

A theoretical study of the hyperfine fields in BCC $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$ alloys

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1990 J. Phys.: Condens. Matter 2 443

(<http://iopscience.iop.org/0953-8984/2/2/019>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.96

The article was downloaded on 10/05/2010 at 21:27

Please note that [terms and conditions apply](#).

A theoretical study of the hyperfine fields in BCC $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$ alloys

H Ebert[†], H Winter[‡], D D Johnson[§] and F J Pinski^{||}

[†] Siemens AG, Research Laboratories, ZFE F1 TPH11, Postfach 3220, D-8520 Erlangen, Federal Republic of Germany

[‡] Kernforschungszentrum Karlsruhe, Institut für Nukleare Festkörperphysik, Postfach 3640, D-7500 Karlsruhe, Federal Republic of Germany

[§] Sandia National Laboratories, Livermore, CA 94551-0969, USA

^{||} Department of Physics, University of Cincinnati, Cincinnati, OH 45221, USA

Received 21 August 1989

Abstract. The hyperfine fields in the substitutionally disordered BCC alloy systems $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$ have been studied by means of charge self-consistent Korringa–Kohn–Rostoker coherent potential approximation (KKR CPA) electronic structure calculations. For the various components, the contribution to the Fermi contact hyperfine field due to core polarisation was found to be proportional to the corresponding local spin moment. The contributions of the conduction band, however, did not show such a simple behaviour and turned out to be dominated by the occupation of the s bands for spin up and down. To study the influence of relativistic effects on the hyperfine fields the corresponding matrix elements for the Fermi contact interaction have been calculated non-relativistically as well as fully relativistically. The importance of contributions to the hyperfine fields coming from non-s electrons have been investigated by performing spin-polarised relativistic linear muffin tin orbital method (SPRLMTO) band structure calculations for hypothetically ordered alloys.

1. Introduction

Nuclear methods are a very powerful tool for the study of magnetic systems because they provide a local probe. This property of experimental techniques that are based on the hyperfine interaction has been used in the past to investigate the variation with concentration of the local magnetic properties in alloys, order–disorder transitions, the influence of short range order, the structure of interfaces and surfaces and so on. Especially in the case of multi-component systems very interesting information on the electronic and magnetic structure can be obtained by these techniques because they allow us to study each of the component separately. With the complexity of the system under investigation, however, the interpretation of the experimental data can get rather complicated and normally has to rely on more or less well justified assumptions. On the other hand, with the availability of high speed computers and the development of new techniques of electronic structure calculation it has become during recent years possible to supply a first-principles description of the above mentioned experiments. In the case of substitutionally disordered alloys, the coherent potential approximation (CPA) alloy theory (Soven 1967) provides a sound basis for a reliable and detailed calculation of the

electronic structure. We have recently used this approach together with the cluster version of the KKR method of band structure calculation (Winter and Stocks 1984) to study the hyperfine interaction in the alloy system $\text{Fe}_x\text{Ni}_{1-x}$ (Ebert *et al* 1988b). In the following, we are presenting results of a corresponding investigation of the alloy systems $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$.

A brief description of our theoretical approach is outlined in the next section. In the following presentation and discussion of our results the main emphasis is on the importance of relativistic effects and the relationship between the Fermi contact hyperfine fields and the partial spin moments of the various alloy components.

2. Theoretical framework

A sound basis on which to investigate the electronic structure of substitutionally disordered alloys is supplied by the KKR CPA method of electronic structure calculation (see, for example, Stocks and Winter 1984). We have used the spin-polarised cluster version of this technique to calculate the magnetic properties of the ferromagnetic alloy systems $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$. Atomic clusters of six shells have been used and energy integrated quantities have been determined by using a complex energy integration path. Exchange and correlation have been taken into account within the framework of local spin density formalism using the parametrisation for the exchange–correlation potential given by Moruzzi *et al* (1978).

The hyperfine fields B_α due to the Fermi contact interaction have been determined in the usual way (see, e.g., Ebert *et al* 1988b) from the resulting spin density m_α ($r = 0$) at the site of the nucleus of component α , which emerged from our self-consistent non-relativistic band structure calculations. The effect of relativistic enhancement of this field has been studied by combining relativistically calculated matrix elements with the non-relativistic band structure (Ebert *et al* 1988b). This approach gives results in good agreement with a consistent scalar-relativistic description of the hyperfine interaction (Blügel *et al* 1987)—note that a combination of the conventional Fermi contact interaction operator and a scalar-relativistically calculated band structure by far overestimates the relativistic enhancement.

