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The influence of the T atom in Co_2TZ on the hyperfine fields (T = Ti, V, Cr, Mn, Fe; Z = Ga, Al)

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Abstract. Hyperfine fields have been calculated by the LMTO-ASA method within the framework of the LSD approximation. The hyperfine field at the Co position in Co_2TZ changes drastically with the T atom from a positive value for the case T = Ti to a negative value for the case T = Fe. The change occurs mainly in the contribution to the hyperfine field from valence s electrons (H_{val}), which is sensitive to the neighbouring magnetic moments. The value of H_{val} is roughly proportional to the 'spin polarization' of the valence s electrons at Co atom positions, which is closely related to the density of states of valence s electrons.

1. Introduction

A great number of measurements of hyperfine fields have been carried out for Heusler alloys with a chemical formula X_2TZ. Heusler alloys have a lattice structure $L2_1$, where each X atom has four T atoms and four Z atoms as the nearest neighbours and each T or Z atom is surrounded by eight X atoms. If X and T atoms are magnetic, they influence each other's magnetic properties. The Mn atom at a T site in X_2MnZ carries a large magnetic moment ((3–4) μ_B), while Mn at an X site in Mn_2VAl carries a small moment (1.2 μ_B) (Nakamichi and Stager 1983). Many Co Heusler alloys with a chemical formula Co_2TZ have been discovered and it was found that the Co atom carries a small magnetic moment (less than 1 μ_B). Webster (1971) observed that the Co and Mn moments in Co_2MnZ are larger for the alloys containing the IVb elements (Z = Si, Ge and Sn) than for the alloys containing the IIIb elements (Z = Al and Ga). Hyperfine fields at Co and Mn sites in Co_2MnZ (Z = Si, Ge, Sn, Al and Ga) have been observed (Kawakami *et al* 1987, Kawakami 1989a, LeDang *et al* 1978, Yoshimura *et al* 1985). The Mn hyperfine field is roughly proportional to the Mn moment, while the Co hyperfine field is not proportional to the Co moment. Furthermore, the experimental results show that the Co hyperfine field in Co_2TZ changes drastically with increasing number of valence electrons of the T atom (T = Ti, V, Cr, Mn and Fe), that is, from a positive value for the case T = Ti to a negative value for the case T = Fe.

The experimental results have been discussed on the basis of energy band calculations by several authors. Ishida *et al* (1982) carried out energy band calculations for Co_2MnSn, Co_2TiSn and Co_2TiAl and showed that the small hump of the density of states near the

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Fermi level determined the small Co magnetic moment of Co_2TZ. Ishida *et al* (1984) calculated hyperfine fields for Cu_2MnAl, Ni_2MnSn, Pb_2MnSn, Pb_2MnSb, Co_2MnSn, Co_2TiSn, Co_2TiAl and Mn_2VAl and showed that the agreement between the calculated values and the experimental ones is reasonable and that the Co hyperfine field in Co_2MnSn has a negative value, while it has a positive one in Co_2TiAl and Co_2TiSn. Fujii *et al* (1990) calculated systematically the hyperfine fields of Co_2MnZ (Z = Al, Ga, Si, Ge and Sn) and showed that the magnetic moments and the hyperfine fields on Co and Mn are influenced by the non-magnetic Z atom.

In this paper, we have calculated the hyperfine fields of Co_2TZ (T = Ti, V, Cr, Mn and Fe; Z = Ga and Al) in order to investigate systematically the influence of neighbouring magnetic moments on the hyperfine fields. We paid special attention to the Co hyperfine fields, because the Co hyperfine field is very sensitive to the circumstances of the Co atom and changes drastically with increasing magnetic moments of the T atom as described above.

2. Density of states and magnetic moments

The energy band calculations were carried out by the LMTO–ASA method (Andersen *et al* 1985) within the framework of the LSD approximation (Janak *et al* 1975). In the partial wave expression of the wave functions, the maximum angular momenta l_{max} were chosen as $l_{max} = 2$ for all of the constituent atoms. The self-consistency was achieved on 85 points in the irreducible Brillouin zone. The density of states (DOS) was obtained by the tetrahedral integration method (Rath and Freeman 1975).

