Simulation of the magnetic sourronding distribution in diluted $A_{56.25}B_{43.75}$ alloys, for different long range order parameter, and its effect on the magnetic properties

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Ordered and disordered $A_{56.25}B_{43.75}$ samples were computationally simulated in a BCC phase, where (A) are magnetic atoms and (B) are nonmagnetic atoms. We obtained the probability distribution of the number of first magnetic neighbors for different long-range order parameters, and simulating in this way the possible hyperfine field distribution of the system. It was found that the average number of near nearest magnetic neighbors decreases quadratically with the long-range order parameter. By using the $1/2$ Ising model and the Monte Carlo method with Metropolis dynamics, the magnetic behavior of the alloy was simulated as a function of dimensionless temperature θ and of the long-range order parameter. It was obtained a para-ferro phase transition when the average number of magnetic bonds per atom exceeds the value 2.37 (bonds/atom); besides the behavior of the mean hyperfine field, for $\theta \to 0$, as a function of the number of mean near nearest neighbors was determined in the light of $1/2$ Ising model.

Keywords: Magnetism; binary alloy; long range order parameter; hyperfine field mean; Monte Carlo.

Se simularon computacionalmente muestras $A_{56.25}B_{43.75}$ en fase BCC, ordenada y desordenada, compuestas por átomos magnéticos (A) y diluidores (B). Se obtuvo la distribución de probabilidad del número de primeros vecinos magnéticos para diferentes parámetros de orden de largo alcance, simulando así la posible distribución de campo hiperfino del sistema. Se encontró que el número medio de primeros vecinos magnéticos disminuye cuadráticamente con el parámetro de orden de largo alcance. Utilizando el modelo de Ising $1/2$ y el método de Monte Carlo con dinámica de Metropolis, se simuló el comportamiento magnético de la aleación como función de la temperatura adimensional θ y el parámetro de orden largo alcance, obteniendo una transición de fase para-ferro cuando el numero medio de enlaces magnéticos por átomo supera el valor 2.37 (enlaces/átomo); asimismo se plantea un posible comportamiento del campo hiperfino medio, para $\theta \to 0$, como función del número medio de primeros vecinos a la luz del modelo de Ising $1/2$.

Descriptores: Magnetismo; aleación binaria; parámetro de orden de largo alcance; campo hiperfino medio; Monte Carlo.

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1. Introduction

The binary alloys composed by magnetic and diluter atoms has been studied because their wide variety of magnetic and structural properties. The experimental studies shows that in this type of alloys (A_pB_{1-p}, A: magnetic and B: diluter) the structural properties depend on the concentration of magnetic atoms and the thermal treatment, as an example, in BCC phase is possible to obtain A2, DO_3, B2 y B32 [1]ordering types. In addition, the role played be the atomic sustitutional disorder in the critical behavior of the system has been the subject of a considerable amount of work from the theoretical [2–4] and experimental points of view [5–7]. One of the most employed experimental technique is the Mossbauer Spectrometry [5].

In previous works, [4–8] the disordering effect on samples of the BCC phase, heterostructures [4] and DO_3 [8] has been simulated, founding that the disorder induce a phase transition from a paramagnetic state to a ferromagnetic state. In Fig. 1, we depict the phase diagram for a system with DO_3 ordering type.

In the present work, we have performed a detailed study of the magnetic neighborhoods of the system $A_{56.25}B_{43.75}$ as the long-range order parameter decreases, from a perfectly ordered phase BCC DO_3 with $S = 1$ (Fig. 2a) up to a total disordered system with $S = 0$ (Fig. 2b).

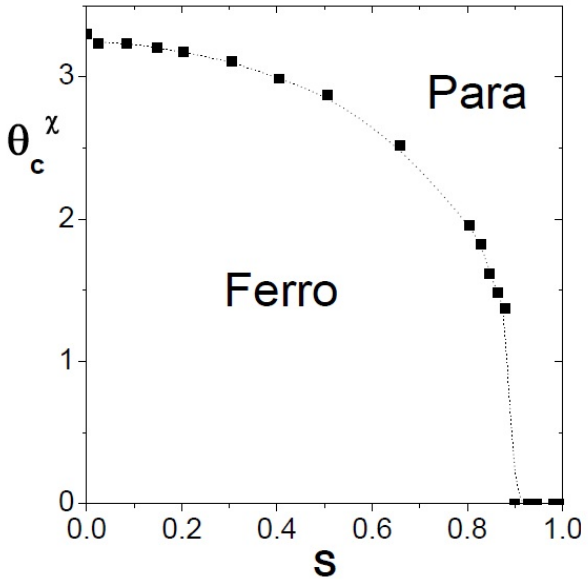

FIGURE 1. Phase diagram of the $A_{56.25}B_{43.75}$ system. Dimensionless temperature θ as a function of the long-rang order parameter S.

