# Formation of magnetic moments on iron impurities in transition-metal hosts

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The role of crystal symmetry for the formation of magnetic moments on iron impurities in transitionmetal hosts is elucidated. To do this, *ab initio* calculations within the framework of the local-spindensity approximation are performed for iron atoms in 3d, 4d, and 5d transition-metal hosts, both for hypothetical bcc structures as well as for the real structures of the hosts. It is shown that the systematics of the formation of magnetic moments is related to the fact that the degree of hybridization among the  $T_{2g}$  and  $E_g$  orbitals depends on the crystal symmetry. The results for the magnetic moments and hyperfine fields are compared with experimental data and with results from other calculations.

# I. INTRODUCTION

The ground-state configuration of an isolated transition-metal atom is determined by Hund's rules and usually exhibits a magnetic moment. If such an impurity atom is dissolved in a metal, the strong intra-atomic Coulomb interactions responsible for Hund's rules compete with the interactions with band electrons. As a result, the ground-state configuration of the impurity atom may be more or less destroyed and the magnetic moment may be reduced to zero. The question whether a transition-metal impurity atom dissolved in a metal exhibits a magnetic moment or not has been investigated both theoretically and experimentally for many years.

Up to the 1980s, theoretical work was essentially based on empirical models.<sup>1</sup> Closest to the starting point of a free impurity atom were the ionic models<sup>2,3</sup> which treat the intra-atomic Coulomb interactions beyond mean-field theory, for instance, by starting from impurity eigenstates constructed by standard atomic-physical methods, and which deal with the coupling of the localized electrons to the conduction electrons by a perturbation approach. In this model, magnetic moments arise because of the intact intra-atomic Hund's rule couplings. At temperatures below the Kondo temperature  $T_K$ , however, the validity of a finite-order perturbation theory breaks down, because physically the moment resonates between its various possible orientations due to the antiferromagnetic interaction with the conduction electrons, and the impurity appears to be nonmagnetic. The ionic mode is valid for most of the metallic systems with 4f impurities and for 3d impurities in sp metal hosts.<sup>4,5</sup>

In the alternative Friedel-Anderson-type models<sup>6-8</sup> it is argued that the coupling between the impurity and host electrons is too strong to be treated as a perturbation. To be able to deal with intra-atomic and interatomic interactions on an equal footing, the Hartree-Fock approximation was applied. Within this approximation a local moment occurs if

$$IZ(E_F) > 1 , (1)$$

where I is Stoner's exchange parameter. This condition

is very similar to Stoner's criterion for elementary ferromagnets with the only difference that  $Z(E_F)$  is the paramagnetic density of states of the impurity atom and not the one of the host. The physical picture (see, for instance, Ref. 9) is the one of an impurity "virtual bound state" at the Fermi level,<sup>8</sup> generated by the scattering of conduction electrons at the impurity potential and described by a local density-of-states function Z(E) for the paramagnetic impurity, which is split and shifted rigidly up or down under the influence of the exchange interaction as in Stoner's model<sup>10</sup> for elementary ferromagnets. As in the ionic model, the state with a static local moment is not the true eigenstate of the system, and the Hartree-Fock approximation should be regarded as an adiabatic approximation to the time-varying local moment, resonating between its possible orientations due to the interaction with the conduction electrons. These spin fluctuations result in a nonmagnetic impurity below the Kondo temperature. They may be suppressed by ferromagnetic exchange couplings between the impurity and the host.

The question whether an impurity atom appears to be magnetic or not thus consists of two parts, namely: (i) Is the formation of a moment possible? (ii) Is this moment stable against fluctuations in orientation?

It is well known that the properties of d impurities in d-metal hosts cannot be described by the ionic model because the strong interatomic interactions destroy the ground-state configuration of the free impurity atom. As a result, the orbital contribution to the magnetic moment of the impurity atom is more or less quenched, and the spin moment appears to be a nonintegral multiple of Bohr's magneton. It is therefore reasonable to analyze corresponding experiments within the Friedel-Andersontype models, as was done for the case of Fe in noble metals.4,5 Indeed, electronic structure calculations<sup>11,12</sup> within the local-spin-density approximation (which may again be regarded as an adiabatic approximation in the sense discussed above) revealed in this case all the essential features of the Friedel-Anderson-type models, i.e., a narrow virtual bound state at the Fermi level with a density-of-states function which is more or less rigidly split under the influence of the exchange interaction.