Contributions to the hyperfine fields coming from non-s electrons cannot be taken into account in a non-relativistic band structure calculation. However, as has been shown by Ebert *et al* (1988a) in the case of the pure elements Fe, Co and Ni a completely relativistic approach gives access to this part of B_α . Because the corresponding spin-polarised relativistic version of the KKR CPA for disordered alloys is not yet available, i.e. a corresponding computer program, we used instead the spin-polarised relativistic LMTO (Ebert 1988) to calculate the non-s contributions to B_α for hypothetically ordered FeCr and FeCo compounds. Although this part of B_α is of dipolar and orbital origin, it will be called orbital (B_α^{orb}) in the following for the sake of brevity. A decomposition of B_α^{orb} into its orbital and dipolar part could in principle be done on the basis of the separation of the matrix elements as has been given by Tterlikkis *et al* (1968) or, more rigorously, by making use of the Gordon decomposition (Baym 1974) of the electronic current (Ebert 1989).

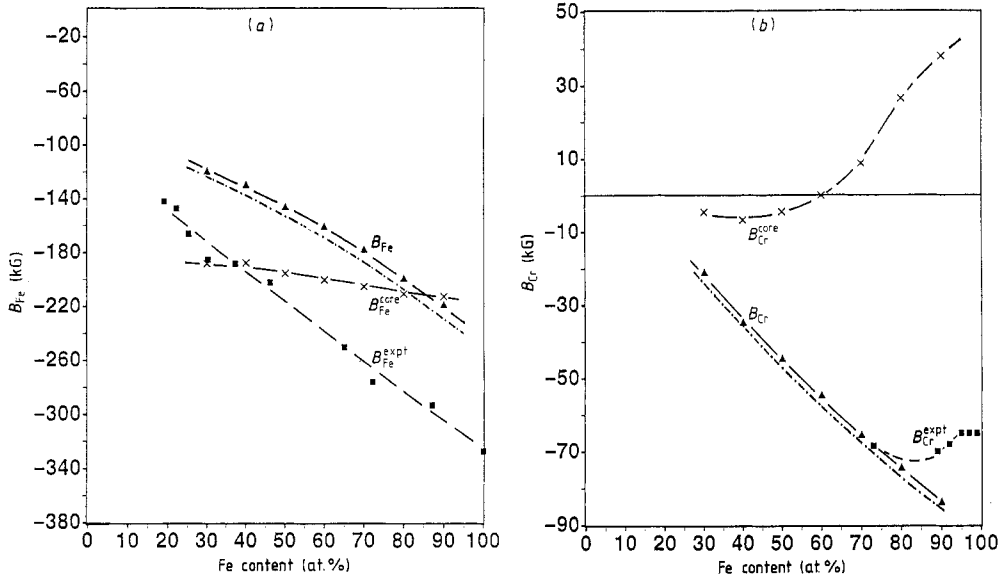


Figure 1. Hyperfine fields for (a) Fe and (b) Cr in BCC $\text{Fe}_x\text{Cr}_{1-x}$. Theory: non-relativistic total (Δ) and core (\times) hyperfine fields; total relativistic hyperfine fields (---). Experiment (\blacksquare): Fe—Johnson *et al* (1963); Cr—Lütgemeier *et al* (1982, 1983).

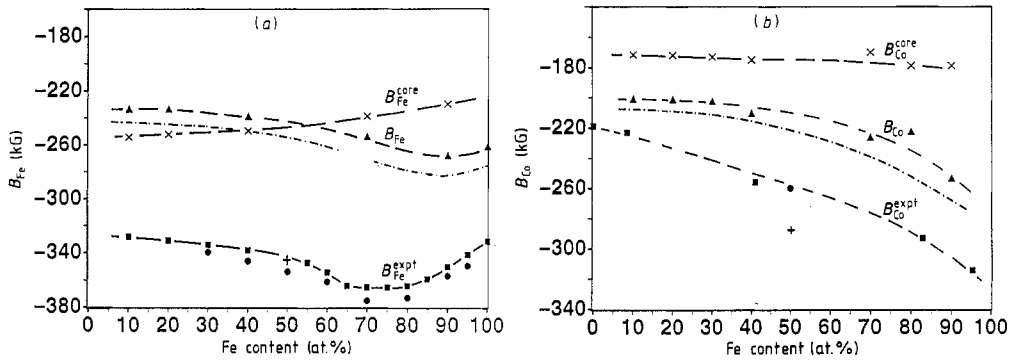


Figure 2. As for figure 1 but for (a) Fe and (b) Co in BCC $\text{Fe}_x\text{Co}_{1-x}$. Experiment: Fe—Johnson *et al* (1963) (\blacksquare) and Hamdeh *et al* (1989) (disordered, \bullet ; ordered, $+$); Co—Arp *et al* (1959) (\square) and Muraoka *et al* (1976) (disordered, \bullet ; ordered, $+$).

