x = 0.2$). For $Y(Co_{0.2}Ni_{0.8})_2$ compound the magnetic susceptibilities decrease in the whole temperature range [15]. As already stated, the Curie-Weiss dependence is shown above temperatures T^* , which also decrease when increasing nickel content. The effective cobalt moments determined at $T > T^*$, supposing that nickel has no magnetic contribution, vary only little in the studied composition range from $3.87 \mu_B/\text{atom}$ ($x = 1.0$) to $3.72 \mu_B/\text{atom}$ ($x = 0.1$) – Fig.4. The YNi_2 shows mainly a Pauli type paramagnetism.

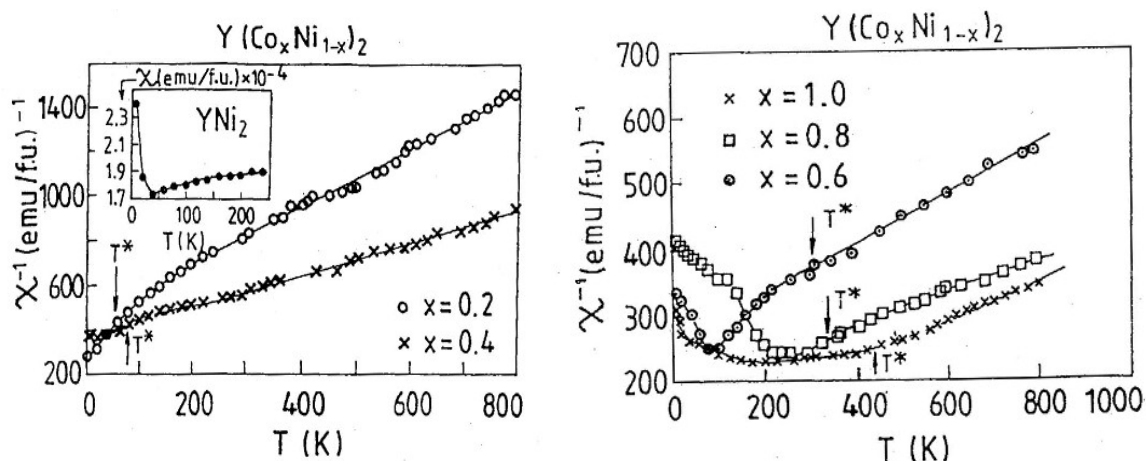


Fig. 3 Thermal variations of reciprocal susceptibilities for $Y(Co_xNi_{1-x})_2$ compounds.

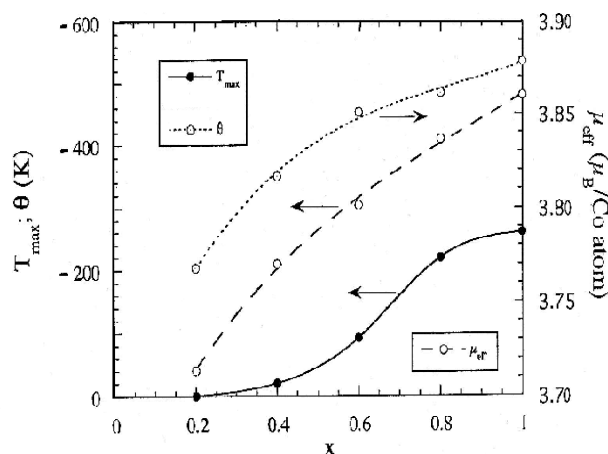


Fig. 4 Composition dependences of the effective cobalt moments, paramagnetic Curie temperatures and T_{max} values in $Y(Co_xNi_{1-x})_2$ system.

The projected band structures for YCo_2 and YNi_2 are plotted in Fig. 5. For YCo_2 , as well as $LuCo_2$, the Fermi level lies just above a sharp peak in density of states (DOS). By alloying with nickel, the Fermi level is shifted gradually towards a region with lower density of states.

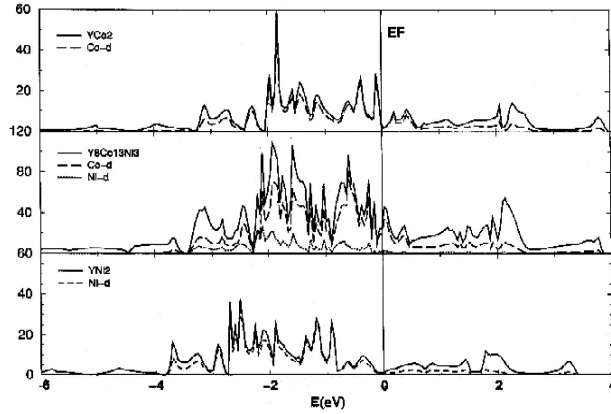


Fig. 5 Projected DOS curves, computed for YCo_2 , $\text{YCo}_{1.625}\text{Co}_{0.375}$ and YNi_2 compounds.