The DOS of d states in Co_2TGa (T = Ti, V, Cr, Mn and Fe) are shown in figures 1(*a*)–(*e*) by the full curve for Co and the broken one for *T*. The Fermi level is indicated by a broken line. First we consider T atoms. In the minority-spin states, the shapes of the DOS are by and large similar for all T atoms. The Fermi level is located in a broad valley in each DOS. Then the occupied minority-spin states are approximately equal for all T atoms. On the other hand, the shapes of the DOS in the majority-spin states are very different for the different T atoms and the occupied majority-spin states increase in the order of T = Ti, V, Cr, Mn and Fe because the potential centred at the T atom becomes deeper in this order. Owing to those characteristics of the d electron's occupancy, the T magnetic moment increases with the atomic number of the T atom except for Fe. (Although there are more majority-spin electrons for Fe than for Mn, the magnetic moment is a little smaller for Fe than for Mn. This is because the occupied minority-spin states of Fe increase after the majority-spin states are mostly occupied.) These features are shown numerically in figure 2(*a*), where the magnetic moments of Co atoms in Co_2TGa are also shown. Next we consider Co atoms.

The Co moment in Co_2TGa changes slowly with the atomic number of the T atom. We consider this fact derived from the DOS of Co and T atoms (denoted by DOS(Co) and DOS(T)). In the majority-spin states, the DOS(T) in the right-hand side of the valley near 0 Ryd shifts gradually to the lower-energy region and the DOS(Co) in the right-hand side of the valley changes shape and becomes higher in the order T = Ti, V, Cr, Mn and Fe. On the other hand, in the minority-spin states, the DOS(Co) and DOS(T) do not change greatly in shape. We consider these features as follows. The potential centred at a T atom becomes deeper with increase in the atomic number of the T atom. As a result, the d bands of T approach and hybridize with the d bands of Co. The difference produced

