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Structural ordering and magnetic properties of arc-melted FeGa alloys

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Abstract

X-ray diffraction, Mössbauer spectrometry and magnetic properties have been performed on FeGa arc-melted binary alloys in order to study the compositional dependence of the structural ordering and magnetic properties of these alloys. The average magnetic hyperfine field at 300 K decreases with increasing Ga content as does the average magnetic moment per Fe atom and a linear dependence between both quantities is found for Ga content up to 20 at. %. The substitution of Fe by Ga atoms increases the lattice parameter and causes a change in the order of the crystal structure that has been modelled using a binomial distribution method. The effect of Ga atoms as near neighbours of Fe on the average magnetic hyperfine field is evaluated.

Keywords: A-Magnetic intermetallics, B-Magnetic properties, B-Order/disorder transformations, F-Mössbauer spectroscopy

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1. Introduction

FeGa alloys have attracted great attention in the last few years due to their superior magnetostrictive properties at low saturation field [1-4]. This quality associated with their high mechanical strengh, good ductility, negligible magnetic hysteresis and low cost [5] makes these materials very promising for sensor and actuator applications.

Recent investigations include the study of the influence of the thermal history and the structural ordering on their magnetostriction [6,7], the phase equilibria and stability of ordered bcc phases in the Fe-rich portion of the FeGa system [8] and the structural transformations in quenched FeGa alloys [9]. Moreover, recently it was found that the addition of Cu to $Fe_{65.5}Cr_4Mo_4Ga_4P_{12}C_5B_{5.5}$ amorphous alloy produces a nanocrystalline microstructure consistent of FeGa nanocrystals embedded in an amorphous matrix [10]. These nanocrystalline alloys are interesting since they would combine a large glass-forming ability with good soft magnetic properties.

However, a Mössbauer study of the FeGa alloy series is still missing. The importance of this study is double. On one hand, structure determination of FeGa alloys by X-ray diffraction is troublesome due to the similarity in the atomic scattering factors of Fe and Ga atoms which results in superlattice reflections of very low intensity. For example, the intensity of the strongest superlattice reflection associated with DO_3 long-range order is calculated to be only 0.6% of the strongest primary reflection. Mössbauer spectrometry, as a short range order sensitive technique, does allow distinguishing between ordered and disordered atomic structures. For nanocrystalline alloys and due to the complexity of their magnetic hyperfine structure, the characterization of the hyperfine parameters of FeGa crystals becomes an essential information.

In the present work, arc-melted polycrystalline $Fe_{100-y}Ga_y$ (y=5, 10, 20 and 25) alloys were prepared in order to study variations in the atomic short range order at room

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temperature with substitution of Fe by Ga. A local model based on a binomial distribution method [11] was used in order to correlate the magnetic hyperfine parameters with the structural ordering of these alloys. The influence of Ga substitution for Fe on the lattice parameter, saturation magnetization, magnetic moment and Curie temperature of these alloys is also reported. The interest of this study is focused in demonstrating that Mössbauer technique is able to supply detailed quantitative data for the structural ordering of such systems as Fe-Ga binary alloy where conventional X-ray diffraction techniques can not resolve an ordered structure due to the similarity between the scattering factors of its constituents.

2. Experimental

$Fe_{100-y}Ga_y$ (y = 5, 10, 20 and 25 at. %) alloys were prepared by arc-melting from pure Fe (99.95%) and Ga (99.999%) in an Edmund-Bühler high vacuum arc-melting system. The arc-melted bottoms (~2 cm diameter and ~0.8 mm thick) were remelted several times to get homogeneous samples.

X-ray diffraction (XRD) patterns were recorded at room temperature using a Brucker AXS D8-Advance diffractometer with Cu K_α radiation on slices ~100 μm thick cut from the bulk samples.

For thermomagnetic (TMG) experiments, the magnetic field of a small magnet (~20 mT) was applied to the sample and the temperature variation of the magnetic force was recorded in a thermobalance (Perkin-Elmer TGA-7) as an apparent weight change of the sample. The Curie temperature, T_C, was determined from low field magnetization curves, by the "kink point" method.

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The saturation magnetization, M_s, was measured on samples ~5 mg at room temperature with a Lakeshore 7407 vibrating sample magnetometer (VSM), using a maximum applied field of 15 kOe.

Mössbauer spectra on the same samples studied by XRD were taken at 300 K in a transmission geometry using a ^{57}Co(Rh) source, with the γ-beam perpendicular to the ribbon plane. The values of the hyperfine parameters were refined using NORMOS [12] and MOSFIT programs [13]. The isomer shift values are quoted relative to α-Fe at 300 K.

3. Results

3.1 X-ray diffraction

X-ray diffractograms of as-cast samples show that the substitution of Fe by Ga shifts the position of diffraction lines corresponding to bcc phase of pure α-Fe to smaller values of 2θ. Figure 1a shows, as an example, the XRD pattern of $Fe_{75}Ga_{25}$ alloy. The increase of the lattice parameter, *a*, caused by Ga addition can be expressed by (Fig. 1b):

$$a = 0.2869(2) + 0.00020(1)y \qquad \text{[nm]} \qquad (1)$$

where *y* is the Ga content (at. %) of the alloy. Additional weak reflections due to the possible occurrence of DO_3 ordering of the structure are not detected. In fact, as it was said above, the similarity between the atomic scattering factors of Fe and Ga makes this detection difficult, unlike for FeSi alloys.