The magnetic behaviour of the above systems can be analysed in the spin fluctuation model. The model considers the balance between the frequencies of longitudinal spin fluctuations, which are determined by their lifetime and that of transverse fluctuations that are of thermal origin. These effects lead to the concept of temperature induced moments. From a strong exchange exchanged paramagnet, as RCO_2 ($R=\text{Lu}, \text{Y}, \text{Hf}$), 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 the above mentioned q values. The average amplitude of spin fluctuations, ξ^2 , increases with temperature and finally reaches an upper limit, at a characteristic temperature T^* . For $T > T^*$, a Curie-Weiss behaviour is predicted, as for systems having local moments. In this model, the moments are localized in q -space.

The temperature dependence of the mean square amplitude of spin fluctuations can be analysed considering the effects of spin fluctuations, for a general model of itinerant electron paramagnetism in the classical Gaussian statistics [16-18]. The contributions to the susceptibilities from the spin fluctuations, in terms of the density of states can be expressed as:

$$\chi_s^{-1} = a_1 - \alpha + (5/3)a_3\xi^2 + (35/9)a_5\xi^4 + (35/3)a_7\xi^6 + \dots \quad (1)$$

where the mean square value of the fluctuating magnetization, ξ^2 , is given by

$$\xi^2 = \frac{3}{2\pi^2} k_B T q_m A^{-1} \left[1 - \frac{\text{tg}^{-1}(q_m \sqrt{A\chi})}{q_m \sqrt{A\chi}} \right] \quad (2)$$

By a_1 , a_3 , a_5 and a_7 are denoted the expansion coefficients of the free energy with respect to the square of magnetization density and α , q_m and A denote the molecular field coefficient, the cut-off wave vector of spin fluctuations and the exchange stiffness constant, respectively.

By limiting the series expansion development up to terms in ξ^2 , we retained in relation (1) only terms in a_1 and a_3 , expressed as [17, 18]:

$$a_1 = \frac{2}{Ng^2\mu_B^2} \left\{ 1 + \frac{1}{6} (\pi k_B T)^2 \left[\left(\frac{N'}{N} \right)^2 - \frac{N''}{N} \right] + \dots \right\} \quad (3)$$

$$a_3 = \frac{g^2\mu_B^2}{2^2 3!} a_1^3 \left\{ 3 \left(\frac{N'}{N} \right)^2 - \frac{N''}{N} + \frac{1}{6} (\pi k_B T)^2 \left[6 \left(\frac{N'}{N} \right)^4 - 13 \frac{N''N'^2}{N^3} + \left(\frac{N'''}{N} \right)^2 + 7 \left(\frac{N''''N'}{N^2} \right) - \frac{N''''}{N} + \dots \right] \right\} \quad (4)$$

We denoted by N the state density at the Fermi level and N' , N'' , N''' and N'''' are their derivatives of the order of one to four.

By fitting the experimental data with relation (1) we determined the α , q_m and A values and, as a result, the temperature dependences of the mean square amplitude of spin fluctuations – Fig.6. Generally speaking, the ξ^2 values are not fully saturated in the studied temperature range ($T < 750$ K) but approach very much to saturation at highest saturation. There is a more evident tendency to saturate, at higher temperatures, as the nickel content increases. This behaviour is in agreement with the decrease of T^* temperatures when nickel content is higher. The lack of full saturation can be connected with the approximation used in determining q_m and A values. We limited the series development for χ up to terms in a_3 . In addition, we neglected the Pauli-type contributions to the susceptibilities, due to mainly the fraction of YNi_2 present in a given compound as well of the core diamagnetism. In spite of the approximation used, the differences between $\langle \xi^2 \rangle^{1/2}$ values, experimentally determined, and the computed ones, at highest temperatures, where nearly saturation was attained, are rather small – Fig.7.

