

Magnetic moments of $\text{Y}(\text{Fe-Co})_{12-x}\text{T}_x$ alloys: A modified magnetic valence approach

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The dependence of the magnetic moment per atom in alloys with the general formula $\text{Y}(\text{Fe, Co})_{12-x}\text{T}_x$ ($\text{T} = \text{Ti, V, Cr, Mo, W, Re}$) on concentration and kind of the added element T has been analyzed in the framework of the magnetic valence concept. A semiempirical method has been used to estimate the contribution of the solute T to the magnetic valence by treating it as a scattering center which introduces additional d states in the energy band scheme of the host. This approach explains the difference in magnetic moments for solute elements in the same column of the periodic table.

1. Introduction

During the last few years considerable attention has been focused on the study of the fairly large class of ternary iron rich rare earth alloys with the general formula $\text{RFe}_{12-x}\text{T}_x$ crystallizing in the ThMn_{12} type structure (tetragonal I_4/mmm) [1, 2] because of their potential application in permanent magnets. The Th site in the body centered tetragonal ThMn_{12} structure is occupied by a rare earth (R) atom while the three inequivalent 8i, 8j, 8f Mn sites are occupied by Fe and T atoms ($\text{T} = \text{Ti, V, Cr, Mo, W, Si}$). Since the RFe_{12} compounds do not exist, the phase stability of the iron rich 1:12 compounds depends mainly on the substitution of T atoms in the Fe sites and their concentration x ($x = 2$ for $\text{T} = \text{V, Cr, Mo, Si}$ and $x \approx 1.2$ for $\text{T} = \text{Ti, W}$).

The saturation magnetization M_s , which determines the maximum theoretically expected energy product $(BH)_{\text{max}}$, arises primarily from the transition metal sublattice. This contribution

can be assessed by studies of the members of the series where R is non-magnetic ($\text{R} = \text{Y, Lu, La}$). Considerable differences of the iron moments for different T atoms have been observed in $\text{YFe}_{12-x}\text{T}_x$ compounds [3] and Mössbauer hyperfine spectra reveal completely different distribution of the magnetic hyperfine fields, respectively [4, 5]. It is known that the $\text{T} = \text{Ti, V, Mo}$ atoms occupy preferentially a part of the 8i iron sites with a statistical distribution of T atoms over these lattice positions [6–8]. A recent study of the spin reorientation transitions in the $\text{RFe}_{10}\text{T}_2$ ($\text{T} = \text{V, Ti, Si}$) series in terms of crystal electric field interactions has shown a variation of the influence of the site occupation from T elements on the total anisotropy energy in these systems [9]. It is obvious, therefore, that the contribution of electronic states from T elements in the 3d-band of the Fe host affects significantly all the magnetic properties in these compounds. A complete understanding of the effect of the T solutes requires spin polarized band structure calculations which involve laborious computations and several approximations in view of the complexity of the systems. Two different approaches of band structure calculations in the

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1:12 compounds $Y(Fe-T)_{12}$ (T = transition metal) have been carried out by Jaswal et al. [10] and Coehoorn [11] in order to reproduce the observed iron magnetic moments. The first of these is a simplified tight binding calculation and leads to unexpectedly large moments ($\approx 1\mu_B$) of T atoms, antiferromagnetically coupled with the iron moments [10]. In the second approach, ab initio calculations for the hypothetical YFe_{12} and YFe_8T_4 compounds have been used to predict by extrapolation the decrease of the magnetization due to substitutions of T atoms in YFe_{12} . Reasonable agreement with experimental data, however, was achieved only when the equilibrium volumes determined from the ab initio calculation were replaced by the experimental volumes. The decrease in magnetic moment due to the T substitution is found to be insensitive to the type of transition metal atom. The experimental data on the other hand show significant variation, as, e.g. in the cases of $YFe_{10}V_2$ and $YFe_{10}Mo_2$ with average moments per Fe atom of 1.6 and $1.3\mu_B$, respectively.