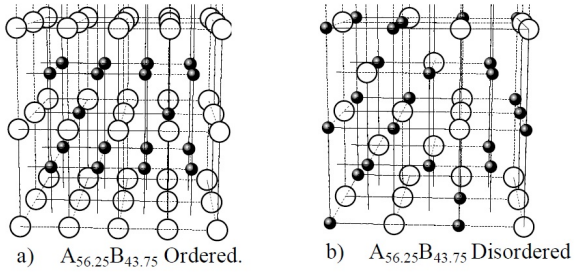

FIGURE 2. (a) Ordered (DO_3) and (b) disordered (A_2) lattices of a binary alloy with a concentration of 56.25% of magnetic atoms (dark spheres) and 43.75% of diluter atoms (white spheres).

2. Theoretical framework

In order to obtain the thermodynamic properties of the $A_{56.25}B_{43.75}$ alloy, using the Ising (1/2) model with interactions between first neighbors ¡nn¿, the Hamiltonian for the system without external applied magnetic field, is given by:

$$H = -J \sum_{<ik>} \sigma_i \sigma_k, \tag{1}$$

where $\sigma = \pm 1$ for magnetic atoms (A) and σ*=0* for diluters atoms (B). $J > 0$ is the exchange energy between the *i-th* and *j-th* spins. For a BCC lattice, the Hamiltonian of Eq. 1 can be rewrited as:

$$H = -\frac{J}{2} \sum_{i=i}^{N_A} \sigma_i \sum_{j=1}^{8} \sigma_{ij} = -\frac{J}{2} \sum_{i=i}^{N_A} \sum_{j=1}^{n_A} \sigma_i \sigma_{ij}, \tag{2}$$

where i runs through the magnetic atoms N_A and j runs through the neighboring magnetic n_A *i-th* spin. Considering the 9 neighborhood types (n_A=0, 1, ... 8), the Hamiltonian becomes:

$$H = -\frac{J}{2} \sum_{n_A=0}^{8} \sum_{i=1}^{N_{nA}} \sum_{j=1}^{n_A} \sigma_i \sigma_{ij}, \tag{3}$$

where N_{nA} is the number of atoms A with n_A magnetic neighbors A. As we have $J > 0$, then as $\theta \to 0$ the product between neighbor spins tends to 1

$$H_{\theta \to 0} = -\frac{J}{2} \sum_{n_A=0}^{8} \sum_{i=1}^{N_{nA}} \sum_{j=1}^{n_A} 1 = -\frac{J}{2} \sum_{n_A=0}^{8} N_{n_A}.n_A, \tag{4}$$

$$H_{\theta \to 0} = -\frac{JN_A}{2} \sum_{n_A=0}^{8} P_{n_A}.n_A = -\frac{JN_A}{2} \left[n_A\right], \tag{5}$$

where P_{nA} is the probability that an atom A has n_A magnetic atoms as its first neighbors, and $[n_A]$ is the average number of magnetic neighbours of an atom. Therefore, the energy of the system is determined by means of the statistical distribution of the magnetic neighbors, *i.e.* by P_{nA}.

3. Results and discussion

To study the effect of the variation in the long-range order parameter with the distribution of neighborhoods, it was initiate with a perfectly ordered DO_3 sample (Fig. 2a) with size $LxLxL$ ($L = 100$ lattice parameters). The calculations were performed by using the algorithm of Aguirre *et al.*, which has been modified in order to calculate the long-range order parameter and introducing a counter of the magnetic neighbours. In this way it was obtained the probability distribution of the magnetic neighbours as a function of the order parameter of the sample. In order to improve the statistical reliability, we have considered ten diferent samples for each value of S.

In Fig. 3, it can be seen some hystograms corresponding to the probability of the 9 types of neighbors for ten different order parameters. This probability distribution determine the possible behavior of the hyperfine field distribution within the sample [5,6]. The hyperfine field is determined, in first approximation, by:

$$H_{hf_{(S)}} = H_{0_{(S)}} + n_A H_{nn_{(S)}}, \tag{6}$$

where H_0 corresponds to a mean field locally present in the sample around the Mossbauer atom and H_{nn} corresponds to the mean magnetic field exerted by a neighbor on the Mossbauer atom and depend on the value of S.

