Theoretical investigation of the magnetic behavior of substitutional Fe impurities in Zn, Cd, and Al hosts

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Calculations for substitutional Fe in Al in the absence of lattice relaxation yield a large value for the magnetic moment at the impurity site. The lack of magnetic response observed experimentally has been attributed to the presence of spin fluctuations. However, more recent calculations show that the moment at the Fe impurity could vanish in the presence of lattice relaxation around the impurity, thus rendering unnecessary a description in terms of spin fluctuations. We have performed electronic-structure calculations to investigate the magnetic behavior of substitutional Fe impurities in Zn, Cd, and Al hosts as a function of lattice relaxation. In the case of Fe in Al, the theoretical results are sensitive to the lattice constant used for fcc Al. If the experimental value is used, the Fe moment decreases drastically but does not vanish at the experimentally observed relaxation values. In the case of Zn and Cd hosts, the calculated moment remains quite large for all reasonable values of relaxation. Our results indicate that a description in terms of spin fluctuations and high values of the Kondo temperature should be used for Fe in Zn and Cd and may also be appropriate to describe Fe impurities in Al. [S0163-1829(98)00511-6]

I. INTRODUCTION

In recent years, owing to advances in experimental techniques, there has been a renewed interest in the problem of impurities in metallic hosts. In particular, nonalloying systems can now be investigated, yielding information about moment formation at the impurity site as the host is varied throughout the periodic table.[1] The Fe impurity is especially well suited for such studies, due to its interesting magnetic properties and its flexibility when used as a probe. Theoretical results can also be of help when addressing the problem of local moment formation at impurity sites in metallic hosts, since values for the moment can be obtained from knowledge of the electronic structure of the impurity system. Electronic-structure calculations for substitutional Fe impurities have been performed in many metallic hosts using different techniques.[2–5] In some systems, the Fe impurity is found to develop local moments, while in other systems the impurity is nonmagnetic. The agreement between theory and experiment regarding local moment formation is impressive, especially if one considers the limitations of the local spin density approximation (LSDA) methods. Some of the discrepancies which originally existed between theory and experiment have been eliminated in the last few years, either by improving sample preparation and experimental techniques in the case of nonalloying systems, or by improved theoretical approaches.

An example of the difficulties which may arise when trying to compare calculated values of the impurity moment with those observed experimentally is illustrated by the case of the Fe impurity in Al. Experiments using different techniques[1,6,7] have found no evidence of magnetic behavior for Fe impurities in Al in the observed temperature range, while first-principles electronic structure calculations[8] performed for substitutional Fe in Al using the Al lattice interatomic distance found a large local magnetic moment at the impurity site. Since dilute alloys of $3d$ transition elements are considered classical examples of systems with spin-fluctuations (SF), the discrepancy had been explained by considering Fe in Al to be a system with SF that has a high Kondo temperature (T_K). However, recent electronic-structure calculations[9,10] which take into account lattice relaxation around the impurity find the Fe impurity to be nonmagnetic. The evidence[10] suggests that substitutional impurities of Cr and Mn in Al do behave as systems with SF, but the Fe impurity in Al is probably nonmagnetic.

In the present work we use the real space (RS) linear muffin tin orbital (LMTO) formalism, within the atomic sphere approximation (ASA), to obtain the electronic structure and magnetic properties of a substitutional Fe impurity in hcp Zn and Cd hosts. Divalent Zn and Cd are located in the column between monovalent Cu, Ag, and Au and trivalent Al in the periodic table. The substitutional Fe impurity is strongly magnetic in Cu, Ag, and Au hosts and the Fe moment does not seem to be very sensitive to lattice relaxation, while the local moment of substitutional Fe impurities in Al was shown to vanish for realistic values of relaxation around the impurity. In this context, the Fe impurity in the divalent Zn and Cd hosts should exhibit an interesting intermediate behavior. To our knowledge, no electronic-structure calculations to determine the magnetic properties of Fe in these systems have been reported. We could find few experiments for Fe in Zn and Cd in the literature. In both cases no significant magnetic response has been observed for the temperature range studied in the experiments.[11,6] It is interesting to note that clear indications of SF with relatively low Kondo temperatures were observed for Cr and Mn in Zn.[11,12] Here we investigate the magnetic behavior of substitutional Fe impurities in Zn and Cd hosts, to determine if a local moment is formed and how it is affected by lattice relaxation around the impurity. We also obtain results and review the earlier theoretical work for substitutional impurities in Al. We hope that the present work will contribute to a better

understanding of the role played by lattice relaxation and (or) SF in these impurity systems.