We present in this paper a simplified method for the interpretation of the experimental data on magnetic moments in $Y(Fe, Co)_{12-x}T_x$ compounds by extending the magnetic valence model [12] based on the Friedel picture of the density of states. Our modification of the magnetic valence model consists of treating the solute transition elements T as scattering centres embedded in Fe positions which produce d resonance states above the Fermi level. The broadening of these levels due to s-d admixture effects leads to a part of the impurity d-state which lies below the host Fermi energy and affects the d band magnetism. In this way the electronic character of the solute is taken approximately into account. It should be noted, however, that the underlying assumption of strong ferromagnetism for the application of the magnetic valence concept remains necessary so that the model is expected to be more successful for the case of Co alloys.

In the following section we briefly review the relations that are used in the magnetic valence model and describe in some detail the semiempirical method that was used in order to calculate the number n_d of d states occupied by the solute.

The basic ideas as well as the numerical parameters that we have used in order to take into account the number of extra d electrons trapped in the impurity d resonance states below the Fermi level have been taken from Harrison's book [13]. The results of these calculations are then applied to the interpretation of available experimental data on $Y(Fe, Co)_{12-x}T_x$ alloys.

2. Electronic states and the magnetic valence of the solute atom

The relation defining magnetic valence Z_m and its connection to the magnetic moment m for a pure metal can be summarized as follows [12]:

$$m = Z_m + 2N_{sp} \quad (1)$$

and

$$Z_m = 2N_d - Z, \quad (2)$$

where Z is the number of valence electrons and N_d is the number of d electrons of the majority spin band. In the cases where the majority spin d bands lie entirely above (early transition metals) or below (late transition metals) the Fermi level, N_d in eq. (2) takes the value of precisely 0 or 5, respectively. It is then clear from the definition (2) that in such cases Z_m is an integer for each column of the periodic table, which can be used to describe the influence on the host system magnetization of a specific element when it appears as a solute in Fe, Co and Ni-based alloys.

For the case of alloys, eq. (1) becomes

$$\langle m \rangle = \langle Z_m \rangle + 2N_{sp}, \quad (3)$$

with

$$\langle Z_m \rangle = \sum_i x_i Z_{mi}, \quad (4)$$

and x_i are the relative concentrations of the constituent atoms. In deducing eq. (3) we have assumed that N_{sp} does not vary significantly by alloying. This assumption is plausible for transi-

tion metal alloys which have similar band structures [12, 14] but it is also valid even if the alloy includes a metalloid element having a larger number of sp electrons as shown by Terakura and Kanamori [15]. The value of $2N_{sp}$ in eq. (3) is between 0.6 and 0.9 [12, 14].

Equations (3) and (4) have been applied very successfully, in the case of strong ferromagnets, to a great number of Fe-, Co- and Ni-based alloys with transition metals and metalloid elements [14]. The most pronounced discrepancy with experiment is found in the case of Fe alloys which do not satisfy the condition of strong ferromagnetism. In addition, the assumption $N_d = 0$ or 5 for early and late solute transition metals is responsible for the failure of the magnetic valence approach to give different magnetic valences Z_m for the elements in the same column of the periodic table. According to this model, for example, the three alloys of the type $YFe_{12-x}T_x$ with $T = Cr, Mo, W$, which have the same valence, would have the same magnetic moment in disagreement with the observed values [3].

In order to improve the magnetic valence approach it is necessary to obtain a quantitative estimate of N_d for the solute transition metals. The effect of the perturbing potential localized at the vicinity of a transition metal impurity in Fe, Co or Ni is to create localized virtual bound d-states which, depending on their relative position with respect to the Fermi level, may be occupied or not. Furthermore, the s-d admixture effects will cause a broadening in energy of the relatively localized impurity d-states, as mentioned above, which spread out into an energy range of Γ as shown schematically in fig. 1. This results, for example, in an early transition metal solute in a finite density of states below the Fermi level and therefore $N_d \neq 0$. The phenomenon can be understood, as proposed by Friedel [16], by considering the impurity as a scattering center for "free" electrons in the host sp-band and d-band (at least those electrons near the bottom of the d-band).