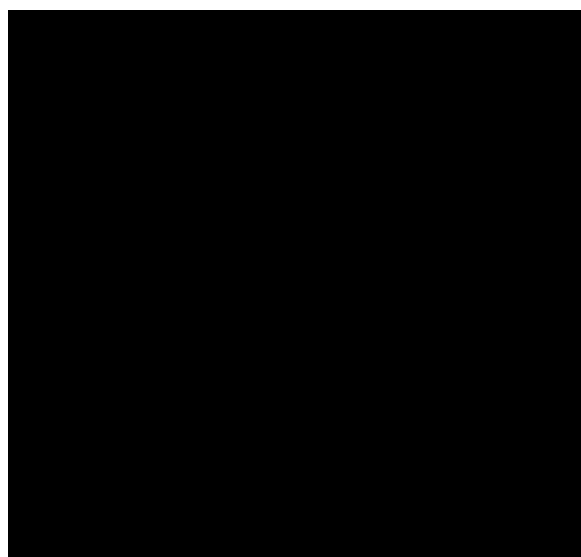


Fig. 6 Temperature dependences of the mean square amplitude of spin fluctuations.

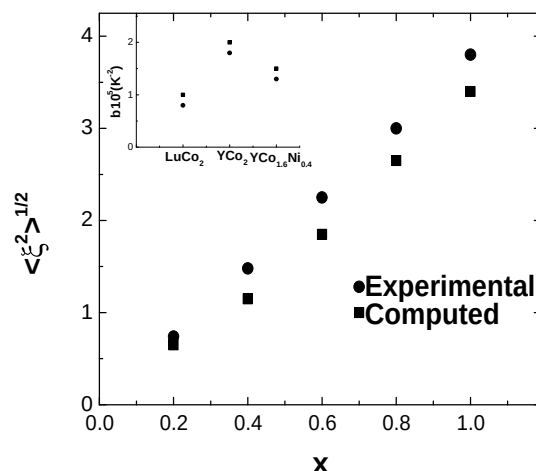


Fig. 7 The computed and experimentally determined values of the mean square amplitude, $\langle \xi^2 \rangle^{1/2}$, of the spin fluctuations. In inset the computed and experimentally determined b values are given.

As above mentioned, in the low temperature range ($T \leq 10$ K) – Fig. 2 - the χ values follow a T^2 type dependence.

$$\chi = \chi_0 (1 + bT^2) \quad (5)$$

Since the maximum in χ vs T values is shifted to low temperatures when increasing the nickel content, no accurate determination of χ values was possible for compounds with $x \leq 0.3$. In the paramagnon model [19] the b coefficient is given by

$$b = \frac{\pi^2}{6} \left[2 \frac{N''}{N} - 1.2 \left(\frac{N'}{N} \right)^2 \right]_{E_F} s^2 \quad (6)$$

where s is the exchange enhanced parameter.

In order to compute the b values we selected a symmetric energy interval around the self-consistent value of the Fermi level in DOS and we used a mean square interpolation scheme in order to analytically analyse the energy dependence of the DOS. This approach allowed us to evaluate the first and second derivative of the DOS at the Fermi level. The b values, computed according to relation (6), describe rather well the experimental data – Fig.7 inset.

The external [20-22] or internal [23,24] fields determine a partial quenching of spin fluctuations. This is reflected by the decrease of the specific heat coefficient γ or of the effective moments. If the magnetic field is sufficiently large so that the Zeeman splitting energy of opposite spin states is comparable to, or larger than the characteristic spin fluctuation energy, then the paramagnons no longer have sufficient energy to flip spins and therefore, the inelastic spin flip scattering is quenched. A magnetic field, H_{eff} , of the order of the characteristic spin fluctuation temperature, $H_{\text{eff}} \propto T_{\text{sf}}$, is requested to quench the spin fluctuations. A partial quenching of spin fluctuations by external fields was evidenced by specific heat measurements on YCo_2 or LuCo_2 [22]. The decrease of the electronic specific heat constant, γ , in field of 10 T, was 4 % for YCo_2 and 10 % for LuCo_2 . A partial quenching of spin fluctuations can be observed by magnetic measurements, when replacing Y or Lu in RCo_2 compounds, by a magnetic rare-earth. The effective cobalt moments decrease as the Curie temperatures, exchange interactions, respectively are greater. In Fig.8 we plotted the effective cobalt moments in RCo_2 compounds as function of the reciprocal exchange field H_{exch}^{-1} , at 4.2 K. There is a linear dependence, $M_{\text{eff}}(\text{Co}) = d + e H_{\text{exch}}^{-1}$, with $e = 2.2 \cdot 10^2 \mu_B \text{T}$. For a variation of the internal (exchange) field of 10 T, the changes in the effective cobalt moments are of ≈ 6 %. This value is close to the diminution of the electronic specific heat constants, as above mentioned, in the same range of external fields, in YCo_2 or LuCo_2 compounds [22].