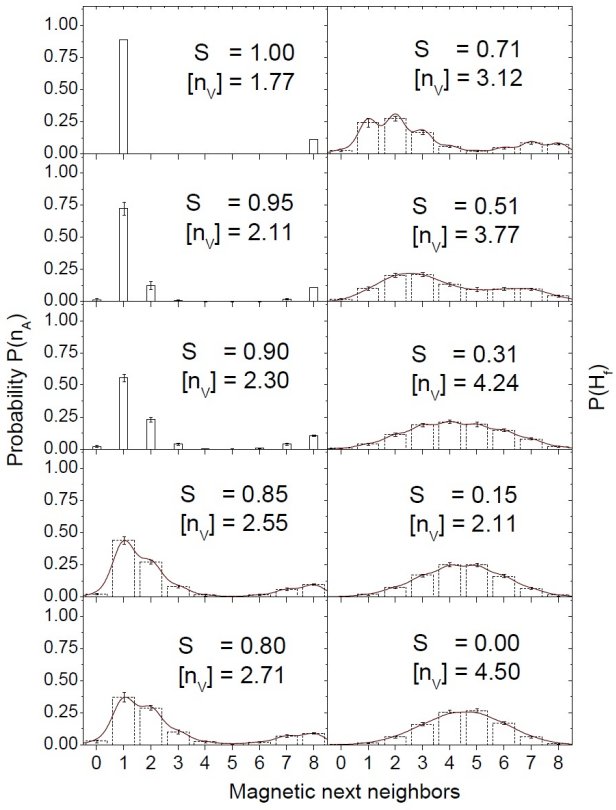

FIGURE 3. Number of bonds probability distributions vs. magnetic neighbors number, for different order parameters for the alloy $A_{56.25}B_{43.75}$. Bars represent the different types of neighborhoods and the curves are a visual guide for the shape of the hyperfine field distribution.

In Fig. 3 we show the distributions corresponding to large (right column) and small (left column) values of the order parameter.

When the sample is perfectly ordered (Fig. 3 with $S = 1$, corresponding to Fig. 2a) the only probably sites are those of atoms that have one or eight magnetic neighbors. These two sites are paramagnetic sites (see Fig. 1), because they do not show long-range magnetic correlations. As the sample is disordered the atoms are redistributed and begin to present different types of paramagnetic sites (Fig. 3, $S = 0.95$ and $S = 0.90$), but the redistribution of atoms is not sufficient to establish long-range correlations. On the other hand, one can see from Fig. 3 that as the order parameter decreases likelihood of new types of neighborhoods are probable (Fig. 3 $S \leqslant 0.85$) and begin to appear magnetic percolation paths within the sample as can be seen in the phase diagram (Fig. 1). Samples present ferromagnetic behavior and the distributions of neighborhoods can be assumed as the hyperfine field distributions (continuous curves in Fig. 3). It is observed how the decrease of the order parameter modifies the original bimodal distribution until a perfect binomial distribution (Fig. 3 $S = 0.0$).

Using the probability distributions from Fig. 3 we obtain the average number of magnetic neighbors $[n_A]$ as function of the order parameter within the sample. As it can see from Fig. 4, $[n_A]$ shows a cuadratic dependence with S as follow

$$[n_A] = n_{A0} + C \cdot S^2, \tag{7}$$

where n_{A0} is the average number of bounds for S=0, and may be obtained by the following expression:

$$n_{Ao} = \sum_{k=0}^{8} \frac{8!}{k!(8-k)!} p^k q^{8-k} k = 8p = 4.5, \tag{8}$$

with p=0.5625. The average number of bounds for S=1 is obtained from

$$[n_A]_{S=1} = 1x\frac{50\%}{56.25\%} + 8x\frac{6.25\%}{56.25\%} = \frac{1}{p}. \tag{9}$$

Equation (7) may be reduced to:

$$[n_A] = 8p\left(1 - S^2\right) + p^{-1}S^2. \tag{10}$$

From Figs. 1 to 4, we may conclude that the critical adimensional temperature increases with the avegare number of magnetic bounds per atom. Fig. 5 shows that the minimum average number of magnetic bonds per atom, it is to have the sample for the existence of phase transition, or equivalently magnetic percolation paths must be equal to 2.371 $\pm$ 0.008 per atom magnetic neighbors.