Quantitative treatments of the transition impurity problem have been given by several authors [15, 17-19] using various approximations.

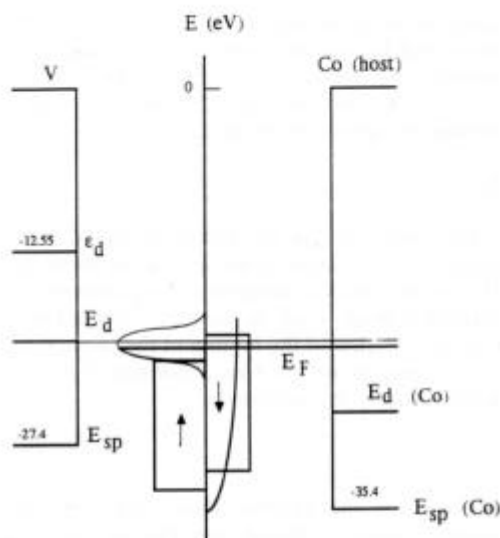


Fig. 1. Schematic representation of the relative position of the energy levels and the density of states for a transition metal solute in Fe, Co or Ni. The energy values pertain to V and Co.

Here we shall use the results given by Harrison [13] which are based on the self-consistent Hartree-Fock treatment by Anderson [17]. We assume that the concentration is small so that we can consider solute atoms as isolated impurities acting as scattering centers and producing d-resonance states around an energy E_d . If the Fermi energy E_F is well above E_d the resonance is completely occupied and it is empty if E_F is much less than E_d .

In the cases where E_d is close to E_F Harrison derives the following relation for n^+ and n^- , the fractional occupation for spin-up and spin-down states of impurity atom, respectively [13]:

$$\tan(\pi n^\pm/5) = \Gamma/[2(E_d^0 + n^\pm U_x - E_F)]. \quad (5)$$

In this expression Γ is the resonance width, E_d^0 is the energy of the resonance without exchange and U_x is the exchange interaction for each pair of d electrons of the same spin on the same atom.

Anticipating the example of $Y(Fe-Co)_{12-x}V_x$

alloys in the next section, where the Y and V atoms will be assumed not to carry a magnetic moment, we shall use eq. (5) for the case of $n^+ = n^- = n_d$. Solving eq. (5) for n_d , we determine N_d appearing in eq. (2) by

$$N_d = 5n_d. \quad (6)$$

The energy E_d^0 in eq. (5) is measured with respect to the bottom of the sp-band of the host. The method used to determine this parameter is illustrated in fig. 1 for the case of V in Co host. First the position of the bottom of the sp-band of V with respect to the free continuum states is determined by the relation:

$$E_{sp} = \varepsilon_d + 8V_{ss}, \quad (7)$$

where ε_d is the Hartree-Fock energy of the atomic d state calculated from Fischer (20) and V_{ss} an appropriate matrix element given by $V_{ss} = -1.4\hbar^2/2\pi m d^2$ [13, Solid State Table], with d the average distance of the nearest neighbours calculated from the atomic volume of the element and $\hbar^2/2\pi m = 7.62 \text{ eV \AA}^2$. In table 1 we have tabulated the terms which appear in eq. (7). Using the computed values of E_{sp} , the position of the impurity d -band in the energy level scheme of the host is

$$E_d^0(V) = [E_{sp}(\text{Co}) - E_{sp}(V)] + E_d(V), \quad (8)$$

where $E_d(V)$ is the energy at the middle of the 3d-band of the V metal obtained from table 20-4 of ref. [13]. The exchange energy U_x is also calculated from atomic data and is tabulated in the same table. The value of I is calculated from the relation given by Heine (21):

$$I = \frac{2W_d}{\frac{n'_l(x)}{j'_l(x)} - \frac{n_l(x)}{j_l(x)}} \quad (l=2), \quad (9)$$

where $j_l(x)$ and $n_l(x)$ are, respectively, Bessel and Neumann functions with argument $x = k_d r_0$ and W_d is the bandwidth. The parameters k_d , r_0 and W_d are also tabulated by Harrison [13]. The

values of I calculated from (9) are given in table 2. We note here that the bandwidth W_d used in this calculation is taken to be that of the solute metal assuming that the local density of states around the impurity is adjusted to come closer to the situation in the solute.