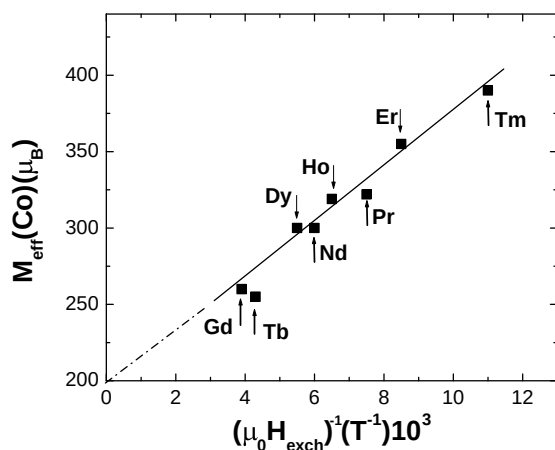


Fig. 8 The effective cobalt moments determined in RCo_2 compounds as function of the inverse exchange fields

4. The effects of exchange interactions on transition metal moments

The substitution of Y or Lu, in RCo_2 compounds, by a magnetic rare-earth induces an order magnetic moment at cobalt site. A magnetic moment of $1.03 \mu_B/\text{atom}$ was obtained by magnetic measurements at 4.2 K in GdCo_2 . This suggests that the cobalt moments are

determined by exchange interactions [2,25]. There seems to be a critical field for the appearance of a moment on cobalt atom.

Previously [26,27], we proposed a model for induced magnetism (or epimagnetism) in which there is a sudden increase of the cobalt moment for a critical field. Then, the magnetic moments increase linearly with exchange fields and finally saturate. The model has been confirmed experimentally by analyzing the magnetic properties of RCo_4B [28] or some RCo_2 [29]–based compounds. In the following we discuss the effect of exchange interactions on the cobalt moments in $\text{Gd}_x\text{Y}_{1-x}\text{Co}_2$, $\text{Gd}(\text{Co}_x\text{Ni}_{1-x})_2$ and $\text{Gd}(\text{Co}_x\text{Al}_{1-x})_2$ systems in which magnetic atoms as Gd or Co, are replaced by Y or Ni(Al), respectively. In this way the exchange interactions are modified.

The composition dependence of the transition metal moments (CoNi) in $\text{Gd}(\text{Co}_x\text{Ni}_{1-x})_2$ system are plotted in Fig.9. There is a great decrease of the transition metal moments for $x \geq 0.8$. Since gadolinium content is not changed, the variation of the magnetizations may be attributed only to the substitution of Co with Ni. In order to have information on Co and Ni magnetic behaviour, band structure calculations were performed [30] – Fig.10. The magnetic moments, thus determined, are listed in Table 1. The cobalt moments, as well as nickel ones, are little dependent on composition. We note that a magnetic moment of $0.12 \mu_B$ was determined in GdNi_2 although previous studies stated that nickel is not magnetic [1]. A value of Ni moment of $0.20 \mu_B/\text{atom}$ ($\mu^L = 0.06 \mu_B$ and $\mu^S = 0.14 \mu_B$) was recently obtained by magnetic circular dichroism measurements [31]. Since in computing Ni moment only the spin value was obtained, this it is in very good agreement with that experimentally determined.

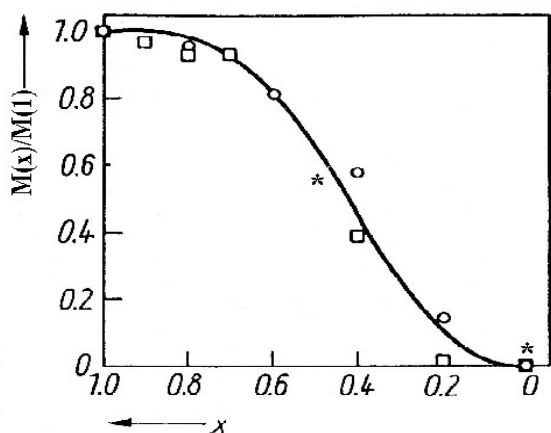


Fig. 9 The composition dependence of the transition metal moments in $\text{Gd}(\text{Co}_x\text{Ni}_{1-x})_2$ system. By * the computed values are plotted. Solid line describes the prediction of relation (7) with $n_c \geq 3$.