The paper is organized in the following way. In Sec. II we briefly introduce the RS-LMTO-ASA scheme used here. In Sec. III we apply the real space scheme to investigate the magnetic behavior of substitutional Fe impurities in Al, discuss our results and compare them to those in the literature. In Sec. IV we calculate the electronic structure and obtain the local moments of substitutional impurities in hcp Zn and Cd hosts. The effect of lattice relaxation on the local impurity moment is also investigated. Finally in Sec. V we present our conclusions.

II. THEORETICAL APPROACH

We use the first-principles, self-consistent RS-LMTO-ASA scheme within the LSDA to determine the electronic structure and magnetic behavior around substitutional Fe impurities in Al, Zn, and Cd hosts in the presence of lattice relaxation. Only a brief introduction to the method will be given here; a detailed description of the scheme and its application to impurities can be found elsewhere.[5,13,14]

The RS-LMTO-ASA scheme is based on the well-known LMTO-ASA formalism[15] and uses the recursion method.[16] The procedure is very similar to the usual reciprocal-space LMTO-ASA formalism, but when solving the eigenvalue problem to find the local density of states (LDOS) we substitute the k-space diagonalization by the real-space recursion procedure. To avoid surface effects, large clusters of a few thousand atoms are normally used. Below, we give a summary of the principal approximations used in the RS-LMTO-ASA scheme. As in the regular LMTO-ASA formalism, we use the atomic sphere approximation, where the space is divided into Wigner Seitz (WS) cells, which are then approximated by WS spheres of the same volume. The LMTO is a linear method and its solutions are valid around a given energy E_ν, normally taken at the center of gravity of the occupied part of the band. In the RS-LMTO-ASA scheme we use a first order Hamiltonian, where terms of the order of $(E-E_\nu)^2$ and higher are neglected. These approximations result in a *tight-binding* Hamiltonian and an orthogonal basis, yielding a simple eigenvalue problem which can be directly solved in real space with the aid of the recursion method. Since it is implemented directly in real space, the RS-LMTO-ASA scheme does not require periodicity. It can be used to treat impurities or other defects,[5,17] and lattice relaxation can be easily introduced[14] even in noncubic systems. In this context we should note that the real space scheme has already been used with success to study interstitial impurities where taking lattice relaxation into account is essential.[14]

The present calculations were performed using large clusters of around 3000 atoms, cut in order to keep the atoms of interest at a maximum distance from the surface. We work within the LSDA with an exchange and correlation term of the form proposed by von Barth and Hedin.[18] Valence s, p and d electrons were considered in the calculations, with a total of nine orbitals per site. For all sites a cutoff parameter $L_{\max}=20$ was taken in the recursion chain and a Beer and Pettifor terminator was used.[19]

III. SUBSTITUTIONAL Fe IMPURITIES IN Al

In this section we will review the problem of Fe impurities in Al, which bears a close relation to our study of Fe impurities in Cd and Zn. The magnetic behavior of substitutional Fe impurities in Al has been investigated using experimental techniques and theoretical first-principles approaches. Even though calculations performed for substitutional Fe in Al at the Al lattice interatomic distance found large local moments at the impurity, no local moment has been observed experimentally.[1,6,7] Dilute alloys of $3d$ elements in Al have been considered classical examples of systems with SF and a high T_K, and experimental evidence for this behavior is found for substitutional Cr and Mn impurities in Al.[1,6,7] Therefore the fact that no significant magnetic response has been observed for Fe in Al had previously been attributed to the presence of SF with T_K in excess of 10^4 K . This picture changed in 1991 when Guenzburger and Ellis[9] performed discrete variational method (DVM) calculations for an $FeAl_{42}$ embedded cluster, and showed that the value of the moment at the Fe site is very sensitive to lattice relaxation of Al nearest neighbors (NN) around the impurity. They argued that the local moment at the Fe site vanishes if reasonable values of the lattice relaxation are considered and that the substitutional Fe impurity is really nonmagnetic. This result would be consistent with experimental observations and would render unnecessary a description in terms of SF. One of the shortcomings of this interesting work was that when no lattice relaxation was assumed, a local moment of $0.96\mu_B$ was predicted, in disagreement with the value of around $1.8\mu_B$ obtained by other approaches.[8] Recently, Papanikolaou *et al.*[10] have reported a systematic study of lattice relaxation effects around $3d$ substitutional impurities in Al, using the full-potential KKR-GF method. The theoretical lattice constant (a_{the}) of the fcc Al host was obtained by energy minimization, and was about 1% smaller than the experimental lattice constant (a_{exp}) value. Due to this fact, the KKR-GF calculated value of Ref. 10 for the local moment of the Fe impurity in Al in the absence of relaxation is around $1.5\mu_B$, slightly smaller than those in the literature[8] which were obtained using the experimental value of the lattice constant. The results of Ref. 10 indicate that the local moment vanishes when Al atoms in the first NN shell around the Fe impurity are relaxed radially towards the impurity site by around 3% of the interatomic distance, while minimization of energy predicts a radial relaxation of 4% on the same scale. The KKR-GF result is in very good agreement with available data from extended x-ray absorption fine-structure (EXAFS) measurements, which give values in the range between 3 and 4% for the relaxation.[10,20] For Cr and Mn impurities in Al, the moments decrease with relaxation, but they are still magnetic for the relaxation which minimizes the energy. Therefore, in Ref. 10 it was concluded that the Fe impurity in Al has no local moment, while Cr and Mn impurities in Al retain their moments and are typical cases of systems with SF and high T_K's.