Using these parameters and Fermi energies E_F ($E_F(\text{Fe}) = 8.8 \text{ eV}$, $E_F(\text{Co}) = 12.49 \text{ eV}$ and $E_F(\text{Ni}) = 12.13 \text{ eV}$ given by band structure calculations [22] we have calculated from eqs. (5) and (6) the values of $2N_d$ and the corresponding magnetic valence for transition metals of the first, second and third rows. The results are given in table 2. For comparison we include also the (integer) values of Z_m calculated on the basis of the simple magnetic valence model [12]. We have used the Fermi energies of the pure Fe, Co and Ni for the corresponding Fe-, Co-, Ni-rich alloys with the

Table 1
Calculated V_{ss} matrix elements for fixed average distances of nearest neighbours, atomic Hartree-Fock d -energy levels ε_d and E_{sp} energies for the bottom of the sp-band.

Transition metal	$-8V_{ss}$ (eV)	$-\varepsilon_d$ (eV)	$-E_{sp}$ (eV)
Sc	10.05	9.35	19.40
Ti	11.69	11.04	22.73
V	14.87	12.55	27.43
Cr	16.39	13.94	30.33
Mn	16.20	15.27	31.47
Fe	16.60	16.54	33.14
Co	17.27	17.77	35.04
Ni	17.43	18.96	36.39
Y	8.35	6.80	15.15
Zr	10.54	8.46	19.00
Nb	12.52	10.03	22.55
Mo	13.77	11.56	25.33
Tc	14.56	13.08	27.64
Ru	15.10	14.59	29.69
Rh	14.96	16.16	31.12
Pd	14.29	17.66	31.96
Lu	9.00	6.62	15.62
Hf	10.84	8.14	18.98
Ta	12.54	9.57	22.12
W	13.62	10.96	24.58
Re	14.31	12.35	26.67
Os	14.78	13.73	28.52
Ir	14.69	15.13	29.82
Pt	14.07	16.55	30.62

Table 2

Resonance width, majority spin contribution and magnetic valence of transition metal impurities in Fe-, Co- and Ni-based alloys. The last column gives the value of magnetic valence according to ref. [12].

Transition metal	Γ (eV)	Fe-host		Co-host		Ni-host		Z_m (SF)
		$2N_\uparrow$	Z_m	$2N_\uparrow$	Z_m	$2N_\uparrow$	Z_m	
Sc	1.131	0.15	-2.85	0.17	-2.83	0.15	-2.85	-3
Ti	1.108	0.19	-3.81	0.23	-3.77	0.19	-3.81	-4
V	1.058	0.33	-4.67	0.49	-4.51	0.33	-4.67	-5
Cr	0.910	0.64	-5.36	1.69	-4.31	0.66	-5.34	-6
Mn	0.830	1.06	-5.94	9.07	2.07	1.12	-5.88	-7
Fe	0.683	9.26	1.26	9.67	1.69	9.31	1.31	2
Co	0.599	9.73	0.73	9.82	0.82	9.73	0.73	1
Ni	0.466	9.86	-0.14	9.89	-0.11	9.86	-0.14	0
Y	1.377	0.14	-2.86	0.15	-2.85	0.14	-2.86	
Zr	1.338	0.17	-3.83	0.20	-3.80	0.17	-2.83	
Nb	1.227	0.21	-4.79	0.26	-4.74	0.22	-4.78	
Mo	1.073	0.27	-5.73	0.38	-5.62	0.28	-5.72	
Tc	0.852	0.38	-6.62	0.71	-6.29	0.40	-6.60	
Ru	0.653	0.93	-7.07	9.30	1.30	1.02	-6.98	
Rh	0.442	9.62	0.62	9.80	0.80	9.65	0.65	
Pd	0.341	9.83	-0.17	9.89	-0.11	9.84	-0.16	
Lu	1.663	0.15	-2.85	0.17	-2.83	0.15	-2.85	
Hf	1.953	0.21	-3.79	0.24	-3.76	0.22	-3.78	
Ta	1.981	0.27	-4.73	0.31	-4.69	0.27	-4.73	
W	1.853	0.32	-5.68	0.39	-5.61	0.32	-5.68	
Re	1.583	0.37	-6.63	0.50	-6.50	0.38	-6.62	
Os	1.321	0.48	-7.52	0.78	-7.22	0.50	-7.50	
Ir	1.004	0.72	-8.28	1.74	-7.26	0.76	-8.24	
Pt	0.789	1.45	-8.55	9.32	-0.68	1.59	-8.41	