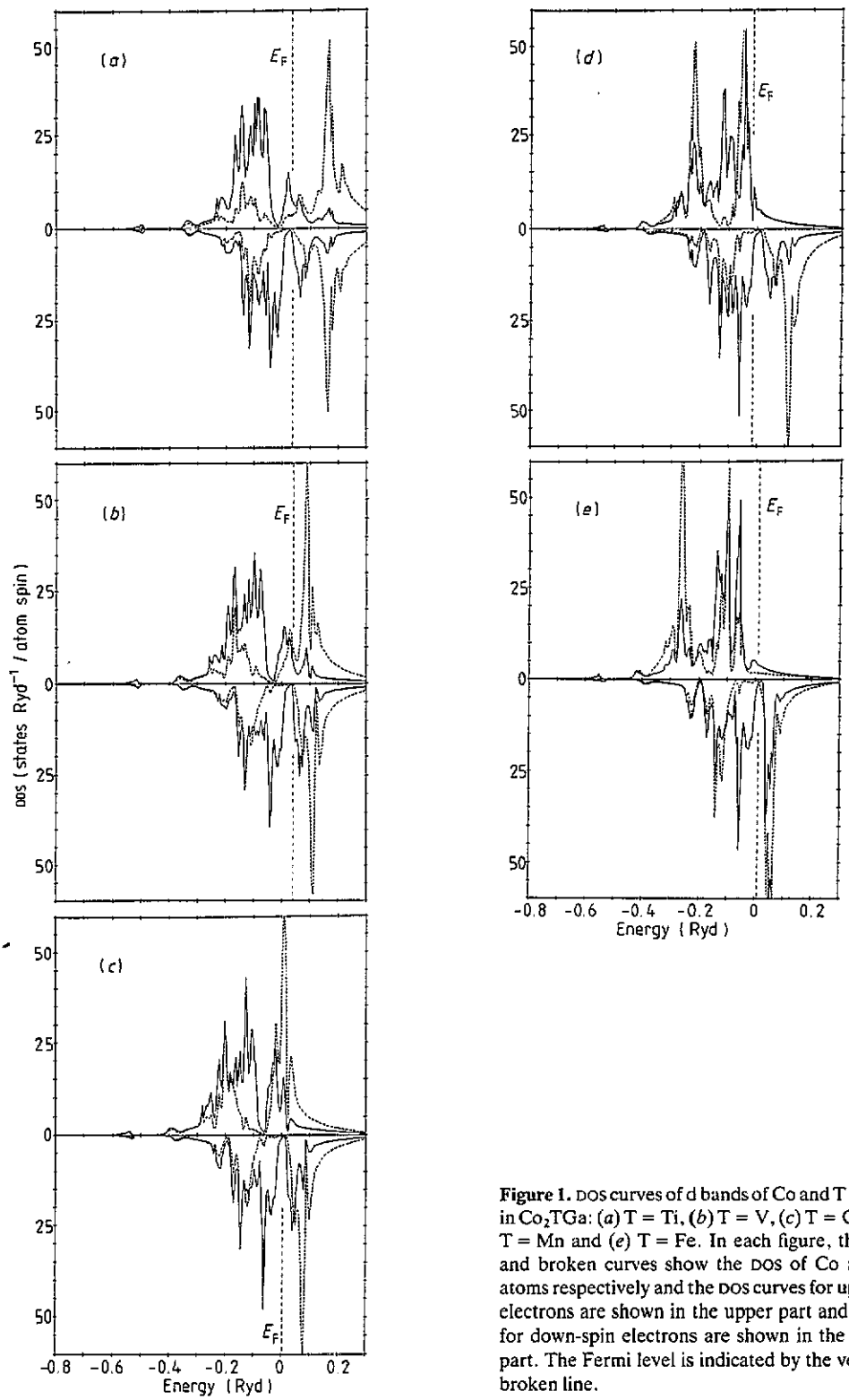

Figure 1. DOS curves of d bands of Co and T atoms in Co_2TGa: (*a*) T = Ti, (*b*) T = V, (*c*) T = Cr, (*d*) T = Mn and (*e*) T = Fe. In each figure, the full and broken curves show the DOS of Co and T atoms respectively and the DOS curves for up-spin electrons are shown in the upper part and those for down-spin electrons are shown in the lower part. The Fermi level is indicated by the vertical broken line.

Table 1. Calculated magnetic moments of constituent atoms in Co_2TZ and those per molecule in μ_B. Experimental values are shown in parentheses.

	Molecule	Co	T	Z
Co_2TiGa	0.97 (0.75[a])	0.59 (0.40[b])	−0.19	−0.01
Co_2VGa	1.95 (1.92[a])	0.93 (1.05[b])	0.09	−0.01
Co_2CrGa	3.01 (2.36[a])	0.96 (0.8[c])	1.14 (1.1[c])	−0.05
Co_2MnGa	4.21 (4.05[a])	0.72 (0.52[d])	2.87 (3.01[d])	−0.10
Co_2FeGa	5.02 (5.13[a])	1.16 (1.0[c])	2.77 (3.10[c])	−0.06
Co_2VAl	1.97 (1.95[a])	0.94 (0.92[b])	0.11	−0.03
Co_2MnAl	4.10 (4.04[a])	0.72 (0.5[d])	2.80 (3.01[d])	−0.13
Co_2FeAl	4.98 (4.96[a])	1.16	2.76	−0.10

[a] Buschow and van Engen (1981).
[b] Ziebeck and Webster (1973).
[c] Kawakami (1989b).
[d] Webster (1971).

by the hybridization causes the change in DOS(Co) in the majority-spin states and the change in the Co moment in Co_2TGa.

The calculated values of the magnetic moments of the constituent atoms of Co_2TGa are compared with the experimental values in table 1. The experimental values of the Co and T moments in Co_2CrGa and Co_2FeGa were estimated as the saturation moments and the hyperfine fields, on the assumption that the hyperfine field may be expressed as the sum of local and transferred terms (Kawakami 1989a). The calculated values of the Co moments are (0.1–0.2) μ_B larger than the experimental values. However, the trend of the variation is in good agreement with the experimental one. Although the Ti moment in Co_2TiGa has been considered to be zero, our result shows that the Ti has a smaller and negative moment (antiparallel to the Co moment).