Here we have employed the RS-LMTO-ASA scheme to calculate the electronic structure around a substitutional Fe impurity in Al in the absence of lattice relaxation using both a_{exp} and a_{the} lattice constants of Ref. 10 for fcc Al. For a_{exp} we find a local moment of $1.9\mu_B$ at the impurity site, much

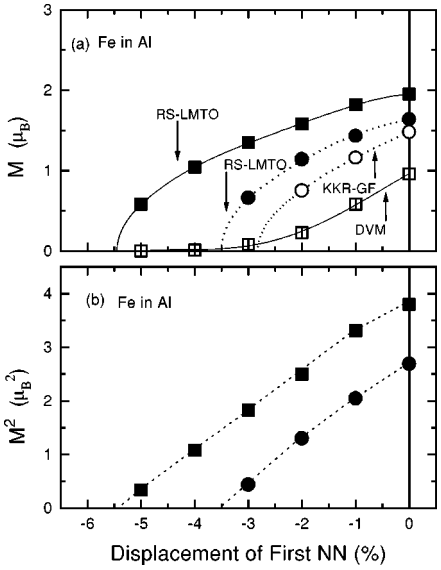

FIG. 1. RS-LMTO-ASA results for (a) local magnetic moment and (b) square of the local magnetic moment of Fe in Al as a function of the radial first-neighbor relaxation towards the impurity (in units of the percentage of the NN distance). Results obtained using the lattice constants a_{exp} (squares) and a_{the} (circles) are shown (see text). For comparison, DVM and KKR-GF results (Refs. 9,10) are also given in Fig. 1(a).

larger than the $0.9\mu_B$ resulting from DVM calculations,[9] and in reasonably good agreement with the values of around $1.8\mu_B$ quoted previously in the literature. When a_{the} was used, we found a smaller value of $1.6\mu_B$, which agrees well with the value of $1.5\mu_B$ obtained using the full potential KKR-GF approach, in the absence of lattice relaxation. We have also performed RS-LMTO-ASA calculations in the presence of lattice relaxation around the Fe impurity. The Al atoms of the first NN shell were displaced radially towards the impurity by a certain distance, expressed as a percentage of the distance between the impurity and the first NN shell in the unrelaxed structure and used to define the relaxation. The RS-LMTO-ASA results for the local moment as a function of the radial first-neighbor relaxation towards the impurity are plotted in Fig. 1(a) for different values a_{exp} and a_{the} of the Al lattice constant. For comparison we also show KKR-GF results[10] obtained using the theoretical value a_{the} and DVM results[9] which were obtained using the experimentally observed value a_{exp} of the Al lattice constant. In Fig. 1(b), we show the square of the magnetic moment *versus* lattice relaxation, which is expected to exhibit a linear behavior for low values of the magnetization.[10] A linear extrapolation of the values in Fig. 1(b) was used to determine the relaxation value for which the moment vanishes in Fig. 1(a). The present RS-LMTO-ASA calculations show a behavior for the impurity moment as a function of lattice relaxation which is very different from that predicted by DVM calculations. On the other hand, the RS-LMTO-ASA results obtained with a_{the} show the same tendencies and agree rather well with the existing full potential KKR-GF results. We note that the good agreement between our RS-LMTO-ASA results and those obtained using the KKR-GF approach is not surprising, since results obtained using these two methods have been shown to agree quite well.[5]