3. Results and discussion

3.1. Fermi contact hyperfine fields and comparison with experiment

The hyperfine fields B_α due to the Fermi contact interaction, which emerged from our non-relativistic calculations for $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$ are shown in figures 1 and 2, respectively. In addition, the core-polarisation contribution to B_α is displayed; this turned out to be nicely proportional to the local spin magnetic moment μ_α . This behaviour obviously obeys a rather general rule, which has been found to be fulfilled under

very different circumstances—for example, for thin films (Lee *et al* 1986) and impurities in ferromagnets (Blügel *et al* 1987). The ratio $R_{\alpha}^{\text{core}} = B_{\alpha}^{\text{core}}/\mu_{\alpha}$ that emerges from our calculations is $-100 \text{ kG}/\mu_{\text{B}}$ for Fe and $-104 \text{ kG}/\mu_{\text{B}}$ for Co in $\text{Fe}_x\text{Co}_{1-x}$. Both values are in good agreement with the results for $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Ni}_{1-x}$ (Ebert *et al* 1988b) as well as the results of Blügel *et al* (1987) for Fe and Co impurities in Ni. For this reason one can say that the ratios R_{α}^{core} are quite universal quantities which are characteristic for the components α . Comparing our theoretical results with experiment, one has to keep in mind that our approach, i.e. the CPA, has only been intended to deal with random alloys. Such randomness is, however, not always found in experiment. In particular, in the case of $\text{Fe}_x\text{Co}_{1-x}$ with x around 0.5, the system tends to order, with a corresponding dependence of the hyperfine fields on the degree of ordering (Muraoka *et al* 1976, Eymery *et al* 1978, Hamdeh *et al* 1989). This can clearly be seen in figure 2, where experimental data are shown for ordered, i.e. tempered, as well as disordered $\text{Fe}_{0.5}\text{Co}_{0.5}$. All other experimental data stem from disordered, i.e. quenched, bulk samples. Comparing the theoretical hyperfine fields with those corresponding to these alloys, one can see that the trend of the various experimental hyperfine fields with concentration is well described by the theoretical fields. For Fe in $\text{Fe}_x\text{Cr}_{1-x}$ $|B_{\text{Fe}}|$ decreases nearly linearly with increasing Cr content. This is in part due to a decrease of its core contribution or partial spin moment μ_{Fe} . More important, however, is the strongly increasing positive conduction band contribution to B_{Fe} . For Cr on the other hand, the core contribution to B_{Cr} is positive for Fe-rich alloys reflecting the antiferromagnetically coupled spin moment in this concentration range. Thus the negative Cr hyperfine field is due to the dominating conduction band contribution, which also determines the decrease of $|B_{\text{Cr}}|$ with increasing Cr content.

In the case of Fe in $\text{Fe}_x\text{Co}_{1-x}$ we again find a change of the conduction band contribution from negative to positive values upon decreasing the Fe content. This behaviour is responsible for the decrease of $|B_{\text{Fe}}|$ on the Co-rich side, which occurs in spite of the increasing contribution $|B_{\text{Fe}}^{\text{core}}|$. For B_{Co} , as for B_{Fe} , there is no strong variation at the Co-rich end of $\text{Fe}_x\text{Co}_{1-x}$. With increasing Fe content the increase of $|B_{\text{Co}}|$ has obviously to be ascribed primarily to its conduction band contribution. In spite of the good qualitative agreement of our results with experiment, one cannot overlook the fact that there are also rather pronounced quantitative deviations in some cases. Because the magnitude of our theoretical fields is always below that of the corresponding experimental values, it is of course tempting to ascribe these discrepancies—as is often done in the literature—to the relativistic enhancement of the Fermi contact hyperfine field. In addition, one has to keep in mind that the theoretical fields in figures 1 and 2 do not contain dipolar-orbital contributions, coming from non-s electrons, that are due to an incomplete quenching of the orbital angular momentum. The importance of both of these relativistic corrections to B_{α} and their possible responsibility for the above mentioned discrepancies is studied in the next section.

3.2. Relativistic corrections to B_{α}

The relativistically enhanced hyperfine fields due to the Fermi contact interaction have been determined as described in § 2. The resulting total fields are shown in figures 1 and 2 by chain lines. For the core as well as for the conduction band contributions the enhancement was in all cases only 5–10%. This obviously shows that the relativistic enhancement cannot account for the discrepancy between the theoretical and experimental fields. Furthermore, one can show that a combination of a scalar-relativistic

Table 1. Orbital hyperfine fields B_{α}^{orb} (in kG) of Fe and Cr in $\text{Fe}_x\text{Cr}_{1-x}$ and Fe and Co in $\text{Fe}_x\text{Co}_{1-x}$, respectively, as deduced from SPRLMTO calculations for hypothetically ordered compounds