3.2 Magnetic properties

The saturation magnetization, M_S, at 300 K, shows a linear dependence with the Ga content, *y*, up to 20 at. % Ga (see Fig. 2a.), that can be expressed by:

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$$M_S = 223(6) - 3.0(5)y \qquad \text{[emu/g]} \qquad (2)$$

The average magnetic moment per Fe atom, $<\mu_{Fe}>$, decreases as the Fe content decreases (Fig. 2b). A linear dependence of $<\mu_{Fe}>$ with y is observed for Ga content up to 20 %, that can be given by:

$$< \mu_{Fe} >= 2.24(3) - 0.004(3)y \qquad [\mu_B] \qquad (3)$$

The different behaviour of M_S and $<\mu_{Fe}>$ below and above y = 20 at. % suggests a change in the structural ordering of the binary alloy.

The Curie temperature, T_C, of the arc-melted alloys decreases monotonously with the Ga content of the alloy as can be observed in Fig. 2c.

3.3 Mössbauer spectrometry

Fig. 3 shows Mössbauer spectra of the studied alloys recorded at room temperature. The hyperfine structure is strongly dependent on Ga content. For $y \leq 20$ at. % a six line pattern is observed, with increasing line widths as the Ga content of the alloy increases. The Mössbauer spectrum corresponding to $Fe_{75}Ga_{25}$ alloy is qualitatively different to those of alloys with lower Ga content, exhibiting additional and sharper lines that suggest some structural change.

The fitting of the spectra was first tried using several independent sextets with free width but only the spectrum corresponding to the alloy with 5 at.% Ga could be satisfactorily fitted using this model. Neither the spectrum of the 25 at.% Ga could be clearly decomposed into two components with proportions 3:1, as could be expected for a stoichiometric Fe_3Ga with a DO_3 structure.

The best fitting of the spectra was attained using a discrete magnetic hyperfine field distribution (HFD) with a linear correlation between the magnetic hyperfine field and the isomer shift of the components of the distribution in order to reproduce the

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asymmetrical shape of the spectra [14]. The quadrupolar splitting was averaged to zero. The obtained HFDs are shown in Fig. 3 (right hand side).

HFDs corresponding to y = 5 and 10 at. % Ga range from 25 to 36 T and show no significant differences: only a small shift of the maximum from 32 T to 31.5 T and a small increase in the width of the distribution from 3.5 T to 4.6 T (for a Gaussian fitting) with increasing Ga content. For y = 20 at. % Ga alloy, the HFD corresponds to a much broader six-line pattern spectrum and ranges from 18 to 36 T with a main maximum at 30.5 T and a shoulder at 21.5 T. The magnetic hyperfine field distribution of $Fe_{75}Ga_{25}$ alloy, that ranges from 16 to 36 T, consists of two clear maxima, labelled as "a" and "b" in Fig. 3, centred at 20 T and 30.5 T and with fraction areas of 0.54 and 0.46, respectively. For a correct fitting of the spectrum it was necessary to add a number of components with magnetic hyperfine fields ranging from 1.5 to 16 T (~ 4 % of the total Fe atoms).

The average magnetic hyperfine field at 300 K decreases with increasing Ga content (Fig. 4a) as does the average magnetic moment per Fe atom, and a linear dependence between these two quantities is found for Ga content ≤ 20 at. % (Fig. 4c).

The decrease of $<B_{hf}>$ with y, for y up to 20 at. %, can be expressed by a linear relation:

$$< B_{hf} >= 33.1(3) - 0.23(2)y \qquad \text{[T]} \qquad (4)$$

The value of $<B_{hf}>$ at y = 0 at. % of Ga is in agreement with the expected value of B_{hf} for pure α-Fe phase at room temperature, 33.0 T. For comparison, Fig.4a also shows the compositional dependence of $<B_{hf}>$ for FeAl [15] and FeSi [16] alloys. A discontinuous jump at 20 at.% metalloid is encountered for FeGa and FeAl alloys, but this jump is not so clear for FeSi alloys.

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The average isomer shift (Fig. 4b) increases linearly with Ga content up to 20 at.% Ga following the relation:

$$< IS >= -0.003(5) + 0.0070(5)y \qquad \text{[mm/s]} \qquad (5)$$

The angle θ, defined by the direction of the magnetic hyperfine field and the propagation direction of the γ rays, can be obtained from the intensities of the second and the third absorption lines of the spectra. For the present alloys, a value of around 55 º reveals the absence of texture of magnetic moments for all alloys.

4. Local order modelling

Using a binomial distribution, the probability, P_{nm}, of a bcc environment with *n* Ga atoms as near neighbours (NN), in the first shell, and *m* Ga atoms as next near neighbours (NNN), in the second shell is given by the expression:

$$P_{nm} = M\left[x_{Ga}^{(NN)}\right]^{n}\left[x_{Ga}^{(NNN)}\right]^{m}\left[x_{Fe}^{(NN)}\right]^{8-n}\left[x_{Fe}^{(NNN)}\right]^{6-m} \qquad (6)$$

where $x_U^{(NN)}$ and $x_U^{(NNN)}$ are the concentration of U atoms (Ga or Fe) in the set of 8 NN atoms of the first shell and in the set of 6 NNN atoms of the second shell, respectively, that surrounds the central Fe atom. The multiplicity, M, can be calculated as:

$$M = \frac{8!}{(8-n)!\,n!}\cdot\frac{6!}{(6-m)!\,m!} \qquad (7)$$

However, the composition of the neighbourhood of the Fe atoms must be strongly affected, not only by the global composition, but also by the ordering of the crystalline structure. In a fully disordered A2 structure, the Ga and Fe positions are indistinguishable and their distribution would be random. Therefore, the atomic composition of the first and second shells is the same, x_{Fe} and x_{Ga}, for Fe and Ga atoms, respectively. However, it is important to note that using Mössbauer spectrometry (MS), from the 15 atoms (one central surrounded by 8 as NN and 6 as NNN) which are probed