3. Hyperfine fields

3.1. Contributions to the hyperfine field

In this paper, we consider only the contribution to the hyperfine field through the Fermi contact interaction and neglect the contribution from the orbital moment because the previous calculation (Ishida *et al* 1983) shows that the Co orbital magnetic moment in Co_2TiAl is small (0.025 μ_B). The calculation was carried out by the LCAO-OPW method and was not self-consistent. Thus, to estimate quantitatively the orbital contribution, we should perform a more accurate calculation. However, we expect the orbital contribution to be small and the general features of the hyperfine fields of Co_2TZ to be explained only by the contribution from the Fermi contact term. The hyperfine field through the Fermi contact interaction is written as follows (Watson and Freeman 1961):

$$H = n\mu_B\chi \qquad \chi = (4\pi/n)\sum(\rho_\uparrow(0) - \rho_\downarrow(0))$$

where n is the number of unpaired electrons, $\rho_\uparrow(0)$ is the density of s electrons at the nucleus for majority-spin states and $\rho_\downarrow(0)$ is the density for minority-spin states. In order

to discuss the hyperfine field in detail, we calculated separately the contributions from inner core s electrons (denoted by H_{core}) and valence s electrons (denoted by H_{val}).

Firstly, we consider, as an example, a single 3d magnetic atom with a net spin (say up or ↑). For this case, the core s electrons of up spin are attracted outside due to the exchange interaction with 3d electrons. Therefore, $\rho_\downarrow(0)$ becomes larger than $\rho_\uparrow(0)$ and so H_{core} has a negative sign, that is, it is antiparallel to its own magnetic moment. On the other hand, the valence s electrons of up spin are attracted inside and H_{val} has a positive sign, that is, it is parallel to its own magnetic moment.

Secondly, we consider the case where the 3d magnetic atom is surrounded by other magnetic atoms with parallel moments. The effect on H_{core} of the neighbouring moments is expected to be small due to the shielding effect. However, the valence s electrons of up spin are attracted outside by the neighbouring moments. This effect contributes negatively to the H_{val}. When the neighbouring moments are antiparallel, the effect contributes positively to the H_{val}. In the following sections, we discuss the hyperfine fields of Co_2TZ on the basis of the above considerations and define the positive direction to be parallel to the Co magnetic moment.

3.2. Hyperfine field at Co in Co_2TZ

Hyperfine fields at the constituent atoms of Co_2TGa are listed in table 2. The calculated values are also compared with the experimental ones in figures 2(*b*) and (*c*). Firstly, we consider hyperfine fields at Co sites (figure 2(*b*)). Although the calculated values are about 20–50 kOe larger than the experimental ones, the trend of the variation with the T atom is in good agreement between our results and experimental ones (figure 2(*a*)). The hyperfine field has a positive value for the cases T = Ti and V, while it has a negative one for the cases T = Cr, Mn and Fe. Its sign changes between T = V and Cr. To interpret this in detail, we consider H_{core} and H_{val} separately. These values are plotted in figures 2(*b*) and (*c*). H_{core}(Co) has a negative value for all T atoms and is roughly proportional to the Co magnetic moment. Thus, the effect on H_{core}(Co) from the neighbouring atoms is small. On the other hand, the H_{val}(Co) varies greatly from positive values for the cases T = Ti, V and Cr to negative values for the cases T = Mn and Fe. Since, for the case T = V, the magnetic moments on the neighbouring V atoms are negligibly small, H_{val}(Co) is determined by the Co moment itself (0.9 μ_B). For the case T = Ti, the Ti atom has a small and negative moment (−0.2 μ_B) but the Co moment is about 0.3 μ_B smaller than that for the case T = V. Therefore, H_{val}(Co) for the case T = Ti is smaller than that for the case T = V. For the case T = Cr, the Cr and Co moments are parallel and their values are approximately equal. In this case, due to the negative contribution from the Cr magnetic moment, the H_{val}(Co) value is smaller than that for the case T = V. For the cases T = Mn and Fe with large moments (about 2.9 μ_B), the negative contributions to H_{val}(Co) from Mn and Fe moments are larger than the positive contribution from the Co moment itself. Then, the H_{val}(Co) value becomes negative. Comparing the case T = Mn with the case T = Fe, the Fe moment is about 0.1 μ_B smaller than the Mn moment and the Co moment is about 0.5 μ_B larger than that for T = Mn. As a result, the positive contribution to the H_{val}(Co) is larger for the case T = Fe than for the case T = Mn. This explains the fact that the absolute value of H_{val}(Co) for T = Mn is larger than that for T = Fe.

Figure 2(*b*) shows that the main variation in the Co hyperfine field H(Co) arises from the H_{val}(Co) part which was discussed in detail in the paragraph above. In this paragraph, we summarize the feature of H(Co). For the case T = Cr where the Cr moment is

Table 2. Calculated hyperfine fields of constituent atoms in Co_2TZ in kOe. Experimental values are listed in the column H_{exp}. The last column shows the difference of s electrons between majority and minority spins. H_{cal} is a calculated value and H_{val} and H_{core} are the contributions to H_{cal} from inner core s electrons and valence s electrons respectively.