	A	A_3B	AB	AB_3	B
A = Fe	14.3	9.5	22.9	5.3	—
B = Cr	—	-0.2	-1.6	1.4	—
A = Fe	14.3	20.5	17.4	16.4	—
B = Co	—	51.0	40.0	55.0	40.7

band structure calculation and the conventional Fermi contact interaction operator (which gives good agreement with experiment in the case of pure Fe) by far overestimates the relativistic enhancement. Blügel *et al* (1987) have recently performed scalar-relativistic calculations of the hyperfine fields of impurities in Ni using a modified expression for the Fermi contact hyperfine matrix element. The relativistic enhancement effects obtained by these authors are in full agreement with the results shown in figures 1 and 2. Furthermore these corrections are too small to bring their theoretical results into quantitative agreement with experiment in the case of Mn and Fe dissolved in Ni. As Blügel *et al* (1987) assume, it is very unlikely that dipolar-orbital contributions to B_{α} can account for the discrepancies found because these corrections should be of positive sign. This assumption was indeed verified by Ebert *et al* (1988a) in the case of the pure elements Fe, Co and Ni, where it turned out that the relativistic enhancement of the Fermi contact hyperfine field is nearly exactly cancelled by the dipolar-orbital contributions coming from non-s conduction electrons. A corresponding study in the case of the disordered alloy systems $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$ would require a spin-polarised relativistic KKR CPA program, which is not available at the moment. For this reason spin-polarised relativistic LMTO (SPRLMTO) calculations [Ebert 1988] have been performed instead for some hypothetically ordered alloys assuming an Fe_3Al or CsCl structure. In the case of $\text{Fe}_x\text{Co}_{1-x}$ this is surely not too serious a simplification, because the influence of disorder is only of minor importance (see, e.g., Schwarz *et al* 1984, Richter and Eschrig 1988). Although one can still expect to get the correct order of magnitude for the dipolar-orbital contributions, this approach is surely more questionable in the case of $\text{Fe}_x\text{Cr}_{1-x}$. The conduction bands contributions emerging from the SPRLMTO calculations were found to be in good agreement with the KKR CPA calculations including relativistic corrections, justifying our approach to some extent. The corresponding non-s contributions to B_{α} are given in table 1. These results clearly demonstrate that, as in the case of pure Fe, Co and Ni (Ebert *et al* 1988a), these corrections cannot be responsible for the deviations between the theoretical and experimental hyperfine fields in figures 1 and 2. Again it is found that inclusion of these terms more or less cancels the enhancement of the Fermi contact hyperfine fields.

In their study of the magnetic properties of Fe, Co and Ni, Ebert *et al* (1988a) speculated on whether inclusion of core contributions coming from non-s electrons could remedy at least to some extent the observed discrepancy. This suggestion can, however, be ruled out on the basis of a recent study of these terms by Ebert (1989) who showed them to be very small and positive, as was the case for the dipolar-orbital conduction band contributions. One should, however, mention here that there is no reason to assume that the dipolar-orbital contributions always have to be of positive sign. As has

been found by Ebert *et al* (1989), in a study of the magnetic properties of 4d and 5d impurities in Fe, these terms can have the the same as well as opposite sign when compared with the dominating Fermi contact contributions due to s electrons.

In summary, one can obviously rule out the possibility that relativistic corrections, although important even for 3d metals, are responsible for the deviations between theoretical and experimental hyperfine fields found in the alloy systems $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$. As already assumed by Blügel *et al* (1987) and Ebert *et al* (1988a) one has therefore to conclude that these discrepancies are caused by shortcomings of the local spin density theory in treating the polarisation of core electrons in terms of a spin-split conduction band.

3.3. The relationship between B_α and the partial magnetic spin moments μ_α

In discussing experimental hyperfine field data, it is often assumed that there is a rather simple relationship between B_α and the partial spin magnetic moment μ_α of the system investigated. Johnson *et al* (1963) suggested that the relationship

$$B_{\text{Fe}} = a\mu_{\text{Fe}} + b\bar{\mu} \quad (1)$$

should hold, but could not obtain reasonable fits to their data in the case of $\text{Fe}_x\text{Co}_{1-x}$, $\text{Fe}_x\text{Ni}_{1-x}$, $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Mn}_{1-x}$. Erich (1969), on the other hand, claims that his Ni hyperfine fields in $\text{Fe}_x\text{Ni}_{1-x}$ fit rather well to an expression analogous to equation (1). As an alternative to equation (1), Menshikov and Yurchikov (1973) have suggested the relation

$$B_\alpha = D_\alpha\mu_\alpha x_\alpha + D_\beta\mu_\beta(1 - x_\alpha) \quad (2)$$

for disordered alloys with components α and β . Also, an even more general expression has been given and used by Takanashi *et al* (1982), Muraoka *et al* (1976) and Stone (1986):

$$B_\alpha = a_0\mu_\alpha + \sum_{i \neq 0} a_i\mu_i \quad (3)$$

which relates B_α to the local magnetic spin moment on site 0 and to those of the surrounding atomic sites i . In the limiting case of an impurity dissolved in a pure magnetic host that is not strongly affected by the impurity, this expression would simplify to

$$B_\alpha = a\mu_{\text{imp}} + b\mu_{\text{host}}. \quad (4)$$

This relation together with the magnetic moments from neutron scattering data leads, in the case of 3d impurities in Fe, to a value of $-70 \text{ kG}/\mu_{\text{B}}$ for the constant a (Stone 1986), which is reasonably close to R_α^{core} given above. For this reason, it seems interesting to investigate whether one of the heuristic relationships between hyperfine fields and magnetic moments given above can be put on a firm theoretical basis and to find in this way a clear meaning for the various coefficients.