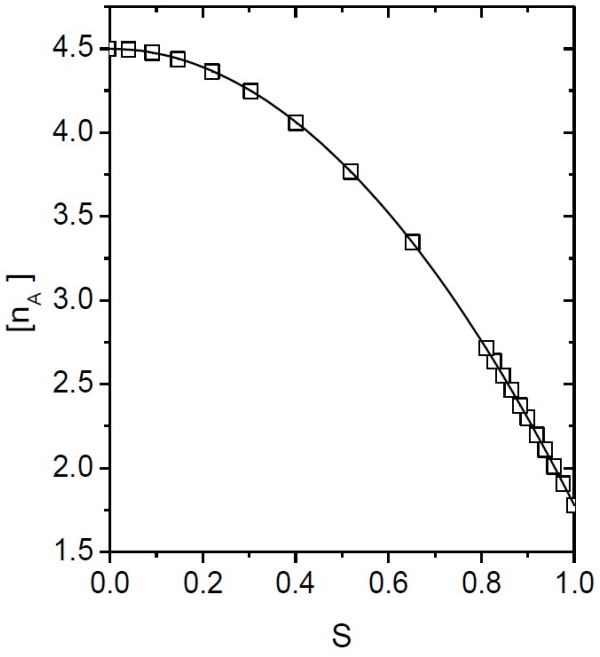

FIGURE 4. Change of the average number of magnetic bonds as a function of S. The squares correspond to the results obtained in the simulation and the continuous line to the Eq. (7).

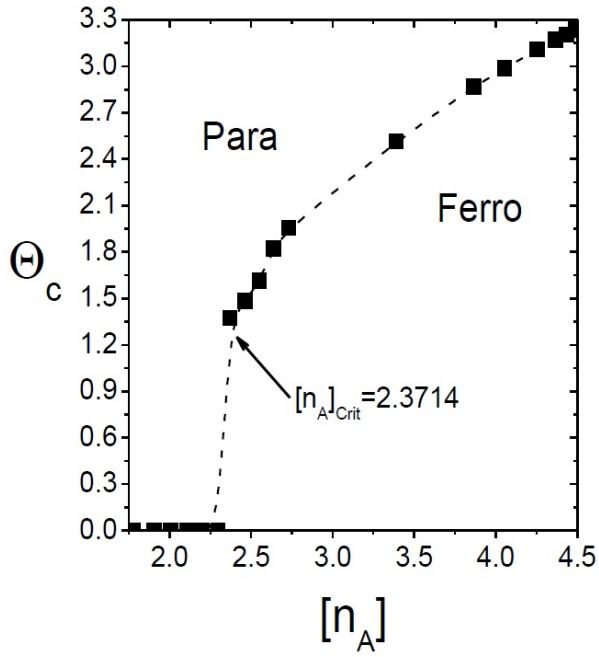

FIGURE 5. Effect of average number of magnetic bonds per atom on the dimensionless critical temperature of the alloy $A_{56.25}B_{43.75}$.

From Fig. 6 we notice that the specific magnetization increases with the average number of bounds, which is consistent with the increases of the hyperfine field as determined by the Eq. (6). For higher values of S, an increase of the average bound numbers induces an increasing of the spins in the percolation routes. This may be observed from Fig. 3, in which it can be noted a decreasing of the probability for atoms with

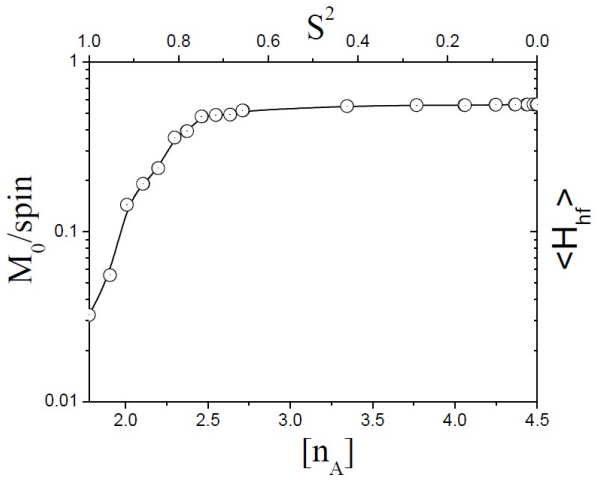

FIGURE 6. Simulated specific magnetization vs. average number of bonds, and of the parameter of magnetic long-range order vs, the possible behavior of the hyperfine mean field.

one or eight neighbors, while increase the probability of atoms with 2, 5, 3, 6, 4, 7 neighbors. When most of the magnetic atoms are part of the percolation paths (Fig. 6, $[n_A] \approx 2.375$) the specific magnetization disminulle its growth rate and begins a process of stabilization to the value 0.5625 and consequently a hyperfine field stabilization mean.

4. Conclusions

We have simulated the probability distributions for the neihgborhoods of magnetic atoms in the $A_{56.25}B_{43.75}$ system obtaining a distribution for the hyperfine mean field as a function of the long-range order parameter.

We have found that the average number of first neighbors is related quadratically with the long-range order parameter by means of the Eq. (10).

Finally, the system presents a phase transition when the average number of magnetic bonds per atom is 2.371 ± 0.008.

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