and form the cluster unit, the central one is forced to be a Fe atom. Therefore, the probabilities for finding a Fe atom or a Ga atom in the neighbourhood of the probe are modified with respect to the global composition ($Fe_{100-y}Ga_y$, with x_{Fe} = (100-y)/100, x_{Ga} = y/100). In fact, the average number of Fe atoms in a group of 15 is $15x_{Fe}$ and the average number of Ga atoms is $15x_{Ga}$. Taking into account that the central probe is a Fe atom, the average number of Fe atoms in the 8 NN plus 6 NNN will be $15x_{Fe}$-1 and, thus, the corrected Fe concentration, $x_{Fe}^{cor} = (15x_{Fe} - 1)/14$, in the NN plus NNN environment is decreased with respect to the global value, and the corrected Ga concentration, $x_{Ga}^{cor} = 15x_{Ga}/14$, is enhanced with respect to its global concentration in the alloy.

In the case of ordered structures, the positions of Ga and Fe atoms in the elementary cell are distinguishable. For a perfect ordered DO_3 structure, only possible for an alloy composition of $Fe_{75}Ga_{25}$, a Ga atom is always surrounded by 8 Fe atoms as NN and 6 Fe atoms as NNN, but for Fe atoms, two different sites are present; namely, 1/3 of the Fe atoms have 8 Fe atoms as NN and 6 Ga atoms as NNN (D site) and 2/3 have 4 Fe and 4 Ga atoms as NN and 6 Fe atoms as NNN (A site). (Table 1).

For alloy compositions $Fe_{100-y}Ga_y$ with y < 25 at. %, there is no possibility for a perfect ordered structure as the number of Fe atoms is in excess and the number of Ga atoms is less than the needed. Therefore, we assume a “maximum ordered” structure in which Ga atoms will be always located in their correct sites and the Ga sites which can not be occupied by Ga atoms will be filled with the exceeding Fe atoms. Thus, “maximum ordered” structure implies that a Fe site will never be occupied by a Ga atom but some Ga sites will be occupied by Fe atoms, resulting three different sites for Fe (Table 1): A and D sites, which are correct Fe sites, and Ga sites occupied by Fe

atoms. The distribution of the 100-*y* Fe atoms will be as follows: 50 will be in A sites, 25 in D sites and 25-y Fe atoms will be substituting Ga atoms.

Each Fe atom in an A site in a perfect ordered DO_3 structure has 4 Ga atoms as NN but for a Ga content lower than 25 at. %, a Fe atom in an A site could have 4, 3, 2, 1 or 0 Ga atoms as NN. Analogously, the possible configurations for a Fe atom in a D site ranges from 6 to 0 Ga atoms as NNN. Finally, a Fe atom in a "Ga atom-site" will always have 0 Ga atoms as NN and 0 Ga atoms as NNN (Table 1).

Taking into account the previous considerations to obtain the concentration of Fe and Ga atoms in the NN and NNN sets of atoms, the probabilities of the different configurations can be calculated using equation (6). The results for disordered and ordered structures are shown in figures 5 and 6, respectively.

5. Discussion

(a) Alloys with low Ga content (≤10 at. %)

Assuming the effect of the Ga atoms on the magnetic hyperfine field to be proportional to the number of Ga atoms in the first shell, *n*, and the number of Ga atoms in the second shell, *m*, the average magnetic hyperfine field can be expressed by:

$$< B_{hf} >= 33 - \sum_{n,m} P_{nm} n \cdot q - \sum_{n,m} P_{nm} m \cdot r \qquad [\mathrm{T}] \qquad (8)$$

where *q* and *r* are the reduction of B_{hf} per Ga atom in the first and the second shell, respectively. The linearity between the reduction of B_{hf} and the number of Ga atoms as NN (or NNN) yielding to *q* (or *r*) is not a strong hypothesis for low Ga containing alloys (expected to be in a disordered structure) as the most probable configurations are those of 0, 1 or 2 Ga atoms as NN or NNN (Fig. 5). For fully disordered systems, the relationships between both $P_{nm}n$ and $P_{nm}m$ with *y* are linear (Fig. 7). Therefore, from equations (4) and (8) it is possible to obtain:

$$q + 0.75r = 2.3 \qquad [T] \qquad (9)$$

It should be remembered that expression (9) has been obtained for compositions for which the most probable environments correspond to n=0, 1 and 2 atoms of Ga.

b) $Fe_{75}Ga_{25}$ alloy

A perfect ordered DO_3 structure (Table 1) cannot explain the fraction areas obtained for the maxima labeled as "a" and "b" of the magnetic hyperfine field distribution of $Fe_{75}Ga_{25}$ alloy (Fig. 3), as the probabilities for the only two possible Fe sites are 2/3 for an A site and 1/3 for a D site.