Table 3

Magnetic valence, average magnetic moment and magnetic moment of Fe atoms in the ternary alloys $YFe_{12-x}T_x$. Experimental values are obtained from Mössbauer and magnetization measurements.

T	x	This work			Williams et al. [12]			Mössbauer $\langle m_{Fe} \rangle$	Magnetization measurements $\langle m_{Fe} \rangle$
		$\langle Z_m \rangle$	$\langle m \rangle$	$\langle m_{Fe} \rangle$	$\langle Z_m \rangle$	$\langle m \rangle$	$\langle m_{Fe} \rangle$		
Ti	1.2	1.09	1.69	2.04	1.06	1.66	2.00	1.87	1.77 ^(a)
V	2.0	0.60	1.20	1.57	0.54	1.14	1.48	1.51 ^(a)	1.61 ^(a)
Cr	2.0	0.49	1.09	1.42	0.38	0.98	1.28	1.56 ^(a)	1.67 ^(a)
Mo	2.0	0.92	1.04	1.35	0.38	0.98	1.28	1.30 ^(b,c)	1.27 ^(b)
W	1.2	0.83	1.51	1.83	0.88	1.48	1.78	-	1.93 ^(a)
Re	1.2	0.83	1.43	1.72	1.15	1.75	2.11	-	1.82 ^(a)

^(a) Verhoef et al. [3].

^(b) Christides et al. [24].

^(c) Denissen et al. [4].

^(d) Christides et al. [25].

^(e) Jurczyk [26].

assumption that the E_F of the host does not change significantly. From the foregoing description of the method of calculation it is seen that the occupation of the d-resonance is mainly determined by the difference $E_d - E_F$ and the width Γ . This introduces a dependence of N_d on the electronic character of the solute due to different values of E_d and results in non-integer values of Z_m . Thus, for example the values of $2N_d$ for Cr and Mo, which have the same number of valence electrons and hence $Z_m = -6$ in the simple magnetic valence model, are now 0.64 and 0.27, respectively, for an iron host. This difference is expected to appear in the magnetic moment as is discussed below in the application to 1:12 alloys.

There are several approximations involved in deriving the values of table 2. The assumption of isolated impurities is not strictly valid for the alloys considered here so that impurity bands should be considered in a more accurate calculation instead of the simple scattering resonances. Furthermore, the transition metal solute may carry a moment in which case n_+ is different from n_- in the previous calculation. Also, since the calculated values of $2N_d$ depend strongly on the difference $E_d - E_F$, anomalies are expected to appear when these two levels are close. This is seen in the instability of the values of table 3 for Mn, Ru and Pt. For these reasons it may be expected that the application of these results would be more successful for the cases of the 1:12 considered here with an early transition metal solute. It is seen that the value of N_d is close to zero for early transition metals as would be expected from the effect of the repulsive potential for 3d electrons which places the resonance far above the Fermi level.

3. Application to $Y(Fe-Co)_{12-x}T_x$ alloys ($T = Ti, V, Cr, Mo, W$)

The modified magnetic valence method which is described in the previous section is applied now to the ternary iron-based alloys with general formula $Y(Fe, Co)_{12-x}T_x$. These alloys are most appropriate for comparison with experimental

results since they are rich in Fe or Co and contain two different transition elements. The average magnetic moment for an alloy can be calculated from eqs. (3) and (4) using for the magnetic valence of Y and the transition metal the new values which are listed in table 2.