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Furthermore, it was argued<sup>4,5</sup> that the Kondo temperature of these systems is strongly reduced by effectively ferromagnetic d-d interactions between Fe 3d and host d-band electrons (resulting in a ferromagnetic spin polarization of the d states of neighboring host atoms) so that the magnetic moments according to the adiabatic approximation can be observed already at low temperatures.

When going from the noble metals to transition metals as hosts, the situation changes drastically. Because of the strong hybridization of the impurity states with the host states which is neglected in the Friedel-Anderson-type models there is a broad impurity band instead of a sharp virtual bound state. Furthermore, there is not simply a rigid shifting of the unpolarized density of states due to the exchange splitting, but in general also a redistribution of the spectral weight within the spin-up and the spindown subbands, respectively.<sup>13-15</sup> This gives rise to covalent magnetism,<sup>16,17</sup> as contrasted against magnetism according to the Stoner model with its rigid shifting of the subbands.

In the present paper we consider mainly the first of the above discussed questions, namely the conditions for the formation of the magnetic moment, whereas there will be only some comments on the stability of the moments against fluctuations in orientation. To do this, a Fe atom in body-centered cubic (bcc) transition-metal hosts is investigated by ab initio calculations within the framework of the local-spin-density approximation and the linearmuffin-tin-orbital theory in atomic-sphere approximation.<sup>18</sup> Special emphasis is given to the role of the hybridization between the impurity states and the host states, which is determined by the symmetry of the bcc lattice and by the location of the Fermi level. To demonstrate this, supercell calculations for hypothetical bcc  $FeT_7$  are performed where T means any metal atom of the 3d, 4d, or 5d series.

If the T matrix in reality does not appear in bcc structure, these results are compared with those for  $FeT_7$  with the actual structure of the T host, and by means of this comparison the role of symmetry may be elucidated.

## **II. OUTLINE OF THE METHOD**

Calculations for hypothetical bcc  $FeT_7$  are performed where T denotes any transition metal or noble metal of the 3d, 4d, or 5d series. The supercell as shown in Fig. 1 is built from a cube with twice the lattice constant of the underlying bcc structure, with T atoms on all corners  $(8 \times \frac{1}{8} = 1)$ , on all mid-points of the edges  $(12 \times \frac{1}{4} = 3)$  and on all face centers  $(6 \times \frac{1}{2} = 3)$ , and with a central Fe atom. Crystallographically equivalent atoms are represented by the same symbol. For instance, all the nearest-neighbor atoms of the central Fe atom (symbol  $\bullet$ ) are of course equivalent, but they are also equivalent to the further distant corner atoms, because these in turn are nearest neighbors of central Fe atoms in neighboring unit cells. In this sense we denote all atoms represented by the symbol • as nearest-neighbor atoms. Proceeding in an analogous way also for the next-nearest-neighbor atoms, it becomes obvious that the whole supercell may be built by the central Fe atom and nearest neighbor as well as next-



FIG. 1. The 8-atom supercell used in the calculations for Fe $T_7$ . The various symbols characterize crystallographically inequivalent sites. Central Fe site:  $\bigcirc$ ; "nearest-neighbor site":  $\bigcirc$ ; see text.

nearest-neighbor atoms. For the lattice constant we insert the theoretical values obtained for the pure bcc T systems.