However, a simple model can explain the experimental values of the fraction areas: 0.54 for peak "a" and 0.46 for peak "b". Let us consider three types of Fe sites: A*, D* and Fe in Ga atoms sites. If Ga and Fe atoms which are not in their correct position were randomly interchanged, the ratio between the populations of A* and D* sites occupied by Fe atoms would remain the same as that of A and D sites in the perfect ordered structure (2:1). From the experimental fraction areas of the peaks, the only possible choice is to assign the whole peak "a", at ~20 T, to A* sites (54 %) and the peak "b", at ~30.5 T, to both D* sites (a half of the number of Fe atoms in A sites, 27 %) and some Fe in Ga sites (the rest of Fe atoms, 19 %). Then, it is possible to calculate a degree of order for our $Fe_{75}Ga_{25}$ alloy. If a statistical set of 100 atoms is considered, 75 atoms of them will be Fe atoms, of which 40.5 will be in A sites, 20.25 in D sites and 14.25 in Ga sites; and 25 atoms will be Ga atoms, of which 14.25 will occupy Fe sites and 10.75 will remain in Ga sites. Therefore, 71.5 % of the atoms are in ordered positions, which can be considered as the degree of order of the system. Although this order parameter is straightforward from the discussion above (the percentage of atoms which are in ordered positions), a comparison with standard parameters will be helpful. An extended model of the Bragg-William-Gorsky model

proposed by Inden [17] yields a description of the atomic distributions in binary bcc solid solutions taking into account nearest and next nearest neighbours. The bcc lattice is divided in four fcc lattices (I, II, III and IV) with a lattice parameter which is double of that of the bcc lattice. In a perfect ordered DO_3 structure, I and II lattices corresponds to the A sites of Fe, the III lattice to the Ga sites and the IV lattice to the D sites of Fe. Any atomic configuration (disordered A2, ordered B2 or ordered DO_3 structures) can be described using three independent parameters [17]:

$$\begin{aligned} X &= \frac{1}{4}\left(p_{Fe}^{I} + p_{Fe}^{II} - p_{Fe}^{III} - p_{Fe}^{IV} \right) \\ Y &= \frac{1}{2}\left(p_{Fe}^{III} - p_{Fe}^{IV} \right) \\ Z &= \frac{1}{4}\left(p_{Fe}^{I} - p_{Fe}^{II} \right) \end{aligned} \tag{10}$$

where p_{Fe}^{L} is the occupation probability of Fe in the lattice L. Therefore, for a disordered A2 structure, X = Y = Z = 0; for an ordered B2 structure $X \neq 0$ and Y = Z = 0 and, for a perfect ordered DO_3 structure ($p_{Fe}^{A\,site}$=2/3, $p_{Fe}^{D\,site}$=1/3 and $p_{Fe}^{Ga\,site}$=0), X = 1/12, Y = -1/6 and Z = 0. In the studied case, X, Y and Z would be:

$$\begin{aligned} X &= \frac{1}{4}\left(p_{Fe}^{A\,site} - p_{Fe}^{Ga\,site} - p_{Fe}^{D\,site} \right) = 0.02 \\ Y &= \frac{1}{2}\left(p_{Fe}^{Ga\,site} - p_{Fe}^{D\,site} \right) = -0.04 \\ Z &= 0 \end{aligned} \tag{11}$$

The actual environment of the Fe atoms in $Fe_{75}Ga_{25}$ alloy in this non-perfect ordered DO_3 structure must be modified with respect to that of the perfect ordered one (Table 1). It is possible to estimate an average effect of the separation from the perfect DO_3 ordered structure, as far as only 43 % of Ga atoms and 81 % of Fe atoms are in correct positions. Considering the calculated disorder and the fact that Ga atoms will occupy both A* and D* sites with the same probability, the modified averaged sites will be:

- Average A* site: 2.5 Ga as NN (43 % of 4 Ga remains in their sites and 19 % of Fe are displaced) and 1.1 Ga as NNN.
- Average D* site: 1.5 Ga as NN and 2.6 Ga as NNN.
- Average Fe site substituting a Ga site: 1.5 Ga as NN and 1.1 Ga as NNN.

The similarity of the average neighbourhood (same first shell) of a Fe atom in a D* site and that of a Fe in a Ga site could explain the overlapping between these two contributions in the magnetic hyperfine field distribution (peak "b"). On the other hand, the non-zero average number of Ga as NN in a D* site could help to explain the shift of peak "b" with respect to 33 T (pure Fe), neglecting the effect of the second shell. This result, in a perfect ordered DO_3 structure, could only be explained by the effect of Ga atoms as NNN as a D site has 0 Ga as NN.

The analysis performed above concerns only to average neighbourhood configurations. The possible deviations from the average configurations, related with a larger number of Ga atoms as NN, can explain the low B_{hf} values necessary to correctly fit the MS spectrum of $Fe_{75}Ga_{25}$ alloy.

Assuming that maxima "a" and "b" are ascribed to the A* and D* sites, respectively, it would be possible to write:

$$2.5q + 1.1r = 13 \qquad [\mathrm{T}] \qquad (12)$$

$$1.5q + 2.6r = 2.5 \qquad [\mathrm{T}] \qquad (13)$$

Both expressions cannot be fulfilled at the same time as this should imply a negative value of $r \sim -2.5$ T. The reason for that could be the non-linearity between $\Delta B_{hf} = 33 - \langle B_{hf} \rangle$ (T) and n and m (i.e. q and r are not constant and independent of n and m, respectively).

c) General dependence of $\langle B_{hf} \rangle$ on the number of Ga atoms as NN

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Assuming the effect of the second shell can be negligible (i.e. the main effect on the magnetic hyperfine field is due to the first shell), it would be possible to obtain the dependence of $<B_{hf}>$ on the average number of Ga atoms as NN, $<n>$, for fully disordered and "maximum ordered" structures (Fig. 8). The average values obtained for ordered and disordered structures differ only for the alloys with 20 and 25 at. % Ga. The actual value for these alloys must lie between these two calculated values. Figure 8 also shows the experimental B_{hf} values corresponding to maxima "a" and "b" of the HFD of $Fe_{75}Ga_{25}$ alloy as a function of their corresponding $<n>$. One single line formed by two linear branches with a slope change at $<n> \sim 2$ can be used to describe the whole set of data. Therefore, it could be concluded that q is not independent of $<n>$. For low $<n>$ values (≤ 2), the decrease of B_{hf} per Ga atom as NN is lower than for values of the average number of Ga atoms as NN bigger than 2. This feature is also described for FeSi alloys [16]. A comparison between figure 8 and figure 4 of ref. [16] shows that, for low $<n>$ (disordered alloys, low Ga content), the effect of Ga as NN is similar to that of Si (slope ~2.5 T per Ga or Si atom as NN), and for $<n> > 2$, this effect is enhanced for both alloy types, but seems to be stronger in the case of Ga than in the case of Si (slope $\geq$15 per Ga atom and ~5.5 T per Si atom as NN).