		H_{core}	H_{val}	H_{cal}	H_{exp}	m_s
	Co	−65.61	100.57	34.96	12.2[a]	0.017
Co_2TiGa	Ti	20.35	−68.61	−48.26		−0.013
	Ga	0.00	−4.49	−4.49		
	Co	−90.79	148.04	57.25	14.3[a]	0.025
Co_2VGa	V	−6.63	−77.58	−84.21	−73[a]	−0.014
	Ga	0.00	−27.82	−27.82		
	Co	−100.33	88.94	−11.39	−35.8[b]	0.015
Co_2CrGa	Cr	−91.80	−47.61	−139.41		−0.010
	Ga	1.06	−64.67	−63.61		
	Co	−79.50	−55.46	−134.96	−171.8[b]	−0.011
Co_2MnGa	Mn	−289.12	77.61	−211.51	−280.0[c]	0.010
	Ga	2.12	−26.19	−24.07		
	Co	−119.73	−10.83	−130.56	−182.0[b]	−0.004
Co_2FeGa	Fe	−276.82	47.84	−228.98		0.003
	Ga	1.59	25.77	27.36		
	Co	−90.87	152.78	57.91	18.0[b]	0.026
Co_2VAl	V	−9.38	−70.64	−80.00	−63.4[b]	−0.014
	Al	0.69	−16.61	−15.92	−7[b]	
	Co	−81.78	−64.46	−146.24	−175.1[b]	−0.013
Co_2MnAl	Mn	−284.77	75.24	−209.53	−280.5[c]	0.009
	Al	2.12	−26.19	−24.07		
	Co	−121.05	−7.28	−128.33	−194.0[b]	−0.004
Co_2FeAl	Fe	−276.45	68.92	−207.53		0.007
	Al	2.88	−9.70	−6.82		

[a] LeDang *et al* (1978).
[b] Yoshimura *et al* (1985).
[c] Kawakami *et al* (1987).

approximately equal to the Co moment, the positive H_{val}(Co) cancels out the negative H_{core}(Co) and H(Co) is approximately equal to zero. For the cases T = Ti and V where the moments on the first neighbours of Co are very small, H(Co) is determined by the Co moment itself and has a positive value. For the cases T = Mn and Fe where the neighbour's moments are large, the effect of the neighbour's moment is very large and the H(Co) value becomes negative.

3.3. Hyperfine field at T in Co_2TZ

The values of H(T) are given in table 2 and the variation with the T atom is shown in figure 2(*c*). It is found that the H_{core}(T) reflects the T magnetic moments and the effect of the neighbour's moments seems to be small due to the shielding effect. For the case T = V, the sign of H_{val}(V) is determined as negative by the neighbouring Co moment, because the V moment is negligibly small. Comparing the case T = Ti with the case