Recently, Blügel *et al* (1987) have calculated the hyperfine fields of 3d and 4d impurity atoms in Ni by means of the KKR Green's function method. In discussing their data they find that a rather small part of the conduction band contribution to $B_\alpha B_\alpha^{\text{cb}}$, should be referred to as 'transferred' and is expected to be essentially proportional to the magnetic moments of the neighbouring host atoms. In addition, there is a dominating local valence hyperfine field which primarily reflects the occupation of the s-like spin-up and spin-down bands (see figure 7 in Blügel *et al* 1987). Stimulated by this work, we investigated

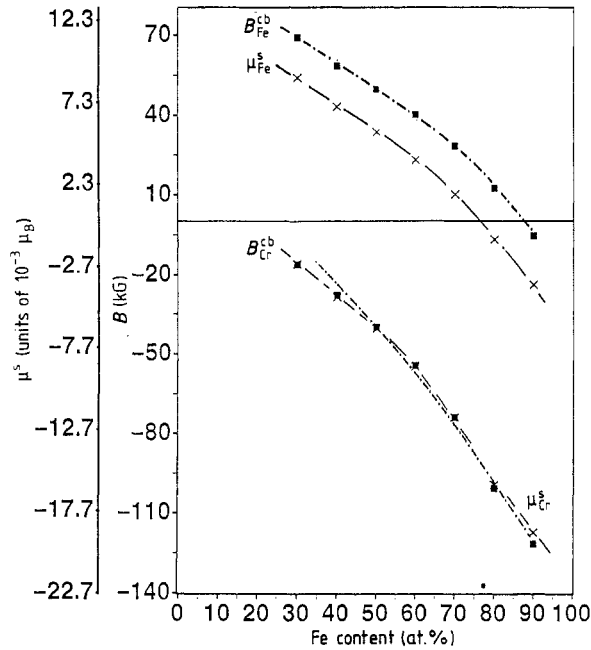


Figure 3. Conduction band contribution to the hyperfine fields B_α^{cb} (\square) and local s moment $\mu_\alpha^s(x)$ for Fe and Cr in BCC Fe_xCr_{1-x} . The fit according to equation (7) using the parameters of table 2 is shown by a chain line.

in an earlier paper on FCC Fe_xNi_{1-x} (Ebert *et al* 1988b) whether this picture can also be applied to concentrated ferromagnetic alloys. Although the concept of transferred hyperfine fields in this case is surely questionable, it could be shown that the population mechanism also plays a dominating role for B_α^{cb} . For Ni and Fe in FCC Fe_xNi_{1-x} it was found that B_α^{cb} goes in parallel with the s-contribution to the spin magnetic moment, μ_α^s , if the concentration is varied. As can be seen from figures 3 and 4, this is also true for Fe, Cr and Co in Fe_xCr_{1-x} and Fe_xCo_{1-x} , respectively. If one multiplies μ_α^s by the spin-averaged hyperfine field per s electron for $E = E_F$, \bar{R}_α^{cb} , which is nearly concentration independent, the result is identical to the μ_α^s -curves in figures 3 and 4, read, however, using the scale for B_α^{cb} . This clearly demonstrates that the concentration dependence of B_α^{cb} is almost completely determined by μ_α^s or, in other words, by the variation of the population of the s bands for spin up and spin down with composition. Obviously this mechanism becomes more important for the magnitude of B_α^{cb} if the total local magnetic moment μ_α becomes smaller—an extreme example for this is Cr in Fe_xCr_{1-x} , where the Cr moment is quite small and B_{Cr}^{cb} stems nearly exclusively from the population mechanism. Furthermore, one finds that the difference between B_α^{cb} and $\bar{R}_\alpha^{cb} \mu_\alpha^s$ is positive in all cases studied and only moderately concentration dependent. Because $\Delta B_\alpha^{cb} = B_\alpha^{cb} - \bar{R}_\alpha^{cb} \mu_\alpha^s$ scales rather well with μ_α with a proportionality constant of +20–22 kG/ μ_B in all cases, it seems plausible to ascribe its occurrence to the distortion of the 4s wave functions by the spin-dependent potential—in analogy to the core polarisation mechanism. If the change in the hyperfine field per s electron due to the distortion of the 4s wave functions is approximated by the difference between the hyperfine fields for spin up and for spin down for $E = E_F$, one gets for the ratio of ΔB_α^{cb} and μ_α a value