The scalar-relativistic calculations were performed within the framework of the local-spin-density approximation based on the functional of von Barth and Hedin<sup>19</sup> in the parametrization of Moruzzi, Janak, and Williams.<sup>20</sup> The linear-muffin-tin-orbital theory [LMTO (Ref. 18)] in atomic-sphere approximation (ASA) was applied (including the combined-correction term). The basis set included angular momenta up to  $l_{max} = 3$ , the maximum momentum being treated with downfolding. In calculations based on the Korringa-Kohn-Rostoker (KKR)-Green's function method<sup>14</sup> an Fe impurity in Nb appeared to be magnetic for  $l_{max} = 2$ , but nonmagnetic for  $l_{max} = 3$ . In our calculations we obtain a nonmagnetic Fe atom in FeNb<sub>7</sub> both for  $l_{max} = 2$  and  $l_{max} = 3$ , in agreement with recent real-space muffin-tin-orbital calculations<sup>21</sup> for Fe in Nb. The results for the magnetic moments and hyperfine fields were tested for convergence with respect to the number of k points used for the Brillouin-zone sampling. For  $FeT_7$  it was sufficient to use 145 k points in the irreducible part of the Brillouin zone. The ratio of the atomic-sphere radii of the T atom and the Fe atom was chosen to be 1.0 for 3d transition metals and 1.1 for 4d and 5d transition metals.

# **III. RESULTS AND DISCUSSION**

#### A. Magnetic moments and hyperfine fields

The magnetic moments for the Fe atom in hypothetical bcc Fe $T_7$  are shown in Fig. 2, together with the induced magnetic moments on the nearest-neighbor T atoms. There is a striking similarity between the 3d, 4d, and 5d series: For T atoms from the group IV and group V there is no magnetic moment on the Fe atom, whereas for all the other T atoms an appreciable Fe moment occurs,



FIG. 2. The magnetic moment of the central Fe atom (full symbols) and of a nearest-neighbor T atom (open symbols) in hypothetical bcc FeT<sub>7</sub> for various T atoms. 3d: triangles; 4d: circles; 5d: squares.

which may even exceed the magnetic moment in pure Fe considerably.

The zero magnetic moment for the Fe atom in Nb agrees with the results from real-space muffin-tin-orbital calculations<sup>21</sup> and from KKR-Green's function calculations<sup>14</sup>  $(l_{max}=3)$  for Fe impurities in Nb. For Mo, our magnetic moment of about  $2\mu_B$  compares with the value of about  $2.5\mu_B$  obtained by the two latter calculations for the Fe impurity in Mo. The disappearance (appearance) of the magnetic moment of Fe in the group-V (group-VI) transition-metal hosts V, Nb, Ta (Cr, Mo, W) was confirmed experimentally.<sup>4,5</sup> Because all the other transition-metal hosts do not crystallize in the bcc structure, we cannot compare our results with experimental data. Riegel and co-workers<sup>4,5</sup> explained the fact that Fe in V, Nb, and Ta appears to be nonmagnetic by the assumption that the d-d exchange interaction between the Fe and the T atom is only weakly ferromagnetic or even antiferromagnetic and thus cannot suppress the spin fluctuations so that the existing magnetic moment resonates quickly between various orientations (see Introduction). In contrast, all the theoretical calculations show that the magnetic moment is not at all formed, anyway.

The induced magnetic moments on the nearestneighbor host atoms are aligned antiferromagnetically for the group-III transition-metal hosts and ferromagnetically for all the other systems with magnetic Fe atoms. We thus would expect that Fe in bcc Y and La appears to be nonmagnetic because of the spin fluctuations, whereas for the other systems the magnetic Fe moment is stabilized against spin fluctuations due to the ferromagnetic interaction. The general trend, i.e., antiferromagnetic Tatom coupling for the left part of the periodic table and ferromagnetic coupling for the right part is correctly reproduced by the very simple model of covalent polarization of Mohn and Schwarz.<sup>17</sup>