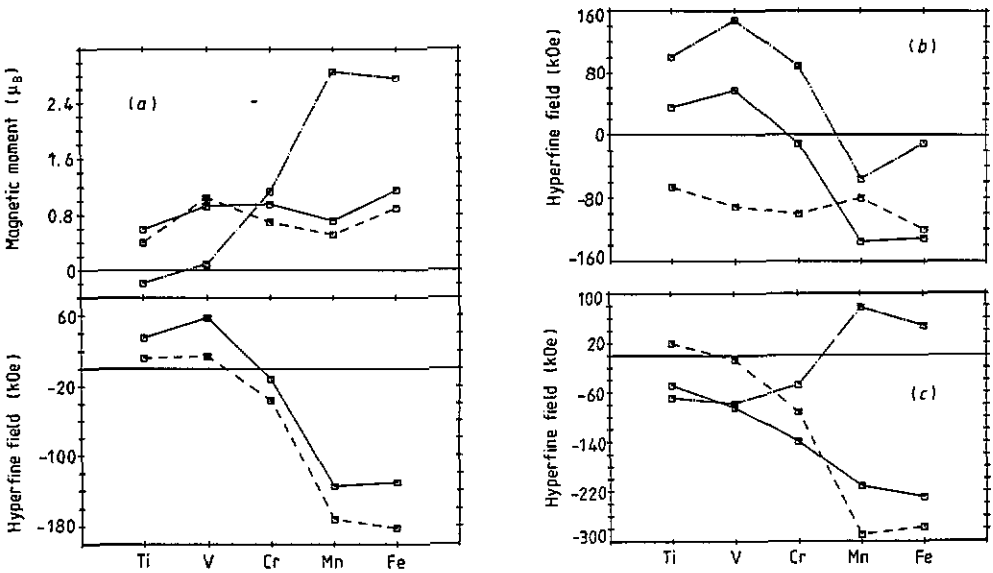

Figure 2. Magnetic moments and hyperfine fields of Co_2TGa(T = Ti, V, Cr, Mn and Fe). Calculated and experimental values are listed in tables 1 and 2. (*a*) Magnetic moments of Co and T atoms are shown in the upper part, where full and chain curves show calculated values of Co and T atoms respectively. A broken curve shows experimental values of Co atoms. Hyperfine fields of Co atoms are shown in the lower part, where full and broken curves show calculated and experimental values respectively. (*b*) Hyperfine fields of Co atoms are shown, where full, broken and chain curves show H_{cal}, H_{core} and H_{val} respectively. H_{cal} is a calculated value and H_{val} and H_{core} are the contributions to H_{cal} from inner core s electrons and valence s electrons respectively. (*c*) Hyperfine fields of T atoms are shown, where full, broken and chain curves show H, H_{core} and H_{val} respectively.

T = V, the absolute value of H_{val}(Ti) becomes smaller because the neighbouring Co moments are smaller for the case T = Ti. For the case T = Cr, since the circumstances of Cr are almost the same as that for the case T = V (the neighbouring Co moments are approximately equal to those for the case T = V) but Cr itself has a moment of about 1 μ_B, a positive contribution to H_{val}(Cr) is induced and H_{val}(Cr) is smaller than H_{val}(V) in magnitude. The positive contribution to H_{val}(Cr) from the Cr moment itself is estimated to be about 30 kOe from the difference between H_{val}(Cr) and H_{val}(V). For the cases T = Mn and Fe where the T atoms have moments of about 3 μ_B, the H_{val}(T) value is positive due to their large moments. The H_{val}(Fe) value is smaller than the H_{val}(Mn) value for two main causes. The positive contribution to H_{val}(Fe) is smaller because the Fe moment is about 0.1 μ_B smaller than the Mn moment, and the negative contribution to H_{val}(Fe) from the neighbouring Co moments is larger because the neighbouring Co moments for T = Fe are about 0.5 μ_B larger than those for T = Mn.

As described above, the hyperfine fields at T atoms in Co_2TGa are induced by the neighbouring Co moment and have a negative sign for T = Ti and V with a negligibly small moment. On the other hand, when the T moment is large as for T = Mn and Fe, the negative contribution to H(T) from its own moment is dominantly larger than the positive contribution. The case T = Cr, where the Cr moment is approximately equal to the neighbouring Co moment, is intermediate between the two cases. Thus, although the T hyperfine fields are negative for all T atoms, the mechanisms are different.

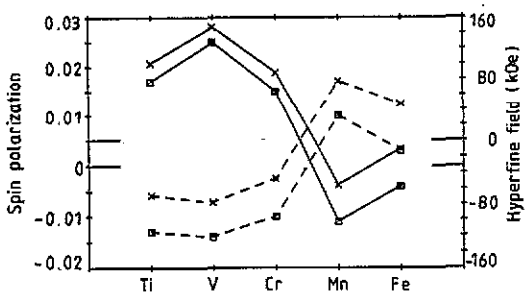

Figure 3. Spin polarizations m_s (square) and hyperfine fields H_{val} (cross) of Co and T atoms in Co_2TGa (T = Ti, V, Cr, Mn and Fe). The full and broken curves show Co and T atoms. H_{val} is a contribution to the hyperfine field from valence s electrons, which is listed in table 2.

3.4. Relation between hyperfine fields and density of states

We have discussed the hyperfine fields at Co and T atoms in Co_2TGa by seeing how the H_{core} and H_{val} values are related to the Co and T magnetic moments. The magnetic moments are mainly determined by the DOS of d states as seen in section 2. In this section, we turn our attention to the DOS of s states and investigate the relation between the hyperfine fields and the DOS.