If one compares the two curves shown in Fig. 1, it is clear that the value of the lattice parameter for fcc Al used in the calculations is extremely important when determining the value of relaxation around the impurity for which the impurity moment vanishes. The KKR-GF calculations, which use theoretical values a_{the} for the lattice constant of fcc Al, indicate that the impurity is nonmagnetic, since the local moment vanishes for reasonably small values of the lattice relaxation. We expect that if the experimental lattice parameter of fcc Al could be used in the KKR-GF calculations, the moment at the Fe impurity would vanish for larger values of first NN shell relaxation, which might be less compatible with the experimentally observed values of the relaxation. This point should probably be investigated further before it can be accepted that for substitutional Fe impurities in Al, the discrepancy between experiment and theory can be completely explained in terms of lattice relaxation around the impurity and that SF play no role.

IV. SUBSTITUTIONAL Fe IMPURITIES IN hcp Zn AND Cd

We have used the RS-LMTO-ASA scheme to obtain the electronic structure and the magnetic properties of a substitutional Fe impurity in hcp Cd and Zn. In both cases, the experimental lattice parameter and c/a ratios were used in the calculations. The calculations were initially performed without lattice relaxation. We found a local moment of $2.6\mu_B$ for substitutional Fe in Zn and a local moment of $2.9\mu_B$ for substitutional Fe in Cd. These values are larger than those obtained for Fe in Al and are comparable to the moments obtained for Fe in Cu and Ag, respectively. But while experimental evidence for local moment at Fe impurities in Cu and Ag exists, no significant magnetic response has been observed for Fe impurities in Zn and Cd in the measured temperature range. We found very few experimental results for Fe in Cd and Zn reported in the literature. Susceptibility measurements below 20 K give no evidence of Curie Weiss behavior for Fe in Zn and indicate a characteristic temperature of the order of 120 K.[11] More recent TDPAD measurements[6] for Fe in Zn and Cd at extremely low concentrations for temperatures between 80 and 300 K have shown no significant magnetic response. They point to T_K's of around 5×10^3 K for Fe in Cd and in excess of 10^4 K in the case of Fe in Zn. We should note that Cr and Mn in Zn are examples of systems with SF that have low T_K's.[11,12] As in the case of Fe impurities in Al, the lack of magnetic response observed for Fe impurities in Cd and Zn could be explained by two distinct physical processes: it could be attributed to SF with extremely high T_K's, or the impurity could be really nonmagnetic. As discussed in the last section, it has been suggested that the Fe impurity in Al is nonmagnetic due to lattice relaxation around the impurity. It is interesting to investigate whether a similar phenomenon could be present in the case of substitutional Fe impurities in Cd and Zn.

Here we have again used the RS-LMTO-ASA scheme to obtain the electronic structure and magnetic properties around substitutional Fe impurities in Zn and Cd in the presence of lattice relaxation. In Fig. 2, we show our results for the local moment of Fe in Zn and Cd obtained with different

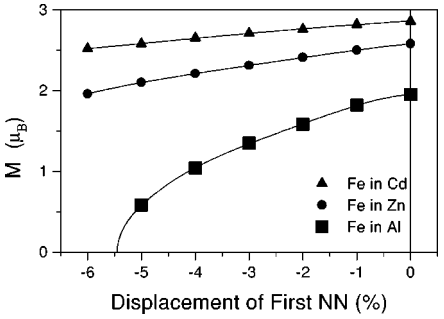

FIG. 2. RS-LMTO-ASA results for the local magnetic moment of Fe in Cd (triangles) and Zn (circles) as a function of the radial first-neighbor relaxation towards the impurity (in units of the percentage of the NN distance). For easy reference we also show the results for Fe in Al (squares), obtained using a_{exp}.

