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Monte Carlo study of the effect of structural long-range order on the magnetic properties of A_9B_7 alloys, where only (A) is magnetic

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Computer simulations were used to create perfectly ordered binary virtual samples, formed by magnetic (56.25%) and nonmagnetic (43.75%) atoms in a BCC phase and with DO_3 order. Subsequently, the samples were disordered and then atomic migration between the lattice sites was simulated; this migration was governed by a migration probability P_m (specified by us) and we achieve the phase A2 for $P_m = 1.0$. An exponential relation was obtained between the long range order parameter (measurable experimental parameter S) and the migration probability (microscopic parameter P_m). Magnetization, susceptibility, the Edward Anderson parameter, and the mean energy as a function of the dimensionless temperature Θ and long range order parameter were calculated using the Monte Carlo method with Metropolis dynamic; they allow us to determinate the critical temperature for samples with phase transition. The saturation magnetization results showed that using the 1/2 Ising model, the disorder induces a para-ferro phase transition due to the substitutional disorder. The highly ordered samples showed a paramagnetic behavior in the entire temperature range, while those samples with migration probability $P_m > 0.06$ have a ferromagnetic phase transition at low temperatures. Additionally, it was found that the critical order parameter is 0.882.
Keywords: Magnetism; binary alloy; long range order parameter; migration probability; Monte Carlo.

Se utilizaron simulaciones computacionales para construir muestras virtuales binarias perfectamente ordenadas, compuestas por átomos magnéticos (56.25%) y diluidores (43.75%) en fase bcc y ordenamiento DO3. Posteriormente, las muestras fueron desordenadas simulando una migración atómica entre los sitios de la red; esta migración esta gobernada por una probabilidad de migración P_m (especificada por nosotros) obteniendo la fase A2 para *Pm = 1.0*. Se obtuvo una relación exponencial entre el parámetro de orden de largo alcance (parámetro medido experimentalmente S) y la probabilidad de migración (parámetro microscópico Pm). Utilizando el método de Montecarlo con dinámica de Metropolis se obtuvieron la magnetización, la susceptibilidad, el factor de Edward Anderson y la energía media como función de la temperatura adimensional Θ y del parámetro de orden de largo alcance; permitiéndonos encontrar la temperatura critica para aquellas muestras que presentan transición de fase. Los resultados de la magnetización de saturación mostraron que usando el modelo de Ising 1/2, el desorden induce la aparición de una transición de fase para-ferro debido a un desorden sustitucional. Para muestras altamente ordenadas se presenta un comportamiento paramagnético en todo el rango de temperaturas, mientras que aquellas muestras con probabilidad de migración $Pm > 0.06$ presentan una transición de fase al estado ferromagnético a bajas temperaturas. Adicionalmente, se encontró que el parámetro de orden crítico es 0.882.
Descriptores: Magnetismo; aleación binaria; parámetro de orden de largo alcance; probabilidad de migración; Monte Carlo.

PACS: 05.10.Ln; 75.30.Et; 75.30.Cr; 75.30.Kz; 75.60.Ej

1. Introduction

Experimental [1] and theoretical [2] studies of binary alloys, composed by magnetic and nonmagnetic atoms, have shown that the way in which atomic components are distributed within the crystalline structure has remarkable impact on the behavior of thermodynamic properties of the system.

By simulation, in 2005 Aguirre [3] showed that the disordering of binary systems (in multilayer structure) have an impact on their critical temperature.

Experimental studies have measured the long-range order parameter [4] (S) and magnetic behavior [5] of such alloys. However, there are no studies showing the correlation between the order parameter (S) and magnetic properties of the system in bulk.

This paper presents a computational description of how the magnetic properties change depending of long-range order parameter in a binary sample (consisting of magnetic and diluter atoms), with a 56.25% of magnetic atoms and an initial structure perfectly ordered (of the BCC DO_3 type) (Fig. 1).

This concentration (56.25%) was chosen because it has the DO_3 order when it is perfectly ordered and is easily constructed as a series of supercells of two lattice parameter ($l = 2a$) with clusters of nine magnetic atoms surrounded by planes of diluter atoms (Fig. 1). Direct interactions between the spins are restricted to clusters of nine atoms and the system will exhibit a global paramagnetic behavior.

2. Theoretical model

The long-range order parameter S (Eq. (1)) determines the regularity and uniformity with which the components are distributed in the crystal structure, with reference to a predetermined atomic configuration [6].

$$S = \frac{r_A - F_A}{1 - F_A} = \frac{r_B - F_B}{1 - F_B} \tag{1}$$

With:

$$r_\alpha = \frac{N^\alpha_{ok}}{N_\alpha}; \qquad F_\alpha = \frac{N_\alpha}{N} \tag{2}$$

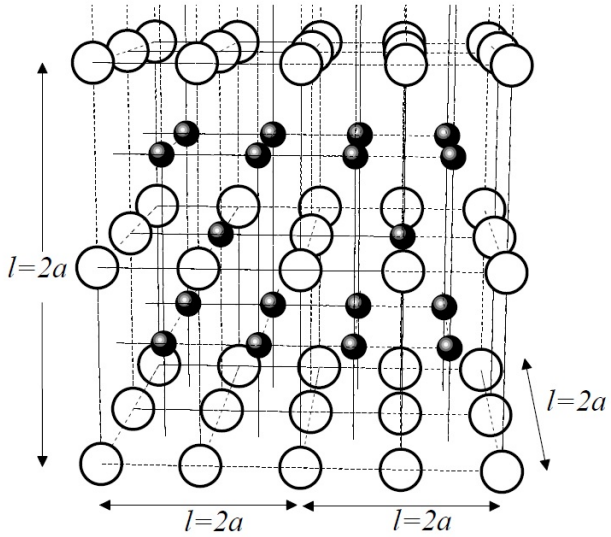

FIGURE 1. Two supercells ($l = 2a$) of a binary alloy with a concentration of magnetic atoms of 56.25% (black spheres) and 43.75% of diluter atoms (white spheres) with a perfect configurationally order (DO_3). a is the lattice parameter. Note the isolated clusters of nine magnetic atoms.

