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Theoretical study of hyperfine and local magnetic properties of Co and Fe clusters in fcc Ag hosts

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We study the behavior of the local magnetic moment and hyperfine fields for Fe and Co grains inside the Ag matrix. Our theoretical calculations are used to discuss the experimental results obtained in the literature by NMR and Mössbauer spectroscopy in Co-Ag and Fe-Ag granular systems and we also considered one Fe impurity in the Co clusters in Ag. We use the first-principles real-space linear muffin-tin orbital–atomic-sphere approximation method to calculate the local magnetic moments and the Fermi contact contribution to the hyperfine fields around Fe and Co atoms in different spatial configurations in Ag hosts: isolated impurities, Fe-Fe and Fe-Co dimmers and precipitates containing 13, 19, and 43 atoms. Special attention is given to the differences between central and interface positions of Fe atoms in the two smallest Co clusters. Our results show that the magnetic moments are almost invariant as a function of the local environment for these systems. The local moments at Co atoms inside clusters in Ag have values around $1.8\mu_B$, very close to the observed value for bulk fcc Co. The hyperfine fields of Co and Fe atoms inside the clusters are much larger than those at the atoms considered as isolated impurities. The Fe and Co hyperfine fields at atoms occupying interface positions do not depend on the size of the clusters in Ag and tend to be less intense than those of the atoms at inner sites. This information may help in the evaluation of grain sizes in these systems.

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I. INTRODUCTION

Since giant magnetoresistance (GMR) has been observed in granular materials,[1,2] many attempts have been made to understand and study these systems. Most of this work has been done by experimental investigations making use of different tools, mainly devoted to the characterization of structural, magnetic, and transport properties. Only a few electronic structure calculations of transition-metal magnetic clusters in a nonmagnetic matrix are reported in the literature.[3,4] In these works the complex magnetic behavior of Fe clusters in Cu hosts is investigated. In Ref. 4 local magnetic moments for clusters with 13 and 19 atoms and in Ref. 3 magnetic moments and hyperfine fields of a cluster with 14 Fe atoms are calculated. Due to the lack of periodicity introduced by the grain in the host matrix, the complexity involved in the theoretical calculations has limited considerably the progress from the theoretical side. In the absence of theoretical results, many unconfirmed assumptions are commonly made to interpret the experimental results, especially concerning grain sizes. It is the purpose of this paper to try to address to some of these issues. Experimental results and theoretical models showed that the GMR properties of granular materials are closely related to structural characteristics, as the distance between the magnetic clusters and their sizes, therefore, a detailed description of such materials is required in order to better understand their behavior. In this direction, different measurements of hyperfine properties of Co-Ag granular systems have recently been presented in the literature.[5–11] The advantage of the use of hyperfine interactions techniques is that they can provide information about small clusters and local environments, which other techniques are usually not able to study. The structural evolution due to annealing in sputtered Co/Ag multilayers was analyzed by the distributions of hyperfine fields, obtained using nuclear magnetic resonance (NMR) in Ref. 8. Mössbauer spectroscopy (MS) was used in Refs. 5–7 to study the formation of Co clusters in fcc Ag, and samples produced by different techniques (coevaporation and ion implantation) were analyzed. The observed spectra suggest the presence of Fe atoms as isolated impurities, as dimmers and inside or at the surface of Co clusters. For one set of the analyzed samples, obtained by coevaporation, they have also observed an additional line assumed to be due to internal oxidation. Furthermore, MS was used to study magnetic and structural properties of vapor-quenched Fe-Ag metastable alloys[9,10] and of $(\mathrm{Co}_{70}\mathrm{Fe}_{30})_{36}\mathrm{Ag}_{64}$ heterogeneous alloy.[11] In this last paper the authors suggest that Mössbauer parameters for Fe-Ag and Co-Ag granular materials should not be drastically different.