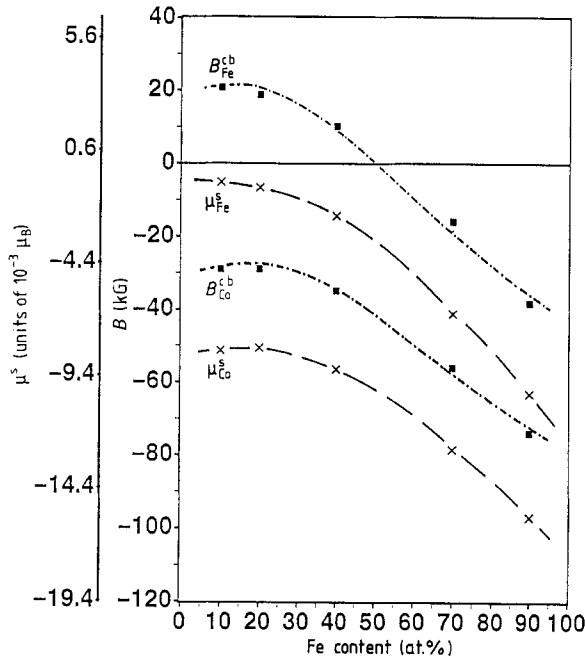


Figure 4. As for figure 3 but for Fe and Co in BCC $\text{Fe}_x\text{Co}_{1-x}$.

between +40 and +50 kG/μ_B for the various components in $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$. Although this estimate seems rather crude, it makes clear that the polarisation mechanism could indeed account for the results found for $\Delta B_\alpha^{\text{cb}}$.

Here we should mention that this point of view differs somewhat from our earlier interpretation of $\Delta B_\alpha^{\text{cb}}$ (Ebert *et al* 1988b) based on our results for $\text{Fe}_x\text{Ni}_{1-x}$. Following the work on impurities in Ni by Blügel *et al* (1987) this contribution to B_α^{cb} has been called 'transferred' to distinguish it from the part in B_α^{cb} arising from the population mechanism. That the term 'transferred' is quite problematical becomes clear from the fact that the population of the s bands is not completely determined by the local electronic properties alone, but depends also on the situation on the neighbouring atomic sites. The partition of B_α^{cb} made above, although giving insight into the various mechanisms determining the conduction contributions to B_α , does not give any information on whether one of the relationships between B_α and μ_α given above should hold or not. This question can, however, be investigated via the following considerations, which give to some extent a justification for the use of the heuristic relation expressed by equation (3). Apart from this, they allow us—at least in principle—to separate B_α^{cb} strictly into local and transferred contributions.

As has already been stated above, B_α^{core} is in all the cases studied so far proportional to μ_α , i.e. for this contribution equation (3) is fulfilled with $a_0 = R_\alpha^{\text{core}}$. To investigate whether there is a theoretical justification for equation (3) for the conduction band contribution, we will ignore orbital effects completely and use the non-relativistic formulation for the remaining Fermi contact interaction in the following. To derive a relation between B_α^{cb} and μ_α it is convenient to introduce a paramagnetic reference system that corresponds to the spin-averaged potential \bar{V} of the ferromagnetic system

studied. Treating the spin-dependent part of the potential as a perturbation $\Delta H = V - \bar{V}$, the corresponding Green's function G_f of the spin-polarised system is given by the Dyson equation

$$G_f = G_p + G_p \Delta H G_f. \quad (5)$$

Here G_p is the Green's function for the paramagnetic reference system and all quantities in equation (5) have to be looked upon as 2×2 matrices with spin indices. In linear approximation, G_f on the RHS of equation (5) may be replaced by G_p . Taking the trace of $\sigma_z G_f$, the spin magnetisation at the site of nucleus α , $m_\alpha(r=0)$, and in this way $B_\alpha = (8\pi)/3 m_\alpha(r=0)$ can be written in terms of G_p and $\Delta V = V_\uparrow - V_\downarrow = \text{Tr } \sigma_z V$. If ΔV is not too large, it should be proportional to the spin magnetisation $m(r)$. Within an atomic cell occupied by an atom of type α , $m_\alpha(r)$ may in turn be approximated by $|\psi_\alpha(r, E_F)|^2 \mu_\alpha$ (Gunnarsson 1976). Because equation (5) implies an integral over the whole space, which may be replaced by a sum over integrals over the various atomic cells, one ends up with a relation between B_α and $\mu_{A(B)}$ of the form

$$B_\alpha = I_{00}^{\alpha\alpha} \mu_\alpha + \sum_{i \neq 0} I_{0i}^{\alpha A} \mu_A \times x_A + \sum_{i \neq 0} I_{0i}^{\alpha B} \mu_B \times x_B \quad \alpha = (A, B). \quad (6)$$

The concentrations $x_{A(B)}$ give the probability that a site i is occupied by an A or B atom of a random disordered binary alloy. The quantities $I_{ij}^{\alpha\beta}$ contain some kind of Stoner-type exchange-correlation integral and are most conveniently expressed in the language of multiple-scattering theory (Staunton 1984, Ebert 1986).