The results for $YCo_{12-x}V_x$ alloys are shown in fig. 2 where the magnetic moment per atom is plotted as a function of V concentration, together with the curve calculated by using $Z_m = -Z$ according to Williams et al. [12] for comparison. Experimental data from a recent investigation of these alloys by Jurczyk [23] are also plotted in the same figure. It is seen that our calculation presents a significant improvement over the simple magnetic valence approach. The correction becomes more important as x increases.

A similar comparison for alloys with formula $YFe_{12-x}V_x$ is shown in fig. 3. Experimental points are obtained both from magnetization measurements and Mössbauer spectra [3]. In the latter case the magnetic moment per Fe has been calculated from the hyperfine field using a conversion factor of $15 T/\mu_B$. For this group of alloys it can be seen that both models give too high values in the low concentration region ($x < 1.5$) where the effect of V is small and the weak

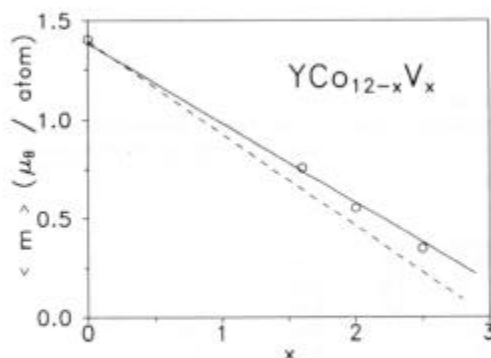


Fig. 2. Average magnetic moments per atom in $YCo_{12-x}V_x$ alloys as a function of V concentration. The full line is calculated with the proposed model. The dashed line is given by the simple magnetic valence model of ref. [12]. Experimental results are obtained from magnetization measurements [23].

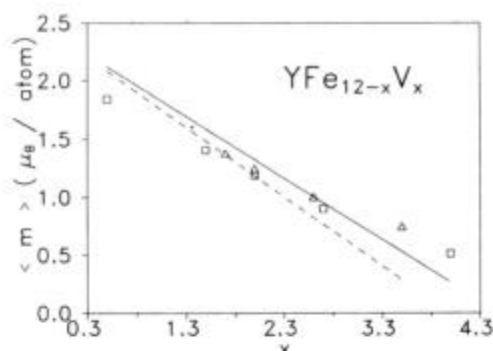


Fig. 3. Average magnetic moments per atom in $YFe_{12-x}V_x$ alloys as a function of V concentration. The full line is calculated with the proposed model. The dashed line is given by the simple magnetic valence model of ref. [12]. Experimental results are obtained from magnetization measurements (x) and Mössbauer data [3].

ferromagnetic character of the Fe-host plays a dominant role. This is expected since the proposed method does not address the major problem in applying the magnetic valence approach to Fe alloys, i.e. the failure of the assumption of strong ferromagnetism for the host Fe. In the range of higher V concentrations where the effect of V is expected to be stronger, the modified model gives values closer to the experimental results.

As another comparison with experimental results, the values of magnetic moments, calculated with our model and that of ref. [12] are listed in table 3 for several $YFe_{12-x}T_x$ alloys ($T = Ti, V, Cr, Mo, W, Re$). For the case of $T = Ti$ a value higher than the experimental is given by both approaches, a result similar to that for low V concentration alloys mentioned above. For the remaining compounds a significant improvement is found in the agreement with experimental data. We note in particular that our calculation leads to different values for $YFe_{10}Cr_2$ and $YFe_{10}Mo_2$ in accordance with experimental results while the simple magnetic valence model would give the same magnetic moment for both alloys since Cr and Mo belong to the same column of the periodic table and therefore are assigned the same magnetic valence in that model.