Table 2 shows that the sign of H_{val} is identical to the sign of the 'spin polarization', m_s (the difference in valence s electrons between majority-spin electrons and minority-spin ones). To clarify the relation between H_{val} and m_s, we plotted these values in figure 3. This figure indicates that the hyperfine field is determined from the charge density of s electrons at the nucleus. However,the contribution H_{val} from valence s electrons is closely related to the 'spin polarization' m_s. That is, H_{val} is not only identical to m_s in sign but also roughly proportional to m_s. Next, we consider the DOS of s states.

In figure 4, the DOS of s states at Co, T and Ga atoms are shown by the full curves. For the case T = Ti (figure 4(*a*)), there is a small peak near the Fermi level in both spin states for Co atoms, while not for Ti and Ga atoms. The small peak is mostly occupied by majority-spin electrons, while not for minority-spin ones. This may be the origin of the positive m_s for Co atoms. The same fact is seen in the DOS of s states for Co atoms in the cases T = V and Cr (figures 4(*b*) and (*c*)). On the other hand, for the cases T = Mn and Fe (figures 4(*d*) and (*e*)), the shapes of the DOS for Co atoms are changed and the peak near the Fermi level in the majority-spin states is smaller than that for the cases T = Ti, V and Cr. This may be the origin of the negative m_s. Concerning the DOS of s states at T atoms, the unoccupied small peak in the majority-spin states approaches the Fermi level when moving from T = Ti to T = Cr and spreads out to the lower energy range for T = Mn and Fe. Thus, the 'spin polarization' m_s changes from negative to positive between T = V and T = Mn.

4. Summary

In order to examine the influence of surrounding magnetic atoms on the magnetic properties of an atom, we calculated the hyperfine fields of Co_2TZ. The Co_2TZ alloys are adequate for this purpose since the magnetic properties of Co atoms in Co_2TZ are easily influenced by the surrounding atoms on account of the small magnetic moment