In the present work we use the real-space (RS) linear muffin-tin orbital (LMTO) formalism, within the atomic-sphere approximation (ASA), to investigate the electronic structure and local magnetic properties of small Fe and Co clusters in fcc Ag hosts. The RS-LMTO-ASA scheme is a first-principles self-consistent approach in the framework of density-functional theory within the local spin-density approximation (LSDA). The main advantage of this method, when dealing with local perturbations, is that the embedding of the defect in the crystal is described correctly, since it can be applied to clusters of several thousands of atoms, avoiding the surface problems which make the embedding so crucial in cluster methods. Because it is implemented directly in the real space, the RS-LMTO-ASA scheme does not require symmetry and is very flexible allowing the study of very complex defects. Another interesting feature is that the computational effort in RS-LMTO-ASA calculations grows lin-

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early with the number of inequivalent atoms. Here we use the RS-LMTO-ASA scheme to obtain local magnetic moments and Fermi contact contributions to the hyperfine fields (HF) for different spatial configurations of Fe and Co atoms in fcc Ag hosts. We have chosen to consider: Fe and Co as isolated impurities; Fe-Fe and Fe-Co dimmers; Fe or Co clusters with 13, 19 or 43 atoms. In all cases Fe or Co were placed as substitutional sites in fcc Ag. As the MS measurements are related to Fe sites, in order to compare our HF results with those presented in the literature, we have considered one Fe impurity in the center of all studied Co grains. For the two smallest Co grains, we have also considered the Fe impurity occupying other positions. Here, we have used a first-principles theoretical approach to study these systems.

The paper is organized as follows: In Sec. II we briefly introduce the RS-LMTO-ASA scheme used here. In Sec. III we show our calculated values and compare them to existing experimental results in the literature. Finally, in Sec. IV, we summarize our conclusions.

II. THEORETICAL APPROACH

In this section, we briefly present the RS-LMTO-ASA method and how it can be applied to the calculation of HF. This scheme has already been used with success in the study of local magnetic moments and hyperfine quantities for different transition-metal systems with local defects as substitutional or interstitial impurities and sets of substitutional impurities, sometimes in the presence of lattice relaxation.[13,14,12,15]

The first-principles and self-consistent RS-LMTO-ASA approach is based on the well-known LMTO-ASA formalism[16,17] and uses the recursion method.[18] 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 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. As in the regular LMTO-ASA formalism, we use the ASA 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, usually 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 neglect. These approximations result in a ''tight-binding'' Hamiltonian and an orthogonal basis, yielding a simple eingenvalue problem which can be directly solved in real space with the aid of the recursion method. Since it is implemented in real space, the RS-LMTO-ASA does not require periodicity and it can be used to treat interstitial or substitutional impurities, precipitates or other defects, and lattice relaxation can be easily introduced even in noncubic systems. We note that all inequivalent sites must be considered. The RS-LMTO-ASA can, in fact, be described as a composition of two self-consistent processes, namely the ''general'' and ''atomic'' parts, one inside the other. In the ''general'' process, given the so-called ''potential parameters'' for all inequivalent sites, the Hamiltonian of the system under study is built up and the eigenvalue problem is solved. In the atomic part, the potential parameters, for each inequivalent site, are calculated. In a periodic metallic system, the Fermi energy (E_F) is determined at each iteration by filling the bands with the correct number of valence electrons. In the case of impurities, the E_F of the system is fixed by the E_F of the host. We calculate the occupation and other moments of the density of states for all nonequivalent sites up to the fixed E_F, keeping the ''potential parameters'' of the rest of the system (outside the perturbed region) at the bulk values. The size of the perturbed region, which varies from system to system, needs to be tested in each case and it is chosen accordingly to give the correct embedding. Here, as usually done, we have used a minimum basis set of nine valence orbitals $(1s,\ 3p,$ and $5d)$ per spin at each site and the core states were not frozen. A more detailed description of the general procedure can be found elsewhere.[19]

The procedure used here for calculating the HF at each site, after the self-consistent electronic structure for a given system is obtained, has been described in detail in previous papers.[12,20–22] As shown in the literature, the hyperfine field for transition metals is usually dominated by the Fermi contact contribution. In a nonrelativistic approach this contribution can be determined by the magnetization density at the nuclear position R through the expression:

$$HF=\frac{8\pi}{3}[\rho^{\uparrow}(0)-\rho^{\downarrow}(0)]\mu_B. \tag{1}$$

Here $\rho^\sigma(r)$ is the electronic charge density per spin and we assume that near the nucleus it can be written as a polynomial expansion:

$$\rho^\sigma(r)=A+Br+Cr^2. \tag{2}$$

We note that in a nonrelativistic approach only the s (core and valence) orbitals contribute to the HF.