4. Conclusion

We have examined the magnetic moments of the series of $Y(Fe, Co)_xT_x$ alloys ($T = Ti, V, Cr, Mo, W, Re$) in the light of the magnetic valence concept, using an estimate for the contribution of the solute atoms to the majority spin band. We have shown that this estimate can be obtained by treating the transition metal atom as an impurity and calculating the number of occupied majority spin states of impurity atoms by resonance scattering theory. The magnetic valence calculated by this approach takes non-integer values and differs for elements in the same column of the periodic table in contrast to the simple model [12]. The improvement in the interpretation of experimental results given by the proposed method are illustrated by an application to $Y(Fe-Co)_{12-x}T_x$ alloys. The agreement of $\langle m \rangle_{cal}$ with $\langle m \rangle_{exp}$ is strongly dependent on the assumption of strong ferromagnetism in the band structure of the host metal.

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References

- [1] K.H.J. Buschow and D.B. De Mooij, in: *Concerted European Action on Magnets (CEAM)*, eds. I.V. Mitchell et al. (Elsevier Applied Science, London, 1989) p. 63.
- [2] J.M.D. Coey, Li Hong-Shuo, J.P. Gavigan, J.M. Gadoogan and Hu Bo-Ping, *Concerted European Action on Magnets (CEAM)*, eds. I.V. Mitchell et al. (Elsevier Applied Science, London, 1989) p. 76.
- [3] R. Verhoef, F.R. de Boer, Zhang Zhi-dong and K.H.J. Buschow, *J. Magn. Magn. Mater.* 75 (1988) 319.
- [4] C.J.M. Denissen, R. Coehoorn and K.H.J. Buschow, *J. Magn. Magn. Mater.* 87 (1990) 51.
- [5] Hu Bo-Ping, Li Hong-Shuo, J.P. Gavigan and J.M.D. Coey, *J. Phys. Condens. Mat.* 1 (1989) 755.

- [6] R.B. Helmholtz, J.J. Vlegaar and K.H.J. Buschow, *J. Less-Common Metals* 138 (1988) L11.
- [7] O. Moze, L. Pareti, M. Solzi and W.I.F. David, *Solid State Commun.* 66 (1988) 465.
- [8] D.B. de Mooij and K.H.J. Buschow, *J. Less-Common Metals* 136 (1988) 207.
- [9] C. Christides, M. Anagnostou, Li Hong-Shuo and A. Kostikas, *Phys. Rev. B*, to be published.
- [10] S.S. Jaswal, Y.G. Ren and D.J. Sellmyer, *J. Appl. Phys.* 67 (1990) 4564.
- [11] R. Coehoorn, *Phys. Rev. B* 41 (1990) 11790.
- [12] A.R. Williams, V.L. Moruzzi, A.P. Malozemoff and K. Terakura, *IEEE Trans. Magn.* MAG-19 (1983) 1983.
- [13] W.A. Harrison, *Electronic Structure and the Properties of Solids* (W.H. Freeman, San Francisco, 1980) Ch. 10.
- [14] A.P. Malozemoff, A.R. Williams and V.L. Moruzzi, *Phys. Rev. B* 29 (1984) 1620.
- [15] K. Terakura and J. Kanamori, *Prog. Theor. Phys.* 46 (1971) 1007.
- [16] J. Friedel, *Nuovo Cim. Suppl.* 2 (1958) 287.
- [17] P.W. Anderson, *Phys. Rev.* 124 (1961) 41.
- [18] A.M. Clogston, *Phys. Rev.* 125 (1961) 439.
- [19] P.A. Wolff, *Phys. Rev.* 124 (1961) 1030.
- [20] C.F. Fischer, *Atomic Data* 4 (1972) 451.
- [21] V. Heine, *Phys. Rev.* 153 (1967) 511.
- [22] L.F. Matheiss, *Phys. Rev. A* 134 (1964) 477, 485.
- [23] M. Jurczyk, *J. Magn. Magn. Mater.* 87 (1990) 1.
- [24] C. Christides, unpublished results.
- [25] C. Christides, A. Kostikas, D. Niarchos and A. Simopoulos, *J. Phys.* 49 (1988) C8-539.
- [26] M. Jurczyk, *J. Magn. Magn. Mater.* 89 (1990) L5.