In summary one can say that a relationship between B_α and μ_α analogous to equation (3) can indeed be derived with a clear interpretation of the various coefficients. One should, however, keep in mind that in doing this a number of assumptions have to be made, among which the linear approximation of equation (5) is without doubt the most questionable. In addition, for equation (3) to be helpful for a disordered alloy system one has to assume that the various terms in equation (6) are not too strongly dependent on concentration. Accepting the linear response behaviour, equation (6) can also be written down straightforwardly using the concept of the generalised spin susceptibility $\chi(\mathbf{r}, \mathbf{r}')$. A corresponding discussion of the Knight shift has been given by Terakura *et al* (1982) and in a more general way by Ebert *et al* (1986). We have tried to use equation (2) to fit our theoretical hyperfine field and magnetic moment data. Although the fit was generally not too bad, in most cases the coefficients turned out to be unreasonably high. Furthermore, the changes for the Fe-related coefficients seemed much too strong on going from $\text{Fe}_x\text{Cr}_{1-x}$ to $\text{Fe}_x\text{Co}_{1-x}$.

Using equation (6) in its configurationally averaged form

$$B_\alpha = a_\alpha \mu_\alpha + b_\alpha \mu_\alpha x_\alpha + b_\beta \mu_\beta x_\beta \quad (7)$$

where a_α corresponds to the on-site coefficient $I_{00}^{\alpha\alpha}$ in equation (6) and the $b_{\alpha(\beta)}$ represent the lattice sums for an occupation of sites i by atoms of type $\alpha(\beta)$, a very satisfying fit of the data could be obtained, as can be seen in figures 3 and 4. The parameters, which are summarised in table 2, are quite reasonable in size. On the other hand, the Fe-related parameters for $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$ again differ much more than one would expect. This does not mean that equations (3) or (7), respectively, are not fulfilled, but presumably indicates that neglecting any concentration dependence in evaluating the parameters a_α and $b_{\alpha(\beta)}$ is not justified. That this auxiliary assumption holds does not seem very likely. Using theoretical results for the hyperfine fields we could show that for

Table 2. Parameters a_α and $b_{\alpha(\beta)}$ according to equation (7) as deduced from a least squares fit to the theoretical data for $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$.

α	β	a_α (kG)	b_α (kG/ μ_B)	b_β (kG/ μ_B)
Fe	Cr	110	-137	-65.3
Cr	Fe	43.9	-87.2	-90.1
Fe	Co	-107	87.4	28.2
Co	Fe	-150	82.1	32.1

$\text{Fe}_x\text{Ni}_{1-x}$ the dependence of B_α on the surrounding atomic environment of an atom α can be expressed by (Ebert *et al* 1987)

$$B_\alpha = B_\alpha^{\text{CPA}} + \sum_{\text{shell } i} \Delta B_\alpha^i (n_{\text{Fe}}^i - \bar{n}_{\text{Fe}}^i) \quad \alpha = \text{Fe, Ni.} \quad (8)$$

Here n_i^{Fe} and \bar{n}_i^{Fe} are the actual and average numbers of Fe atoms in an atomic shell i around a central atom occupied by an atom of type α . B_α^{CPA} is the configurationally averaged hyperfine field for the central atom and ΔB_α^i determines the deviation from B_α^{CPA} due to occupation fluctuations in shell i (for a more general discussion on the interpretation of ΔB_α^i see Johnson *et al* (1989)). The coefficients ΔB_α^i can straightforwardly be related to the coefficients in the lattice sums of equation (6) and turned out to be concentration dependent in a non-negligible way in the case of $\text{Fe}_x\text{Ni}_{1-x}$. This is in full accordance with the statement given by Hamdeh *et al* (1989) that for $\text{Fe}_x\text{Co}_{1-x}$ the Fe-related nearest neighbour coefficient decreases with Co content and changes sign for $x = 0.5$. Their experience that even for diluted alloys parameters up to the fifth-neighbour shell are significant is also in full accordance with our earlier findings (Ebert *et al* 1988b).

Thus one has to conclude that a relationship between B_α and μ_α as expressed by equations (3), (6) or (7) can be justified by theoretical arguments and also by the results of calculations for the occupation fluctuation parameters ΔB_α^i . On the other hand, these equations seem normally only of limited usefulness in discussing experimental data, because of the concentration dependence of the various parameters.