Mössbauer spectrum of $Fe_{80}Ga_{20}$ alloy has turned to be the most complex of the studied alloy series. Its HFD shows two broad and overlapped maxima, which can be ascribed to a mixture of the disordered A2 and ordered DO_3 phases. The large number of relevant contributions for both fully ordered and maximum disordered approaches (see figures 5 and 6) prevents a further discussion on the hyperfine structure of this alloy. In fact, the structure of this alloy can be considered as a transition between low Ga containing alloys ($\leq$ 10 at. %), which can be described by a disordered structure,

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and $Fe_{75}Ga_{25}$ alloy, which can be described using a DO_3 ordered structure with small perturbations.

4. Conclusions

The substitution of Fe by 5, 10, 20 and 25 at. % Ga in arc-melted polycrystalline FeGa binary alloys causes a decrease of the Curie temperature, the average magnetic hyperfine field, $<B_{hf}>$, and the average magnetic moment, $<\mu_{Fe}>$ per Fe atom at 300 K. A linear dependence of $<B_{hf}>$ and $<\mu_{Fe}>$ with Ga content, and therefore between these two quantities, is found for Ga content up to 20 at. %.

The change in the ordering of the crystal structure with increasing Ga content of the alloy was modelled using a binomial distribution method taking into account both the nearest neighbours and the next nearest neighbours shells. Low Ga containing alloys (≤ 10 at. %) present a disordered A2 structure and the $Fe_{80}Ga_{20}$ alloy shows a mixture of both A2 and DO_3 phases. The alloy $Fe_{75}Ga_{25}$ does not present a perfect ordered DO_3 structure, as could be expected for its stoichiometry and a degree of order of 71.5 % was calculated. The modelled actual environment of the Fe atoms in a non-perfect ordered DO_3 structure (for $Fe_{75}Ga_{25}$ alloy) can explain the experimental features of its magnetic hyperfine field distribution using only a nearest neighbours approximation. The decrease of the magnetic hyperfine field per Ga atom in the nearest neighbours shell is ~2.5 T for a number of Ga ≤ 2 and ~5.5 T for higher number of Ga atoms.

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Table 1. Definition of the different Fe sites in a perfect ordered DO_3 structure and in a "maximum ordered" structure for $Fe_{100-y}Ga_y$ alloys.

Structure	Site	NN Fe atoms	NN Ga atoms (n)	NNN Fe atoms	NNN Ga atoms (m)
Perfect ordered DO_3 y=25 at.%	Fe atom in D site	8	0	0	6
	Fe atom in A site	4	4	6	0
	Ga atom site	8	0	6	0
"Maximum ordered" y<25 at. %	Fe atom in D site	8	0	≥ 6	≤ 6
	Fe atom in A site	≥4	≤ 4	6	0
	Fe atom in a Ga atom site	8	0	6	0

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Figure captions

FIG. 1. (a) XRD pattern corresponding to $Fe_{75}Ga_{25}$ alloy and (b) lattice parameter, *a*, of the bcc phase of FeGa alloys as a function of the Ga content of the alloy.

FIG.2. (a) Compositional dependence of the saturation magnetization, M_S; (b) average magnetic moment per Fe atom, $<\mu_{Fe}>$, at 300 K and (c) Curie temperature, T_C, of $Fe_{100-y}Ga_y$ alloys.

FIG. 3. Transmission Mössbauer spectra at 300 K and their corresponding fitting (solid line) and magnetic hyperfine field distributions of $Fe_{100-y}Ga_y$ alloys.

FIG. 4. (a) Compositional dependence of the average magnetic hyperfine field, $<B_{hf}>$; (b) average isomer shift, $<IS>$, of FeGa alloys. For comparison, it is also shown the compositional dependence of $<B_{hf}>$ for FeAl [12] and FeSi [13] binary alloys on (a). (c) Average magnetic hyperfine field, $<B_{hf}>$, as a function of the average magnetic moment per Fe atom, $<\mu_{Fe}>$, at 300 K.

FIG. 5. Probabilities, P_{nm}, of a Fe site to have *n* Ga atoms as NN, in the first shell, and *m* Ga atoms as NNN, in the second shell for a fully disordered A_2 structure, calculated using equation (6), for the different studied alloys.

FIG. 6. Probabilities, P_{nm}, of a Fe site to have *n* Ga atoms as NN, in the first shell, and *m* Ga atoms as NNN, in the second shell for a "maximum ordered" DO_3 structure, calculated using equation (6), for the different studied alloys.

FIG. 7. Summatories of the products $P_{nm} \cdot n$ and $P_{nm} \cdot m$, as a function of the Ga content for $Fe_{100-y}Ga_y$ alloys.

FIG. 8. $<B_{hf}>$ dependence on the average number of Ga atoms as near neighbours, $<n>$, for both fully disordered and "maximum ordered" structures. The experimental B_{hf}

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values corresponding to maxima “a” and “b” of the HFD of $Fe_{75}Ga_{25}$ alloy are also shown.