values of the lattice relaxation. As in the case of Al, only relaxation of the first NN shell was included. The 12 Zn and Cd impurity NN were relaxed radially towards the impurity by a given percent of their unrelaxed distance to the impurity site. For easy reference we also show in Fig. 2 the results for Fe in Al, obtained using a_{exp}, and already shown in Fig. 1(a). It is clear that there is a systematic tendency for the impurity moment to decrease as the value of the relaxation is increased, but for Cd and Zn hosts the decrease is small and the impurity moment remains significantly large for all reasonable values of the relaxation. Unrealistic relaxations, in excess of 10%, would be needed for the Fe moment to vanish in Zn, and even larger values would be required in the case of Cd. Since Cd and Zn have hcp stuctures, we have also changed the c/a ratio by relaxing the NN in the impurity plane while keeping the others at the unrelaxed position, but no drastic decrease of the local moment was observed. Our calculations also show that the local moment is not very sensitive to small variations of the lattice parameter. It is interesting to compare the behavior of the Fe impurity in divalent hcp Zn and Cd and in trivalent fcc Al. The d band in Cd and Zn is deep and interacts very little with the $3d$ levels of the Fe impurity, which are close to the Fermi level. In this sense, when $3d$ impurities are considered, Zn and Cd behave as simple metals. As in other simple metals (including Al), the LDOS at the Fe impurity is dominated by a resonant $3d$ peak, which will be broadened by hybridization with s-p electrons. The existence of a local impurity moment can then be simply understood by using the concept of the virtual bound state introduced by Friedel. Within this model, differences in lattice structure (fcc for Al and hcp for Cd and Zn) are probably less important than the differences in electronic density associated with free-electron-like states of the host, when determining the LDOS and magnetic properties at the impurity site. Recent self-consistent calculations,[21] where the free-electron-like states were introduced using a jellium model, show that the electronic density associated with valence free-electron-like states of the host plays a very important role in the formation of local impurity moments, with lower electronic densities favoring impurity magnetism. The electronic density of the host (defined here as the number of s and p valence electrons per unit volume) is larger in trivalent Al than in divalent Zn and Cd. Therefore, if the simple concept of virtual bound states is used, we find that the tendency towards moment formation should be weaker for Fe in Al than for Fe in Zn or Cd. This has been confirmed by our more accurate RS-LMTO-ASA calculations.

To have a better feeling for the differences between the behavior of the moment at the Fe impurity in trivalent Al and divalent Zn and Cd we have performed non-spin-polarized calculations and obtained the LDOS per spin at the Fermi level $N(E_F)$ for several values of the lattice relaxation. The stability of the impurity moment is usually related[5,14,23] to the local density of states at the Fermi level $N(E_F)$ at the impurity site and the Stoner parameter I through the Stoner-like criterion $I \cdot N(E_F) > 1$. If the result for $N(E_F)$ at the impurity site, obtained in absence of spin polarization, is larger than I^{-1}, the impurity is expected to develop a local magnetic moment. In Fig. 3, we show the non-spin-polarized LDOS for substitutional Fe in Al [Fig. 3(a)], Zn [Fig. 3(b)], and Cd [Fig. 3(c)] for several values of first NN relaxation around the impurity. The horizontal solid line represents the limiting value I^{-1} for the local density of states at the Fermi level $N(E_F)$, above which, according to the Stoner-like criterium, the impurity should develop a local magnetic moment. Here, the LSDA value of 0.068 Ry given by Janak[22] for the Stoner constant I of Fe was used. It is clear from Fig. 3 that the Stoner condition is well satisfied for Zn and Cd hosts in the absence of lattice relaxation around the impurity, but barely satisfied in the case of Al host. As the lattice relaxation is introduded, the resonance gets broader and the value of $N(E_F)$ decreases. In the case of Cd and also Zn, the Stoner condition continues to be satisfied, but for Al it ceases to be fulfilled and the impurity moment vanishes.

Our results indicate that in the case of substitutional Fe impurities in Zn and Cd, the introduction of lattice relaxation has no drastic effect on the magnetic properties, and the local moment at the Fe site remains significantly large for all reasonable values of relaxation around the impurity. The theoretical results indicate that the substitutional Fe impurity in Cd and Zn is magnetic and that the local moments are reasonably large. We suggest that the lack of significant magnetic response observed experimentally in the measured temperature range is due to SF and extremely high T_K values in these systems.

Finally, we should stress that the present calculations are valid for substitutional impurities. Fe is expected to enter substitutionally in the Zn lattice as it does in the case of Mo and Tc, hosts of similar atomic size. The situation is less clear in the case of Cd, which is similar in size to Zr where both substitutional and interstitial Fe sites are known to be occupied. But since Fe atoms in interstitial sites are very compressed, they usually have negative values of the isomer shift IS as observable in the Mössbauer effect. Early Mössbauer data[24] for Fe impurities in Cd and Zn show large positive values for the IS, indicating that the Fe impurity occupies substitutional sites in both hosts. It would be interesting to repeat the experiments using the more modern ''in beam'' techniques to verify whether significant interstitial site occupation could also be present in these hosts.