To stress the important role of symmetry for the formation of magnetic moments (see also Sec. III B) we have in addition performed calculations for Fe in 4dtransition-metal hosts with the real structure of the host (instead of exclusively bcc structure). The supercells for the fcc (hcp) structure contained 16 (8) atoms. For the lattice parameters we inserted the experimental values. The results for the magnetic moments on the Fe atom and the nearest-neighbor T atom are shown in Fig. 3, together with the old results from Fig. 2 for the bcc structure. On the extreme left-hand side (Y) and on the extreme right-hand side (Pd, Ag) of the periodic table there is only a small difference between the results for two different structures. This has to do with the formation of virtual bound states on the Fe atoms, see Sec. III B. Dramatic differences arise in between. For Zr in the hcp structure the substitutional Fe atom appears to be magnetic, in agreement with the experimental and theoretical (real-space LMTO-ASA, KKR-Green function) results given by Metz *et al.*, <sup>22</sup> whereas in the bcc structure the Fe atom was nonmagnetic. Vice versa, for Tc and Ru in the hcp structure the Fe atom is nonmagnetic, whereas it is magnetic in the bcc structure. We are not aware of any experimental results for Tc, but for hcp Ru our finding is confirmed by experiments<sup>4,5</sup> as well as by LMTO Green's function calculations,<sup>23</sup> albeit only for a slightly contracted Ru host. The existence of an Fe moment in hcp Y and in fcc Rh, Pd, and Ag was found also experimentally,<sup>24,4,5</sup> and by other theoretical work (Y: Jund et al.;<sup>25</sup> Pd: Mohn and Schwarz;<sup>17</sup> Oswald, Zeller, and Dederichs;<sup>26</sup> Ag: Podloucky, Zeller, and Dederichs<sup>12</sup>). The induced magnetization on the neighboring T atoms of the hcp host (Fig. 3) is rather small, except for Pd (in agreement with Oswald, Zeller, and Dederichs<sup>26</sup> and Mohn and Schwarz<sup>17</sup>), Zr and Y. In the latter case, there is an antiferromagnetic alignment of the Fe moment and the moment of the nearest-neighbor T atom. According to Riegel and co-workers,<sup>4,5</sup> the substitutional Fe atom should therefore appear to be nonmagnetic due to spin fluctuations, in contrast to the experimental observation.24

For completeness, Fig. 4 shows the magnetic hyperfine



FIG. 3. The magnetic moment of a substitutional Fe atom (circles) and of a nearest-neighbor T atom (triangles) in various 4d hosts, with the real structure of the 4d host (full symbols) and with a hypothetical bcc structure (open symbols).

60

30

0

-30

hyperfine field [T]

ı



## B. Local density of states and interpretation

The results presented in Sec. III A are now interpreted in terms of the local density of electronic states, Z(E). Figure 5 presents the density of states for the perfect bcc T atom host (left side) of the 4d series and for the central Fe atom (right side) in bcc Fe $T_7$ , obtained from a calculation without spin polarization (paramagnetic state). In addition, the contributions from the d states with  $E_g$  $(3z^2-r^2,x^2-y^2)$  and  $T_{2g}$  (xy,xz,yz) symmetry are shown. Quite similar results are obtained for the 3d and



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FIG. 5. Density of states for the perfect hypothetical bcc transition-metal host (left side) and for the Fe atom in hypothetical unpolarized bcc FeT<sub>7</sub> (right side). Solid line: full density of states; dashed line: contribution of  $T_{2g}$  states; dotted line: contribution of  $E_g$  states. The vertical line denotes the Fermi level.

the 5d series.

The density of states for the T atom host exhibits the same qualitative features throughout the series, i.e., essentially a four-peak structure, whereby the highestenergy peak is predominantly of  $E_g$  character, the two intermediate peaks are dominated by  $T_{2g}$  states, and the lowest-energy peak is of mixed character. The main difference when going from Ag to Y is the location of the Fermi energy  $E_F$ . For Ag the Fermi energy is above the highest-energy peak of  $E_g$  symmetry, and then it drops to lower energies in the band when going from the right side of the periodic table to the left side, passing the  $E_g$  peak and entering the  $T_{2g}$  dominated region of the two intermediate peaks for the first time for Nb. The density of states for the T atoms which are nearest neighbors of the Fe atoms in FeT<sub>7</sub> looks very much like the one of the pure bcc T matrix.