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FIGURE 1

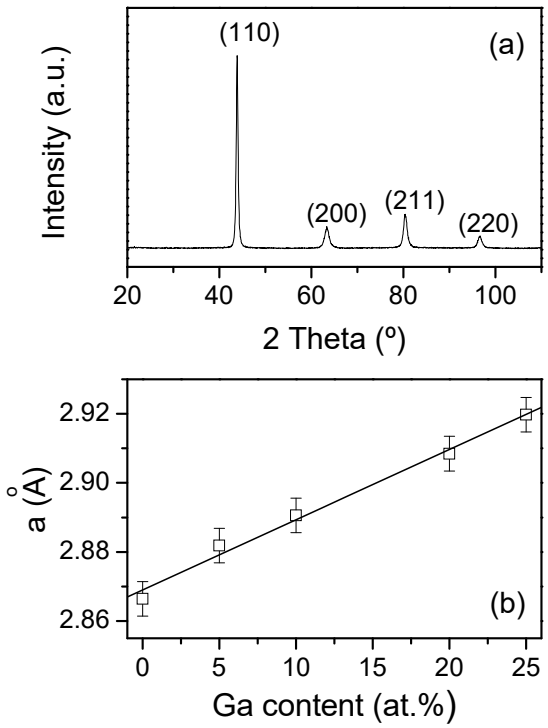

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FIGURE 2

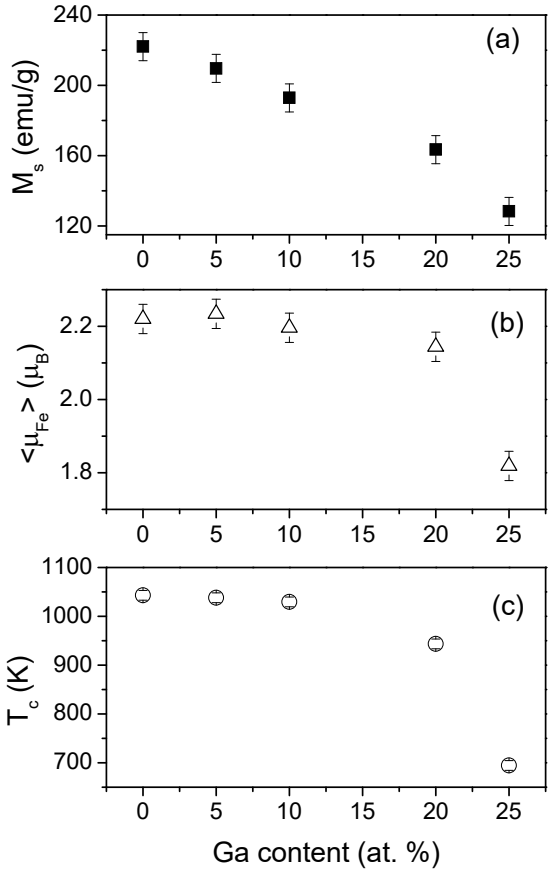

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FIGURE 3