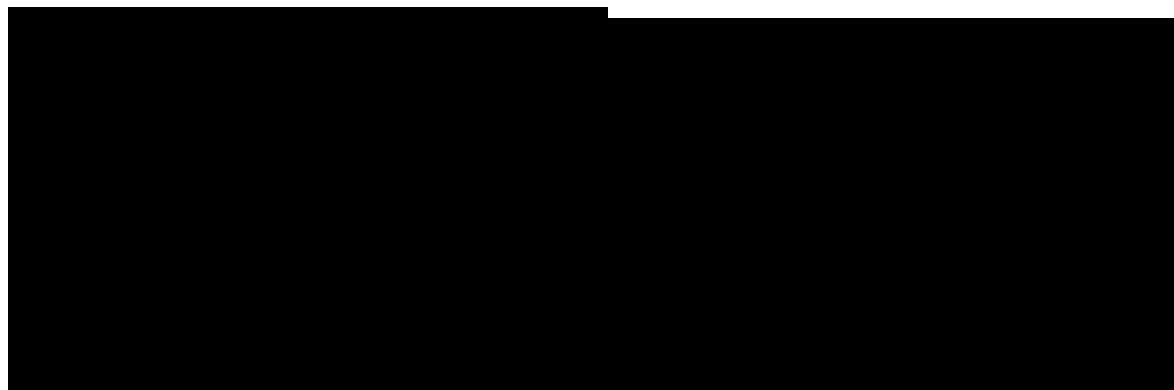


Fig. 10 Projected DOS curves for GdCo_2 and GdCoNi compounds.

The analysis of the data from Table 1 suggests that cobalt and nickel moments, as already stated, are little dependent of composition. Thus, the high decrease of the transition metal moments at $x \geq 0.8$ can be attributed only to the loss of cobalt moments at sites where the exchange interactions are smaller than a critical value. This can be correlated with a minimum number of cobalt atoms coupled by exchange interactions. Thus, a statistical model can be used in order to determine the critical exchange field. In this model [32] the magnetic moment of cobalt is lost if there is a smaller number of cobalt atoms as nearest neighbours than a critical value, n_c . The mean magnetic moment for a composition x can be described by:

$$\langle M_{Co} \rangle = \sum_{n > n_c} M_{Co}(x) P_n(x) \quad (9)$$

Table 1. Magnetic moments of Co and Ni determined from band structure calculations in $Gd(Co_xNi_{1-x})_2$ compounds.

Compound	M_{Co} (μ_B /atom)	M_{Ni} (μ_B /atom)	$M_{5d}(Gd)$ (μ_B)	M_{Gd} (μ_B /atom)
GdCo ₂	1.22	–	-0.53	-7
GdCoNi	1.11	0.14	-0.43	-7
GdNi ₂	–	0.12	-0.30	-7

We denoted by $P_n(x)$, the probability for a cobalt atom to have n nearest neighbour similar atoms. Considering a random distribution of Co and Ni atoms on $\bar{3}m$ sites, we have

$$P_n(x) = \frac{6! x^n (1-x)^{6-n}}{(6-n)! n!} \quad (10)$$

Relation (9) describes well the composition dependence of (Co,Ni) moments, supposing that cobalt has a magnetic moment M_{Co} ($x=1$) if there are $n \geq 3$ Co nearest neighbours and is nil if this number is smaller than $n_c = 3$. From these data we can estimate the critical field for the appearance of cobalt moment. By using paramagnetic measurements we evaluate the molecular field coefficients characterizing the interactions between cobalt atoms. A value $J_{Co-Co} = 3.3 \cdot 10^{-22}$ J was obtained. This corresponds to a critical field $H_c = 70$ T for the appearance of cobalt moment, when considering the presence of three atoms in a cluster. This value agrees with that suggested previously by our studies [27, 28] or other data from literature [29].

The critical field for the appearance of cobalt moment can be also estimated in $Gd_xY_{1-x}Co_2$ compounds. For this purpose, the molecular field coefficients were determined by using paramagnetic measurements or by fitting the temperature dependence of the magnetization, by using a two sublattices model, in the molecular field approximation [33]. The cobalt moments as function of the exchange fields, thus determined, are plotted in Fig. 11. In the same figure the data obtained in case of $Gd(Co_xAl_{1-x})_2$ and $Gd(Co_xNi_{1-x})_2$ systems are also included. A transition from nonmagnetic to magnetic state of cobalt is shown also at $H_{crit} \cong 70$ T. The cobalt moments then increase linearly with a slope of $(3 \cdot 10^2)^{-1} \mu_B/T$ and above $\cong 150$ T saturate.