V. CONCLUSIONS

We have performed electronic structure calculations in order to investigate the magnetic behavior of substitutional

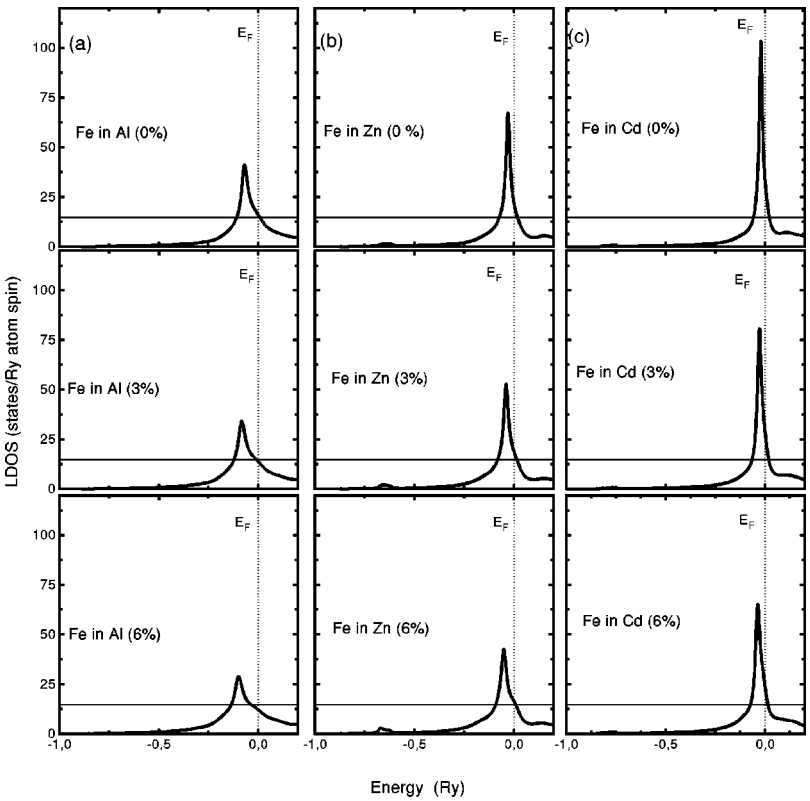

FIG. 3. Non-spin-polarized local density of states obtained using the RS-LMTO-ASA scheme for (a) Fe in Al, (b) Fe in Zn, and (c) Fe in Cd. The results are shown for three diferent values of the radial first-neighbor relaxation towards the impurity. The solid line represents the Stoner-like limit $1/I$ for $N(E_F)$, above which the impurity tends to be magnetic (see text).

Fe impurities in Al, Zn, and Cd as a function of the lattice relaxation around the impurity. We find that for substitutional Fe in Al, the magnetic properties depend strongly on the value of the lattice parameter used for fcc Al. When the theoretical lattice parameter of Ref. 10 is used, the Fe moment vanishes for relaxations of 3.5%, comparable to the value of around 3% obtained by the full potential KKR-GF, which indicates that the Fe impurity in Al is nonmagnetic. But when the experimentally observed value of the lattice parameter of fcc Al is used in the calculations, the impurity moment decreases drastically, but vanishes only for very large values of the assumed relaxation, in excess of 5.5%. These values are not compatible with experiment, indicating that the Fe impurity may retain some moment and that further investigation is needed to rule out the existence of SF with a high T_K in this system.

The introduction of Fe impurities into Cd and Zn presents problems and few experimental results are available. They show no significant magnetic response in the measured temperature range. Our calculations for Zn and Cd indicate that large local moments exist at the substitutional Fe impurity in both hosts and that these moments are not very sensitive to lattice relaxation around the impurity. The moment of Fe in Zn decreases from $2.6\mu_B$ in the absence of relaxation to $2.0\mu_B$ when a relaxation of 6% is assumed. The decrease is even smaller for substitutional Fe in Cd where we find that the moment goes from an unrelaxed value of $2.9\mu_B$ to a value of $2.5\mu_B$ when a relaxation of 6% is included. We conclude that in the case of Zn and Cd hosts, the substitutional Fe impurity should retain its local magnetic moment in the presence of lattice relaxation around the impurity. These results suggest that the lack of significant magnetic response observed experimentally in the measured temperature range is due to SF with high T_K values in these systems. In conclusion, our results indicate that a description in terms of SF and high T_K values is applicable to Fe in Zn and Cd and may also be appropriate to describe Fe impurities in Al.

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