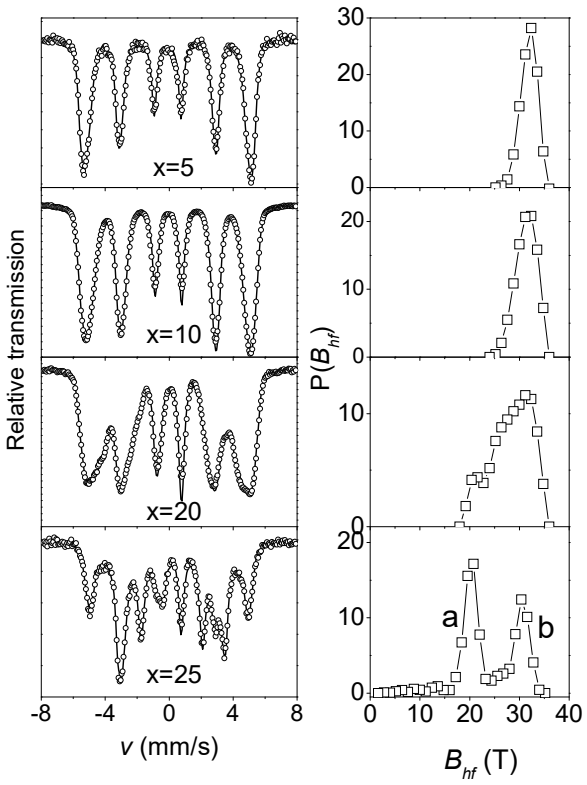

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FIGURE 4

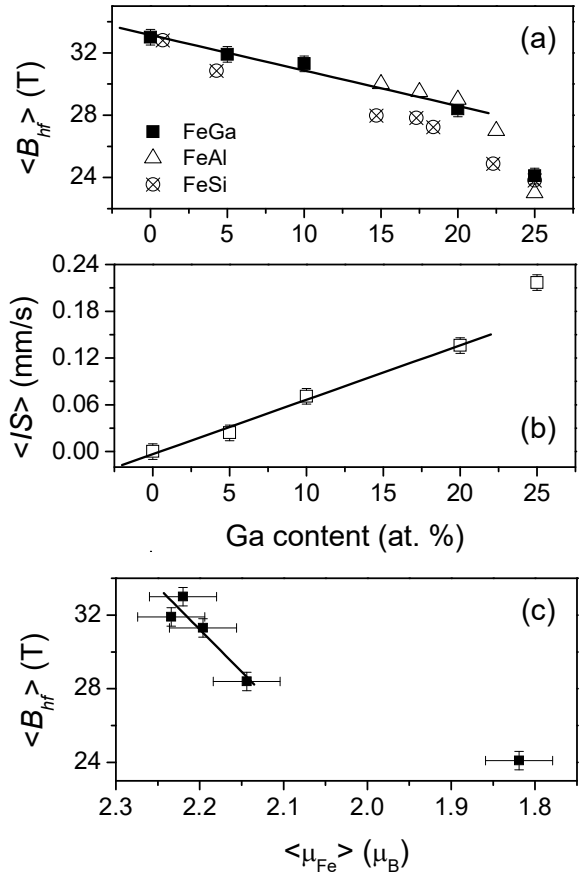

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FIGURE 5

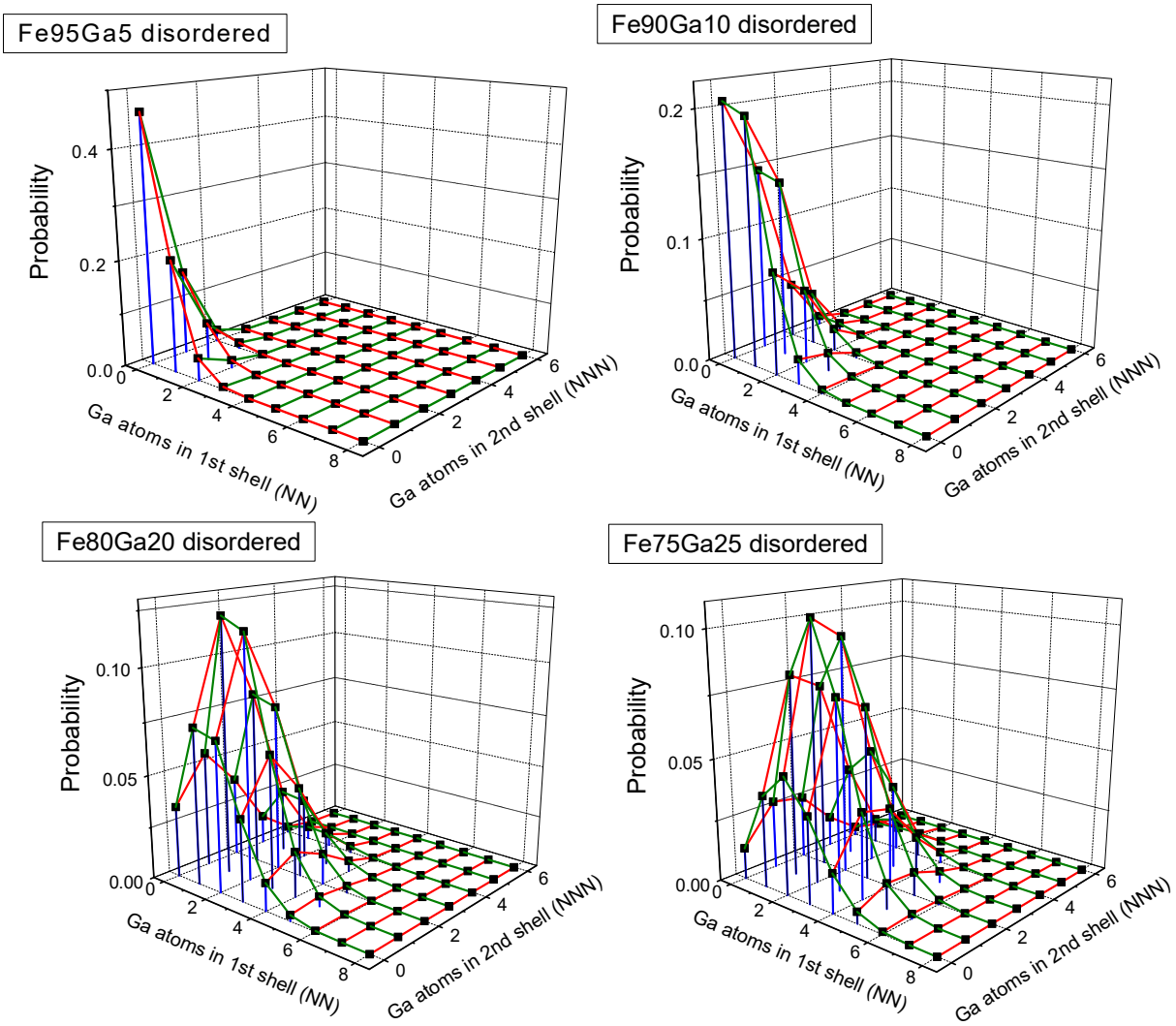

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FIGURE 6