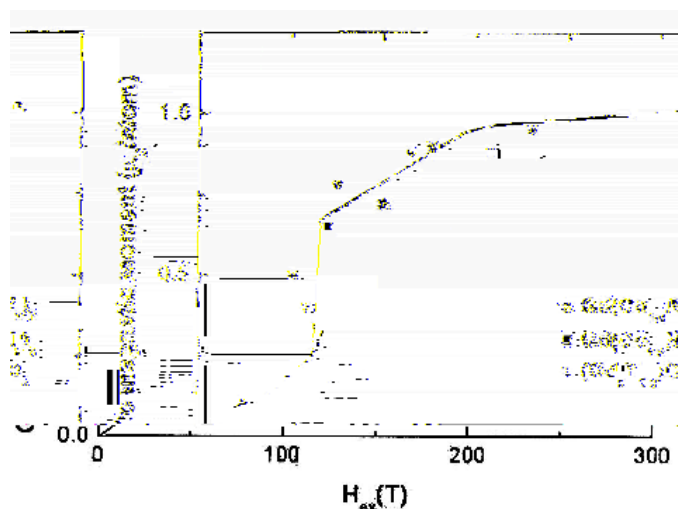


Fig. 11 The variation of cobalt moments, at 4.2 K, as function of the exchange fields.

The dependence of the iron moments on the exchange fields in $(\text{Gd}_x\text{Y}_{1-x})\text{Fe}_2$ compounds is plotted in Fig.12 inset. A linear variation, in all the composition range, was shown, described by the relation $\Delta M_{\text{Fe}}(\mu_B) = (18.10)^{-2} \Delta H_{\text{exch}}(\text{T})$. This suggests that the iron moments are not so sensitive as cobalt to the exchange interactions, showing a more localized behaviour. We also analysed the variations of iron moments in $(\text{Gd}_x\text{Y}_{1-x})\text{Fe}_n$ and $\text{Gd}(\text{Fe}_x\text{Al}_{1-x})_n$ series with $n = 2, 3$, where Gd is replaced by Y or Fe by Al. In this way the exchange interactions are modified. We note that in GdFe_3 -based compounds the iron atoms occupy different sites in lattice, having different magnetic contributions. In this case we considered only the mean iron moments. The composition dependences of iron moments experimentally determined and those computed are plotted also in Fig. 12. There is a rather good agreement between the two sets of data showing that the proportionality relation between the variation of the magnetic moments and of exchange fields is valuable also for other types of structures than Laves phase.

Fig. 12 The dependence of the iron moments on the exchange fields in $(\text{Gd}_x\text{Y}_{1-x})\text{Fe}_2$ system (inset) and the computed and experimentally determined variations of the iron moments in $(\text{Gd}_x\text{Y}_{1-x})\text{Fe}_n$ and $\text{Gd}(\text{Fe}_y\text{Al}_{1-y})_n$ compounds with $n = 2$ and 3.

The present band structure calculations show that small magnetic moments are also induced on nickel atoms in RNi_2 compounds with magnetic rare-earths. These values are by nearly two order of magnitude smaller than those of rare-earth moments and cannot be

determined by magnetic measurements since are of the order of experimental errors. Experimental evidence of Ni moment was shown only by magnetic circular dichroism in GdNi₂ compound [31].

5. R5d band polarization

The gadolinium 5d band polarization, M_{5d} , in GdM₂ (M=Fe,Co,Ni) Laves phase compounds are plotted in Fig.13 inset, as a function of the transition metal contributions to the magnetization, M_d . There is a linear increase of M_{5d} vs M_d . The extrapolation at $M_d \rightarrow 0$ leads to a value of 5d band polarization, $M_{5d}(R)$, which can be attributed only to local 4f-5d interactions. The above data suggest that the R5d band polarizations are determined both by local 4f-5d and 5d-3d short range exchange interactions. Thus:

$$M_{5d} = M_{5d}(R) + M_{5d}(0) \quad (11)$$

The contributions to 5d band polarization from local 4f-5d exchange interactions can be determined in compounds where M elements are not magnetic or by the extrapolation procedure mentioned above. In case of gadolinium compounds a value $M_{5d}(R) \cong 0.27 \mu_B$ was obtained, parallel oriented to the rare-earth moment. The study of 5d band polarizations in RCo₂ compounds with heavy rare-earths suggests that this contribution is proportional to De Gennes factor, $G = (g_J - 1)^2 J(J+1)$, $M_{5d}(R) = \alpha G$ with $\alpha = 2.1 \times 10^{-2} \mu_B$. Supposing that the above two contributions described by relation (11) are additive, the effects of 5d-3d short range interactions on the 5d bands polarizations, $M_{5d}(0)$, were determined. The exchange interactions of given R atoms with neighbouring M ones are described by the Hamiltonian:

$$H = JS_{5d} \sum_i S_{3di} \quad (12)$$

where J is the exchange integral and i is the number of neighbouring 3d atoms having S_{3di} spin.