III. RESULTS AND DISCUSSION

In the present work we have chosen to study the following systems embedded in fcc Ag: (a) one isolated impurity of Fe or Co, (b) Fe-Fe and Fe-Co dimmers, and (c) spherical clusters composed by a central atom and one, two or three first shells of neighbors (13, 19 or 43 atoms, respectively) . In all these cases, the Fe and Co atoms occupy substitutional positions in fcc Ag hosts. The systems with embedding clusters will be labeled by the number of Fe and Co atoms they contain. Just for a rough comparison, if we estimate the size of these clusters considering them as spheres with the corresponding volumes occupied by the Co and Fe atomic spheres, the clusters studied here would have diameters 7.5, 8.5, and 11 Å , respectively. To calculate the local density of states we used the Beer-Pettifor terminator,[23] and we have taken a cutoff parameter $LL=20$ in the recursion chain. We performed nonrelativistic calculations with an exchange-correlation term of the form proposed by von Barth and Hedin.[24] In all cases, the defects are placed in substitutional positions around the central region of a cluster with 3078 atoms, in a fcc arrangement, with lattice parameter $a_0=4.07$ Å .

We have estimated the influence of lattice relaxation effects on our results. In order to do that, we have calculated

TABLE I. Local magnetic moments (μ_B) and hyperfine fields (T) at the Fe sites for isolated impurity, Fe-Fe dimmer, Fe_{13}, Fe_{19}, and Fe_{43} clusters. The nonequivalent sites in a given system, are identified by an index indicating the neighborhood (from the position labeled by 0) where that atom is placed, in a fcc Ag host.

System	Site	μ	HF
Fe	0	3.07	−10.9
Fe-Fe	0	2.92	−13.6
Fe_{13}	0	2.86	−34.0
	1	2.94	−22.4
Fe_{19}	0	2.90	−33.9
	1	2.92	−27.7
	2	2.96	−23.5
Fe_{43}	0	2.88	−37.2
	1	2.87	−35.5
	2	2.88	−30.0
	3	2.91	−22.6

the system with 12 Co and one Fe in the central position decreasing in 10% the distance between the central atom and its nearest neighbors (NN). The changes that we have found in the absolute values of the magnetic moments are less than $0.2\mu_B$ and are about 4 T for the HF. However, as for all atoms the variations were in the same direction, the general trends and the comparative behavior remained unchanged. Experimental results from the literature suggests a difference smaller than 2 T in HF of Co atoms due to strain effects in Co-Ag systems,[8] which is smaller than the inaccuracy of our calculations due to the LSDA.[25] Therefore, in order to simplify our calculations, we neglect relaxation effects in the following discussion.

A. Fe clusters

Our results for local magnetic moments and hyperfine fields for one isolated Fe impurity, Fe-Fe dimmer, and Fe clusters in fcc Ag are presented in Table I. As all atoms in the same shell are equivalent, the nonequivalent sites of the clusters will be identified by the index of its neighborhood with respect to a chosen central position, which will be denoted by 0 as the 0th shell.

From Table I, we see that the local magnetic moments at Fe sites in these systems are all very similar, all of them with a value around $3\mu_B$. The isolated impurity has the highest moment, of $3.07\mu_B$, and when the dimmer is formed it decreases by $0.15\mu_B$. Our value for the local moment at an isolated impurity can be compared to previous results in the literature. Using the Korringa-Kohn-Rostoker Green-function method, Papanikolaou *et al.* have obtained a local moment of $3.06\mu_B$ for Fe in Ag,[26] in an excellent agreement with our results. For the Fe clusters in Ag, we can see from Table I that atoms placed at inside positions have local moments smaller than those at the interface (largest shell index at each system). The Fe atoms at the interface tend to have local moments close to the value found for the dimmer. Also, the difference between the local moments for Fe atoms at inside and interface positions tends to be slightly smaller as the size of the cluster increases. This can be seen by comparing the values $0.08\mu_B$, $0.06\mu_B$, and $0.03\mu_B$ observed, respectively, for Fe_{13}, Fe_{19}, and Fe_{43}. The values we found for Fe atoms in the Fe_{19} cluster show a decrease in the local moments for inner sites (closed to the 0 site), and inside the Fe_{43} cluster they are almost equal, oscillating between $2.88\mu_B$ and $2.87\mu_B$, while the atoms at the interface have moments of $2.91\mu_B$. This behavior indicates that the local moments for atoms inside the clusters tend to be equal and the moments at the interface sites slightly larger than those, but these differences are very small.