4. Summary

By means of self-consistent KKRCPA band structure calculations, the electronic structure of random $\text{Fe}_x\text{Cr}_{1-x}$ and $\text{Fe}_x\text{Co}_{1-x}$ alloys has been studied. The Fermi contact hyperfine field was, from these calculations, found to be in satisfying agreement with experimental data. It could be shown that the quantitative deviations between theoretical and experimental fields, which are most pronounced for Fe, do not stem from a relativistic enhancement of the Fermi contact hyperfine field nor from dipolar-orbital contributions. It has therefore to be concluded that these shortcomings have to be ascribed to problems of local spin density theory in dealing properly with the polarisation of inner core electrons due to a spin-split conduction band.

The various contributions to the Fermi contact hyperfine field have been studied in detail, showing the core contribution to be proportional to the local spin magnetic moment. Theoretical justification for a frequently used linear relationship between the

hyperfine field and the spin magnetic moment on surrounding atomic sites could be given. However, this interrelation seems to be of limited use in interpreting experimental data because of the concentration dependence of the relevant expansion coefficients.

Note added in proof. Results for the Fermi contact hyperfine fields in $\text{Fe}_x\text{Co}_{1-x}$ similar to those presented here have also been recently found by Akai (1989).

References

- Akai H 1989 *Mater. Sci. Forum* **37** 211
 Arp V, Edmonds D and Petersen R 1959 *Phys. Rev. Lett.* **3** 212
 Baym G 1974 *Lectures on Quantum Mechanics* (New York: Benjamin)
 Blügel S, Akai H, Zeller R and Dederichs P H 1987 *Phys. Rev. B* **35** 3271
 Ebert H 1986 *Thesis* University of Munich
 ——— 1988 *Phys. Rev. B* **38** 9390
 ——— 1989 to be published
 Ebert H, Drittler B, Zeller R and Dederichs P H 1989 to be published
 Ebert H, Strange P and Gyorffy B L 1988a *J. Phys. F: Met. Phys.* **18** L139
 Ebert H, Winter H, Gyorffy B L, Johnson D D and Pinski F J 1987 *Solid State Commun.* **64** 1011
 ——— 1988b *J. Phys. F: Met. Phys.* **18** 719
 Ebert H, Winter H and Voigtländer B 1986 *J. Phys. F: Met. Phys.* **16** 1133
 Erich U 1969 *Z. Phys.* **227** 25
 Eymery J P, Raju S B and Moine P 1978 *Phys. Lett.* **68A** 260
 Gunnarsson O 1976 *J. Phys. F: Met. Phys.* **6** 587
 Hamdeh H H, Fulk B and Pearson D H 1989 *Phys. Rev. B* **39** 11233
 Johnson C E, Ridout M S and Cranshaw T E 1963 *Proc. Phys. Soc.* **81** 1079
 Johnson D D *et al* 1989 to be published
 Lee J E, Fu C L and Freeman A J 1986 *J. Magn. Magn. Mater.* **62** 93
 Lütgemeier H, Bohn H G and Dubiel S M 1983 *J. Magn. Magn. Mater.* **31–34** 547
 Lütgemeier H and Dubiel S M 1982 *J. Magn. Magn. Mater.* **28** 277
 Menshikov A Z and Yurchikov E E 1973 *Sov. Phys.–JETP* **36** 100
 Moruzzi V L, Janak J F and Williams A R 1978 *Calculated Electronic Properties of Metals* (New York: Pergamon) p 15
 Muraoka Y, Shiga M, Yasuoka H, Nakamura Y 1976 *J. Phys. Soc. Japan* **40** 414
 Richter M and Eschrig H 1988 *J. Phys. F: Met. Phys.* **18** 1813
 Schwarz K, Mohn P, Blaha P and Kübler J 1984 *J. Phys. F: Met. Phys.* **14** 2659
 Soven P 1967 *Phys. Rev.* **156** 809
 Staunton J 1984 *PhD Thesis* University of Bristol
 Stocks G M and Winter H 1984 *The Electronic Structure of Complex Systems* ed. P Phariseau and W M Temmerman (New York: Plenum) p 463
 Stone N J 1986 *Low-temperature Nuclear Orientation* ed. N J Stone and H Postma (Amsterdam: North-Holland) p 351
 Takanashi K, Yasuoka H, Kawaguchi K, Hosoi N and Shinjo T 1982 *J. Phys. Soc. Japan* **51** 3743
 Terakura H, Hamada N, Oguchi T and Arsada T 1982 *J. Phys. F: Met. Phys.* **12** 1661
 Tterlikkis L, Mahanti S D and Das T P 1968 *Phys. Rev.* **176** 10
 Winter H and Stocks G M 1984 *Phys. Rev. B* **27** 882