Due to high symmetry of the structure, the M and R atoms occupy only one type of site in lattice and thus only one $M_{5d}(0)$ value is expected for all sites in a given compound. The 5d-3d exchange interactions act as an internal field, H_{exch} , on 5d bands and induce an additional polarization to that determined by 4f moment. By using the molecular field approximation, the internal field can be written as $H_{\text{exch}} = N_{5d-3d} M_d$ where N_{5d-3d} is the molecular field coefficient describing the exchange interactions between R and M atoms. We showed already that above the critical field, which determines appearance of magnetic M moment, the M_d values are proportional to the exchange field. Thus, it results that $M_{5d}(0) = \gamma M_d$. The analysis of the magnetic properties of Gd_xY_{1-x}Co₂ system showed that the molecular field coefficients describing the exchange interactions between Gd and Co are $N_{\text{GdCo}} = 110 \pm 10$ and not dependent on composition. By using this value and supposing that the 5d band polarization can be described by the same relation, as a function of exchange field, as for Co 3d moments, $M_{5d} = (3 \cdot 10^{-2})^{-1} \mu_B/T$, we obtained that $M_{5d} \cong 0.19 M_d$. This relation, in spite of used approximation, is in rather good agreement with that experimentally determined, $M_{5d} = 0.12 M_d$ – Fig.13. This suggests that sensitivity of 5d band polarization to the exchange interactions is of the order of induced cobalt moments.

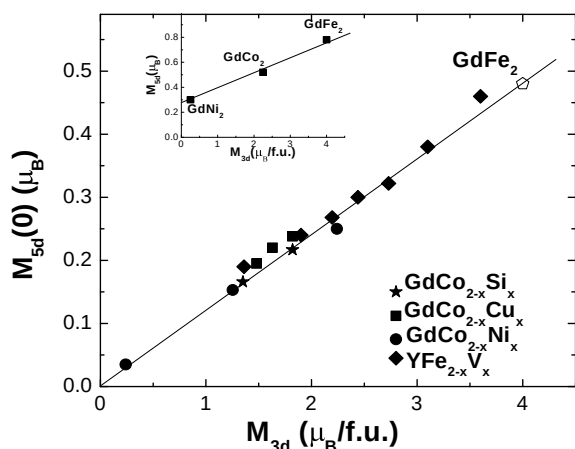


Fig. 13 The $M_{5d}(0)$ band polarizations in some Laves phase compounds as a function of the transition metal moments. In the inset, the total M_{5d} band polarizations are plotted as a function of 3d magnetic moments for RM_2 ($M=Fe, Co, Ni$) compounds.

6. Conclusion

The exchange enhanced paramagnets $Y(Co_xNi_{1-x})_2$ and $LuCo_2$, at $T \leq 10$ K show a T^2 dependence of the magnetic susceptibility. Above a characteristic temperature, T^* , a Curie-Weiss type behaviour was shown. The determined cobalt effective moments are close to that of Co^{2+} ion. The above behaviour is well described by the spin fluctuations model [35]. By using band structure calculations we computed the contributions of (CoNi) to the mean square amplitude of spin fluctuations. The values thus obtained, agree rather well with those experimentally determined.

A critical exchange field, $H_{crit} = 70$ T, was estimated, as necessary to induce an ordered magnetic moment on cobalt, at 4.2 K. The presence of small nickel moments in RNi_2 compounds, with heavy rare-earths, was shown by band structure calculations. Iron shows a more localized behaviour. The effect of exchange interactions on M_{Fe} values is nearly one order of magnitude smaller than for cobalt.

The effect of local 4f-5d and range 5d-3d exchange interactions on the R5d band polarizations were evaluated. The induced 5d band polarization by 4f-5d local interactions is proportional to the De Gennes factor while that due to 5d-3d short range interactions is proportional to transition metal moments of neighbouring atoms to a given R.