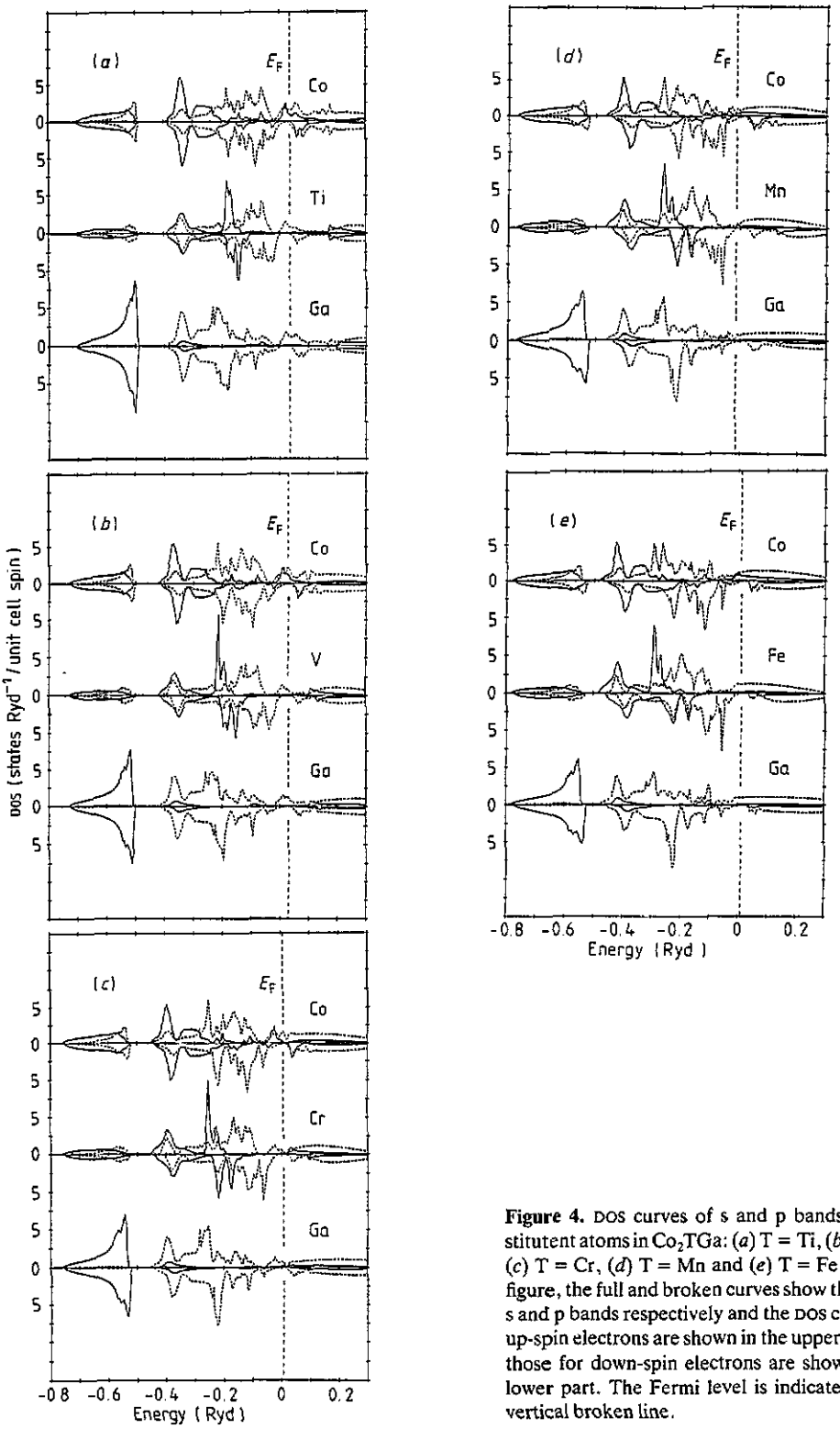

Figure 4. DOS curves of s and p bands of constitutent atoms in Co_2TGa: (*a*) T = Ti, (*b*) T = V, (*c*) T = Cr, (*d*) T = Mn and (*e*) T = Fe. In each figure, the full and broken curves show the DOS of s and p bands respectively and the DOS curves for up-spin electrons are shown in the upper part and those for down-spin electrons are shown in the lower part. The Fermi level is indicated by the vertical broken line.

on Co sites. The hyperfine field at Co atoms in Co_2TZ changes drastically not only in magnitude but also in sign through the different T atoms. When the hyperfine field is divided into two contributions (H_{core} and H_{val}), H_{core} is antiparallel and roughly proportional to the magnetic moment of the T atom but H_{val} strongly depends on the surrounding moments. The drastic change in the hyperfine field H(Co) with the T atom comes mainly from the H_{val}(Co) part which is roughly proportional to the 'spin polarization' of valence s electrons of Co atoms.

We considered first the hyperfine field at Co atoms in Co_2TZ. The value of H_{val}(Co) is positive when the surrounding moments are small for the cases such as T = Ti, V and Cr but negative when the surrounding moments are large, for the cases such as T = Mn and Fe. The hyperfine field H(Co) has a positive value for the cases T = Ti and V, because the absolute value of the positive H_{val}(Co) is larger than that of the negative H_{core}(Co), but a negative value for the cases T = Mn and Fe because both values of H_{core}(Co) and H_{val}(Co) are negative. For the case of T = Cr, the positive H_{val}(Co) is mainly cancelled out by the negative H_{core}(Co) and so H(Co) has a small and negative value.

We considered second the hyperfine field at the T atom in Co_2TZ. For T = Ti and V, H_{core}(T) is negligibly small on account of its own small magnetic moment and H_{val}(T) has a negative value due to the surrounding Co moment. Therefore, the hyperfine fields at Ti and V atoms have negative values. For T = Cr, Mn and Fe, the sign of H_{core} is negative and its value is roughly proportional to its own moment. Concerning H_{val}(T), there are two contributions; the positive contribution from its own moment and the negative one from the surrounding Co moments. The positive contribution becomes larger with increasing moment of the T atom in the order T = Cr, Mn and Fe. Summing up these contributions, the hyperfine fields are negative for T = Cr, Mn and Fe. Thus, the hyperfine fields are negative for all of Ti, V, Cr, Mn and Fe, though those for Ti and V are mainly determined by the surrounding Co moments and those for Cr, Mn and Fe by the moment of the T atom.

Similar calculations were carried out for Co_2TAl (T = V, Mn and Fe). The results are consistent with those for Co_2TGa and are listed in tables 1 and 2.

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