The calculated HF at an isolated Fe impurity in Ag is also presented in Table I. This value of −10.9 T disagrees with the experimental values in the literature, −3.6 T (Ref. 27) and −1.2 T,[28] but is very similar to the value −10 T from another theoretical calculation.[29] Part of this discrepancy can be attributed to a well-known failure of the LSDA to describe correctly the electronic behavior in the core region where the *s* electrons contribute to the HF. Without employing a fully relativistic treatment we are also neglecting other contributions to the hyperfine field. We note however that the discrepancy between measured and calculated HF in the case of a single Fe impurity in Ag is far beyond the usual errors. This suggests that this is due to a specially complex magnetic situation that can be destroyed otherwise. Nevertheless, although absolute HF values are expected to have a relatively large uncertainty, due to a cancellation of errors in the present case, we still can compare relative values for the HF at different sites with measurements. We note, however, that one should be careful when adopting this kind of procedure, since a cancellation of errors as a rule is not expected to be held. Despite that fact, the results for the clusters show a much better agreement with the experiments. In Ref. 9 the Mössbauer spectra for $Ag_{1-x}Fe_x$ indicated average HF's from 21 to 33 T when the Fe concentration ranged from 0.2 to 0.8. This shows that the presence of other Fe atoms and the enlargement of the precipitates increases the intensities of the HF. Our theoretical results shown at Table I presents exactly the same trend. Comparing our results for each Fe system we can see a strong growth in the intensity of the HF from the case of the isolated impurity and dimmer to the grains, and a minor enhancement when we compare interface and inner sites. We should note that these differences in magnitude of the HF's are certainly beyond the intrinsic LSDA theoretical errors (mentioned above) thus allowing the present analysis. We also note that the behavior of the HF's goes in the opposite direction of the small changes observed in the local moments. We can also see that the sites at the interfaces have similar HF's around 23 T for all three clusters.

B. Co clusters with Fe impurities

The systems with Co clusters we have studied are formed by 12, 18 or 42 Co atoms plus one Fe impurity as substitutional clusters inside fcc Ag. The spatial configurations we have considered were (a) the Fe atom at the central position in all cases, (b) the Fe atom at the interface of the grain for the 13-atom cluster, and (c) the Fe atom in the first and in the second NN shell of the central position for the 19-atom cluster. As before, we name 0 the central position of the Co cluster that can be occupied by Co or Fe atoms. We have also calculated one Co as an isolated impurity and the Fe-Co

TABLE II. Local magnetic moments (μ_B) and hyperfine fields (T) at the Fe sites for one Fe plus a Co cluster in fcc Ag hosts. The systems system are identified by the number of Co atoms in the cluster and by the neighborhood (from the position labeled by 0) where the Fe atom is placed (see text).

System	μ	HF
Fe-Co	2.97	-12.6
Fe^0Co_{12}	3.07	-25.4
Fe^1Co_{12}	3.06	-18.1
Fe^0Co_{18}	3.05	-24.4
Fe^1Co_{18}	3.05	-21.6
Fe^2Co_{18}	3.05	-17.4
Fe^0Co_{42}	2.98	-26.0

dimmer. The notation we will establish here is as follows: we name Fe^nCo_{12}, Fe^nCo_{18}, and Fe^nCo_{42} the clusters with 12, 18, and 42 Co atoms respectively, where the index n denotes the shell where the single Fe impurity was placed. If the Fe atom is in the center, all Co atoms in a given neighboring shell will be equivalent, and we will call Co^n one atom in the Fe nth neighborhood. If the Fe impurity is placed at any other position, this special symmetry is broken and we have more than one nonequivalent Co atom in each shell of neighbors of the central atom. In these cases, we will use two indexes to denote this site: a first index that, as before, denotes the neighborhood where the atom is placed related to the central site; one additional alphabetic index which increases with the distance to the Fe impurity that indicates the different sites in the same nearest-neighbor shell of the central site.