References

- [1] E.Burzo, A.Chelkovski and H.R.Kirchmayr, Landolt Bornstein Handbuch, vol. 19d2, SpringerVerlag, Berlin, 1990 and references
- [2] E.Burzo, Solid State Commun. 20, 1569 (1976)
- [3] A.E.Clark, Handbook on the Physics and Chemistry of the Rare-Earths, vol. 2, Ed. R.A Gschneidner, L.Eyring, North Holland, Amsterdam, 1979, p.231
- [4] KH.J.Buschow, Phys. Stat Solidi (a) 7, 199 (1971)
- [5] M.A.Ruderman and C.Kittel, Phys. Rev. 96, 99 (1954); T.Kasuya, Progr. Theor. Phys. 16, 45 (1956); K.Yoshida, Phys. Rev. 106, 893 (1957)
- [6] W.E.Wallace and J.T.Swearingen, J.Solid State Chem. 8, 37 (1973); W.E.Wallace, E.P.Ganaphaty and R.S.Craig, J. Appl. Phys. 50, 2327 (1979)
- [7] I.A.Campbell, J Phys. F: Metal Phys. 2, L 47 (1972)

- [8] O.K.Andersen, Phys. Rev. B 12, 3060 (1975)
- [9] O.K.Andersen and O.Jepsen, Phys. Rev. Letters 53, 2571 (1974)
- [10] O.K.Andersen, O.Jepsen and O.Glotzel, in Highlights of Condensed Matter Theory, Eds. F.Bassani, F.Fumi and M.P.Tossi, North Holland, New York, 1985
- [11] R.O.Jones and O.Gunarson, Rev. Mod. Phys. 61, 689 (1989)
- [12] U. von Barth and L.Hedin, J. Phys. C5, 1629 (1972)
- [13] V.Ansimov, J.Zannen and O.K.Andersen, Phys. Rev. B 44, 943 (1991):
A.I.Lichtenstein, J.Zannen and V.I.Ansimov, Phys. Rev. B 52, R 5467 (1995)
- [14] V.I.Ansimov, F.Aryasetiawan and A.I.Lichtenstein, J. Phys.: Condens Matter. 9, 967 (1997)
- [15] E.Burzo, D.Givord and L.Chioncel, J. Appl. Phys. 83, 1779 (1998)
- [16] L.Chioncel, E.Burzo, R.Tetean and V.Pop, Mol. Cryst. Liq. Cryst. 415, 107 (2004)
- [17] M.Shimizu, Phys Letters 81 A, 87 (1981)
- [18] M.Shimizu, Rep. Progr. Phys. 44, 21 (1989)
- [19] M.T.Beal-Monod, Physica B 109, 1837 (1982); M.T.Beal-Monod and J.M.Lawrence, Physica B 21, 5400 (1980)
- [20] M.T.Beal-Monod, S.K.Ma and D.R.Fredkin, Phys. Rev. Letters 22, 928 (1968)
- [21] W.F.Brinkman and S.Engelsberg, Phys. Rev. 169, 417 (1968)
- [22] K.Ikeda, K.A.Gschneidner, R.J.Stiermann, J.W.E.Tsang and O.D.Mc Masters, Phys. Rev. B 29, 5039 (1984)
- [23] E.Burzo and R.Lemaire, Solid State Commun. 84, 1145 (1992)
- [24] E.Burzo, Rom. J. Phys. 43, 319 (1998)
- [25] E. Burzo, Phys. Rev. B 17, 1414 (1978)
- [26] E. Burzo, Rev. Roum. Phys. 23, 689 (1978)
- [27] E.Burzo, J. Less Common Met. 77, 251 (1981)
- [28] E.Burzo, N.Plugaru, I.Creanga and M.Ursu, J. Less Common Met. 155, 281 (1989)
- [29] N.N.Duc, T.D.Hien, P.E.Bromer and J.J.Franse, J. Magn. Magn. Mater. 104-107, 1252 (1992)
- [30] E.Burzo and L.Chioncel, J. Opt. Adv. Mater. (2004), in press
- [31] M.Mizumaki, K.Yano, I.Umehara, F.Ishikawa, K.Sato, A.Koizumi, N.Sakai and T.Muro, Phys. Rev. B 67, 132404 (2003)
- [32] E.Burzo, D.P.Lazar and M.Ciorascu, Phys. Stat. Solidi (b) 765, K 145 (1974)
- [33] L.Neel, Ann. Phys. 3, 137 (1948)
- [34] E.Burzo and M.Balanescu, J. Solid State Chem. 37, 1 (1981)
- [35] T.Moriya, J.Magn.Magn.Mater. 100, 201 (1991)