The shape of the density of states curve for the Fe atom depends on the degree of hybridization with the surrounding T atoms. For FeAg<sub>7</sub> the Fermi level is above the highest-energy peak in the density of states of the Ag atoms. In contrast, because of charge neutrality, the d density of states for the Fe atom must have a considerable weight above  $E_F$  so that the local d band below  $E_F$  is filled with the correct number (6) of d electrons. Because there are no d states available for hybridization at  $E_F$  in the Ag host, a narrow density-of-states peak arises for the Fe atom, which represents the virtual bound state of the Friedel-Anderson-type models (see Sec. I). As a result, the local Fe density of states at the Fermi level,  $Z(E_F)$ , is very large. The situation is very similar to the one found for Fe impurities in fcc Ag.<sup>12</sup> There, the d density of states for Ag at the Fermi level is also very low and almost no hybridization with the Fe d states occurs. As a result, the magnetic moments for Fe in fcc and bcc Ag are quite similar (Fig. 3).

When going from Ag to Pd, the *d* density of states in the Pd host is a bit larger at  $E_F$  than the one of Ag, i.e., the hybridization with the Fe *d* states is stronger and the virtual bound state is broadened. Thereby, the  $T_{2g}$  part is more strongly broadened than the  $E_g$  part. This results from the fact that for Fe in a transition-metal host the hybridization with the nearest-neighbor *T* atoms is stronger than the one with the next-nearest-neighbor atoms (see Fig. 7 of Morinaga, Yukawa, and Adachi<sup>28</sup>) and that the nearest-neighbor hybridization is dominated



by the  $T_{2g}$ - $T_{2g}$  part (Fig. 8 of Morinaga, Yukawa, and Adachi<sup>28</sup>). This becomes obvious by looking at the relative orientation of the various *d* orbitals in the bcc structure, i.e., it is related to the structural symmetry.

When going further to the left side of the periodic table, the process continues, i.e., there is a further broadening of the Fe density of states. Due to the hybridization with the host atom d states, a structure occurs in the local density of states at the Fe atom in the energy range of the intermediate  $T_{2g}$  peaks of the host. This structure is again more pronounced for the  $T_{2g}$ states than for the  $E_g$  states because of the strong  $T_{2g}^{-}$ .  $T_{2g}$  nearest-neighbor hybridization. By integrating the density-of-states curve up to  $E_F$  we find that the numbers of occupied  $E_g$  and  $T_{2g}$  states at the Fe atom remain roughly constant throughout the 4d series. Because the  $E_g$  peak is only gradually broadened, the Fermi level must remain in this peak when going to the left-hand side of the periodic table in order to maintain the correct number of occupied  $E_g$  states. Therefore, the density of states at  $E_F$ ,  $Z(E_F)$ , is rather large up to T=Mo. For the case of Nb, the Fermi level enters the energy range where the host density of states is strongly dominated by

the  $T_{2g}$  symmetry, and the corresponding structure in the Fe density of states is strongly piled up, both for the  $E_g$  and for the  $T_{2g}$  states. In order to maintain the correct number of states, the remainder of the original virtual bound-state peak shrinks and the Fermi level moves out of this peak, i.e.,  $Z(E_F)$  decreases. When proceeding from Nb to Zr and finally to Y, the hybridization of the Fe states with the host atom d states becomes weaker, because there are only few host d states available for hybridization and because the lattice constant increases quickly, inducing a narrowing of the bands. The Fe density of states in Y therefore again looks like the one of a broadened atomic state. To maintain charge neutrality, the Fermi level must be located in the corresponding peak, resulting in a large value of  $Z(E_F)$ .

The paramagnetic Fe density of states in FeT<sub>7</sub> at the Fermi level,  $Z(E_F)$ , is shown throughout the 3d, 4d, and 5d series in Fig. 6. As discussed above, it is very large at the right-hand side of the series because of the formation of the virtual bound state, and it is minimum for group IV and V of the transition metals. Within the framework of Stoner's theory of magnetism<sup>10</sup> we can now predict for which transition-metal hosts a magnetic moment on the





FIG. 6. The local density of states at the Fermi level for Fe in hypothetical unpolarized bcc Fe $T_7$ . The horizontal line represents the limit below which according to Stoner's theory of magnetism no magnetic moment on the Fe atom can be formed. 3d: triangles; 4d: circles; 5d: squares.