Our results for the local magnetic moments and HF at the Fe sites for the Fe-Co dimmer and for clusters with the Fe surrounded by Co in fcc Ag hosts are present in Table II. From these results we see that in all studied situations the local magnetic moments at the Fe sites have values around $3\mu_B$. We note that this reflects the fact that the majority band is almost full and the minority band is almost empty, so the local moment is saturated. Concerning the HF values for this type of granular systems, the experimental results found in the literature[6,7] suggest values of around -31 T for Fe atoms inside the cluster and values in the range between -25.3 and -29.0 T for atoms at their surfaces. They also suggest that the HF should be more intense for larger clusters. Our results presented at Table II show that the HF's at the central Fe atoms (Fe^0) have almost the same magnitude (around -25 T) in the three Co clusters. So, contrary to the experimental assumption, we see no indication that they become more intense for larger clusters. In the clusters with 12 and 18 Co (plus one Fe) shown at Table II the ratios of the Fe HF at surface atoms (atoms with the largest numerical index in each system) to the Fe HF at the central atom are 0.7 and 0.9, respectively. These results are in excellent agreement with the suggested ratio in the range 0.8–0.9 inferred from the experiments mentioned above. So, although we cannot predict with precision the exact magnitudes of the HF's, our theoretical results clearly indicate the tendency of a decrease in the HF magnitudes for Fe atoms near the interfaces of the clusters, but with values almost independent of the size of the grains.

TABLE III. Total magnetization and average Co local magnetic moments in the clusters, in μ_B units.

System	Total	Average
Fe^0Co_{12}	28.90	1.82
Fe^1Co_{12}	24.98	1.83
Fe^0Co_{18}	35.81	1.82
Fe^1Co_{18}	35.46	1.80
Fe^2Co_{18}	35.25	1.79
Fe^0Co_{42}	77.56	1.78

In Table III we show our results for the average Co local magnetic moments in the situations we have studied and the corresponding total magnetization. We have found average moments of around $1.8\mu_B$ for the Co atoms in the clusters, with a very small decrease when the cluster is made larger. In Table IV we present our results for local magnetic moments at each Co site in the Fe-Co, Fe^nCo_{12}, Fe^nCo_{19}, and Fe^nCo_{42} systems. The results for an isolated Co impurity is also shown. This value is in excellent agreement with previ-

TABLE IV. Local magnetic moments (μ_B) and hyperfine fields (T) at the Co sites for isolated Co impurity and Co clusters with one Fe impurity in fcc Ag hosts. The nonequivalent sites in a given system are identified by an index indicating the neighborhood (from the position labeled by 0) where that atom is placed and, when necessary, an extra alphabetical index indicating the distance to the Fe impurity, in a fcc Ag host (see text).

System	Site	μ	HF
Co	0	1.66	-6.6
Fe-Co	1	1.52	-10.5
Fe^0Co_{12}	1	1.82	-15.4
Fe^1Co_{12}	0	1.91	-22.9
	1*a*	1.80	-15.5
	1*b*	1.83	-14.5
	1*c*	1.83	-14.5
	1*d*	1.83	-14.5
Fe^0Co_{18}	1	1.83	-18.7
	2	1.80	-15.5
Fe^1Co_{18}	0	1.90	-21.9
	1*a*	1.83	-18.6
	1*b*	1.84	-17.5
	1*c*	1.85	-17.5
	1*d*	1.85	-17.3
	2*a*	1.78	-16.1
	2*b*	1.72	-15.8
	2*c*	1.63	-14.7
Fe^2Co_{18}	0	1.93	-21.2
	1*a*	1.83	-18.6
	1*b*	1.85	-17.4
	1*c*	1.84	-16.9
	2*a*	1.64	-14.9
	2*b*	1.63	-15.0
Fe^0Co_{42}	1	1.88	-22.9
	2	1.83	-19.7
	3	1.71	-15.2