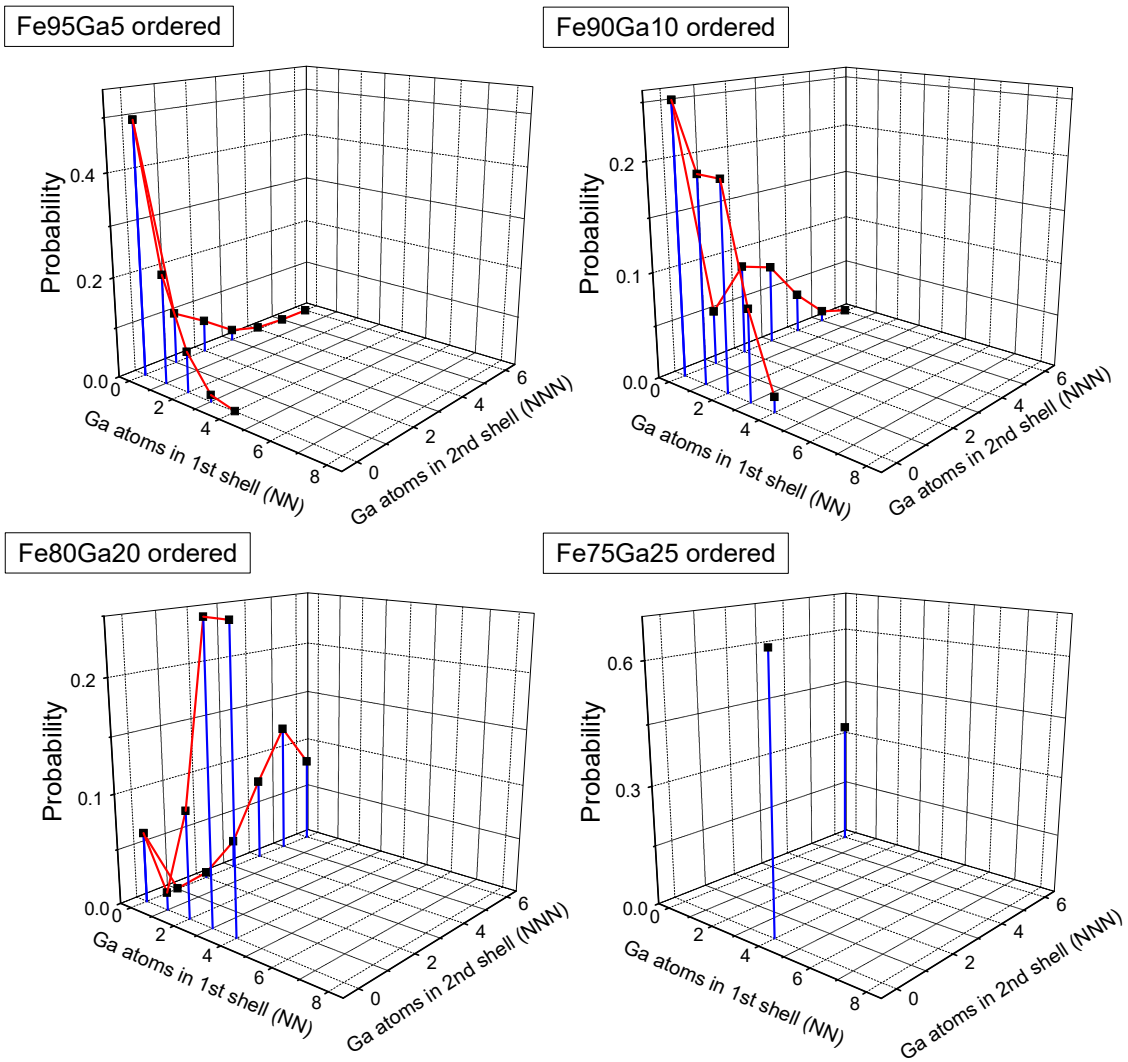

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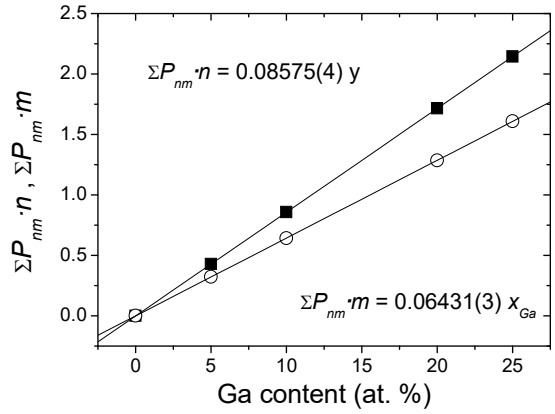
FIGURE 7



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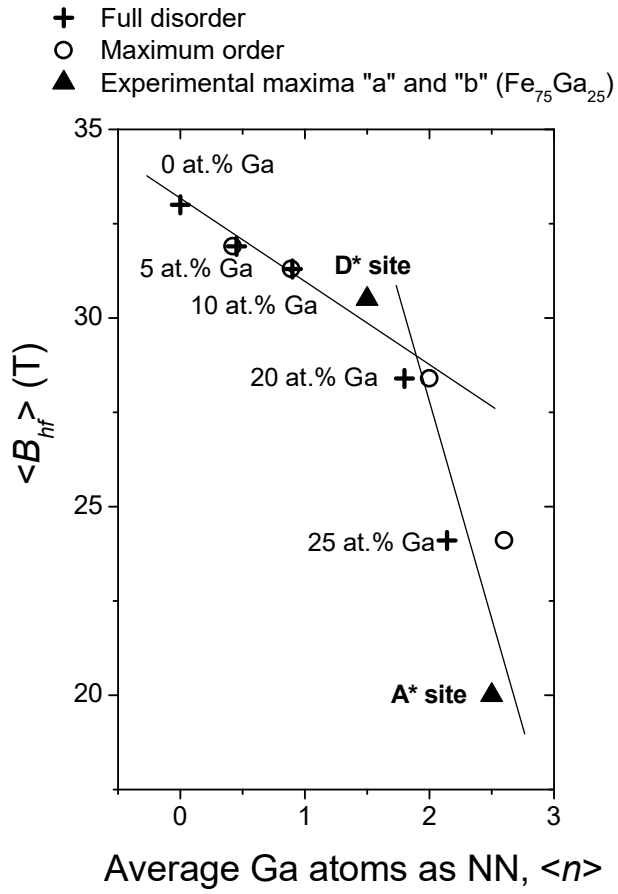
FIGURE 8