Fe atom is expected. To do this, we insert for the Stoner parameter, which represents an intra-atomic interaction and which therefore is only slightly influenced by the chemical surrounding, the value I=0.068 Ry for pure Fe. The dashed horizontal line in Fig. 6 represents the limit of the density of states, below which according to Eq. (1) no formation of a magnetic moment is possible. Indeed, this is the case for the group-IV and group-V transition metals, in perfect agreement with the results from our spin-polarized band-structure calculations (Fig. 2).

The mechanism of magnetism is now discussed from the viewpoint of the Stoner theory<sup>10</sup> and the theory of covalent magnetism<sup>16</sup> by means of the spin-polarized density of Fe states in FeT<sub>7</sub> (Fig. 7). In the conventional version of the Stoner theory, magnetism is related to a rigid shift of the spin-up and spin-down bands under the action of the exchange field. The theory of covalent magnetism accounts for the fact that due to the exchange interaction the two spin systems feel different effective potentials and thus experience different hybridization effects, leading to



FIG. 7. The spin-polarized density of Fe states in hypothetical bcc Fe $T_7$ . Left side: majority band; right side: minority band. Solid line: full density of states; dashed line: contribution of  $T_{2g}$  states; dotted line: contribution of  $E_g$  states. The vertical line denotes the Fermi level.

a redistribution of the spectral weight in the two subbands. Figure 7 clearly shows that the Stoner model in its conventional version is not adequate. Comparing carefully the density of states for the minority spins with the corresponding paramagnetic density of states (Fig. 5), it becomes obvious that there is, in addition to a rigid shift, also a small redistribution of the spectral weight. For instance, for the Mo system the  $E_g$  peak is higher in the minority-spin band than in the paramagnetic band, and the displacement of the  $E_g$  peak with respect to its location in the paramagnetic state is stronger than the one of the  $T_{2g}$  peaks. The majority-spin states are shifted to lower energies and thus experience a stronger hybridization with  $T_{2g}$  states of the host. As a result, there is a strong redistribution of the spectral weight in the majority band, and the resulting density of states resembles to some extent the one of the host. However, these covalent effects have only a small influence on the magnetic moments, because the majority band is nearly saturated (especially for Ag, Pd, and Rh), and therefore the redistribution of spectral weight in the majority band does not matter too much.



## **IV. CONCLUSIONS**

We have investigated the mechanism of the formation of a Fe magnetic moment in a bcc transition-metal host by supercell calculations within the local-spin-density approximation for hypothetical bcc Fe $T_7$ , where T denotes any 3d, 4d, or 5d transition metal. The emphasis was on the role of symmetry of the transition-metal host. It was shown that the systematics observed for the formation of magnetic moments in these systems is related to the fact that in a bcc structure the nearest-neighbor interaction is dominated by  $T_{2g}$ - $T_{2g}$  hybridization. To elucidate the role of symmetry further, we have contrasted the hypothetical bcc Fe $T_7$  systems to systems with an Fe atom in a T host of the real structure (i.e., bcc, fcc, or hcp). Indeed, in the latter case (where our results can be directly compared with experimental data) the systematics for the formation of Fe moments are totally different.

The physical picture emerging from this paper is the basis for the interpretation of the magnetization data for the ternary system  $Nb_{1-x}Mo_x$  with 1% Fe. Jaccarino and Walker<sup>29</sup> proposed a model for the concentration dependence of the experimentally observed magnetization in these random alloys based on the assumption that a Fe atom carries a certain magnetic moment if it has not more than one Nb atom as nearest neighbor, whereas it is nonmagnetic otherwise. This interpretation has been roughly confirmed by *ab initio* supercell calculations<sup>15,30,31</sup> (albeit the details are different from the pure Jaccarino-Walker model). The role of Nb as contrasted to Mo for the destruction of the Fe moment becomes obvious from the results of the present paper.

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