ous theoretical results in the literature.[26] Comparing the single impurity with the Fe-Co dimmer we see that the local moment at a single Co atom is slightly reduced by the presence of a neighboring Fe atom. We also see that the local magnetic moments at the Co atoms in the central positions are about $1.9\mu_B$. For atoms at the surface (again denoted by the highest numerical index in each system) it becomes slightly smaller, approaching the local moment value for the isolated impurity. We note that they differ in less than $0.3\mu_B$ and the differences are more considerable between sites in different shells than between different sites in the same shell. This is due to the fact that Co atoms belonging to different NN shells can have more Ag atoms in their neighborhood and thus have a more perturbed environment. In the case of different sites in a given shell we are just replacing a Co by a Fe atom. Since Fe atoms are more similar to Co than to Ag atoms the band structure and, as a consequence, the local moment is less perturbed in this case.

In order to evaluate the Co grains sizes in measured granular systems, it is a common practice to assume that the local magnetic moment of each Co atom in the sample has the same value as the bulk fcc Co.[11,30] In Ref. 30 the value used was $1.77\mu_B$. The magnitude and the small sensibility of the average local moments shown at Table III, as well as the individual values presented at Table IV, supports this assumption used in the literature to evaluate the Co grain sizes.

The NMR spectra for Co-Ag granular materials reported in Ref. 8 shows distributions of HF's with two peaks. The first is around -17.5 T and the second near -21.6 T, which are related to Co atoms inside and at the grain boundary. Our results for the HF at central Co atoms are around -22 T as can be seen from Table IV. For the 13-atoms cluster this value is -22.9 T and for the two clusters with 19 atoms (where the Fe impurity is placed at the first and at the second NN shell of the central site, the HF's at the central Co are -21.9 and -21.2 T, respectively. For Co atoms at the surfaces of the clusters the HF's are in all calculated cases around -15 T. In the clusters with 13 atoms, this value is in the range between -15.5 and -14.5 T. The Co sites at the surfaces of the 19-atom clusters (placed at the second neighboring shell of the central site) have HF's in the range between -16.1 and -14.7 T. Finally, the Co atoms at the surface of the cluster with 43 atoms (with the Fe impurity in the center) have a HF of -15.2 T. These HF results reproduces very well the experimental observations for both grain boundary and internal atoms in Co-Ag granular systems. Moreover, we note that the influence of the Fe atoms on the Co HF's seems to be a weak enlargement of the intensities, as Co atoms in a same shell but with different distances from the impurity have similar HF values, differing by less than 2T, and being more negative when the Fe impurity is closer.

The behavior of the HF at the Co sites is similar to that observed for Fe sites. Both are dependent on the position relative to the interface. We have observed that the HF at an isolated impurity is sensibly weaker than at the dimmer and at the sites in the clusters. This means that the HF at a given site tend to be stronger when there are more magnetic atoms in its neighborhood and, therefore, when the atom is in an inner position of the magnetic cluster. Comparing the HF values at Fe sites in the Fe dimmer and in the Fe-Co dimmer and also comparing the HF's at Fe sites in Fe clusters and clusters with the Fe surrounded by Co, we found that when Fe atoms of the environment are replaced by Co atoms, the Fe HF becomes smaller. However, the general trends of the HF behavior for Fe in Fe and Co grains are similar.

IV. CONCLUSIONS

We have studied the magnetic and hyperfine behavior for small Co and Fe substitutional clusters in fcc Ag from a local point of view. Our theoretical results for Co-Ag granular systems are in agreement with the suggestion based on measurements, found in the literature, that the local magnetic moments at Co sites are almost independent of the position occupied by the atom. We note, however, that small changes were observed. We have found a similar behavior for Fe clusters and for Fe impurities in Co clusters. The presence of a Co neighbor increases the local magnetic moment at another Co atom but does not sensibly affect the local moment at a Fe site.

We have theoretically supported the HF trends inferred from measurements present in the literature. For all studied clusters we observed an increase in the magnitudes of the HF's at inner sites and at interface positions the HF's were found to be almost independent of the size of the clusters. In addition we found that the Fe HF becomes smaller when Fe atoms from neighboring shells are replaced by Co atoms. However, the general trends of the HF behavior for Fe in Fe and Co grains are similar.

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