where r_A (r_B) is the fraction of atoms A (B) occupying right A (B) lattice sites, and F_A (F_B) is the fraction of atoms A (B) in the solution ($F_A = 0.5625$ and $F_B = 0.4375$). When the long-range order is perfect the fraction of atoms that are well placed is equal to unity ($r_A = 1$) and therefore $S = 1$. When the atomic arrangement is perfectly random $r_\alpha = F_\alpha$ and $S = 0$.

To study the magnetic response of the system the spin-1/2 Ising model is considered. In this model the magnetic atoms (A) have net spin σ ($\sigma = \pm 1$) and diluter atoms (B) have no net spin ($\sigma = 0$).

The Hamiltonian of the system, without external magnetic field, is expressed as:

$$H = -J \sum_{\langle ik \rangle} \sigma_i \sigma_k \tag{3}$$

where the symbol $\langle ik \rangle$ means that the sum is performed on the nearest neighbor (first neighbors) and J is the exchange energy between *i-th* and *j-th* spins.

3. Results and discussion

To analyze the effect of the order parameter in $A_{56.25}B_{43.75}$ binary system it was initially built a DO_3 ordered sample (Fig. 1) in a bcc lattice with sized $L \times L \times L$ ($L = 10$ lattice parameters). To disorder the sample it was used the Aguirre's algorithm [7], which uses by they called the Migration Probability (P_m). P_m provides the probability that an atom in a lattice site exchanges position with another atom in another lattice site.

In this study, samples were disordered and the order parameter was calculated by Eq. (1), taking as reference the initial sample DO_3.

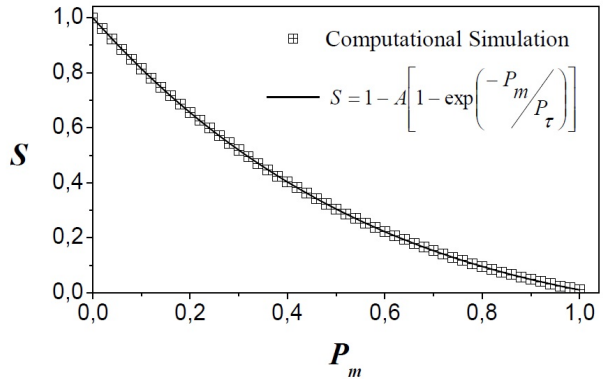

FIGURE 2. Shows that the migration probability P_m (statistical effect of microscopic thermal actions, mechanical or otherwise) produces an exponential decay in the order parameter S (parameter experimentally measurable by X-ray diffraction [5]).

The exponential decay was excellently fitted by:

$$S = 1 - A \left[1 - \exp\left(\frac{-P_m}{P_\tau} \right) \right] \tag{4}$$

where $A = 1.2461 \cong [1 - \exp(-P_\tau^{-1})]^{-1}$ and $P_\tau = 0.6121$ are constants.

After constructing the virtual sample, Monte Carlo's thermal scans were performed (with Metropolis dynamic) for a dimensionless temperature ($\Theta = k_B T/J$) varying from 8.00000 to 0.10102 ($\pm 5 \times 10^{-5}$). For each temperature the properties were analyzed with 8×10^4 Monte Carlo steps and 5×10^3 MC thermalization steps. ZFC process was emulated by changing the temperature according to the relationship $\theta_{k+1} = 0.99\theta_k$, where k and $k+1$, are the present and back state, respectively.

Figure 3 shows the behavior of: (a) the susceptibility, and (b) the Edward Anderson factor Q_{EA} (fourth cumulant of the magnetization) as a function of dimensionless temperature (θ), for different order parameters (S). Lambda peaks are ob-

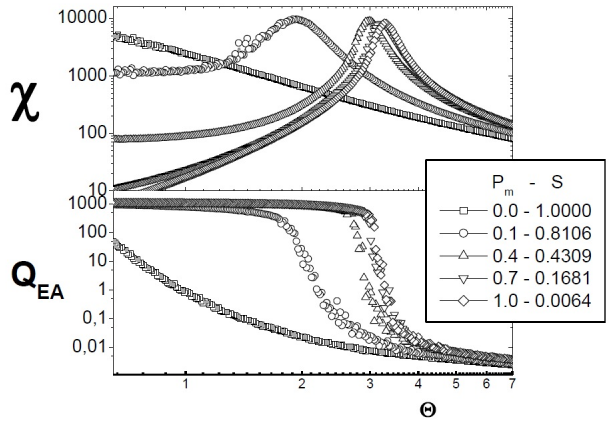

FIGURE 3. Susceptibility (γ) and Edward Anderson (Q_{EA}) factor vs. dimensionless temperature (θ), for different long-range order parameter (S). For $S = 1.0$ the structure is DO_3.

served in susceptibility curves that match with abrupt jumps in $Q_{EA.}$ This means that there is a phase transition from a ferromagnetic to a paramagnetic state at the peak temperature. The perfectly ordered sample ($P_m = 0.0$ and $S = 1.0$) has not phase transition, when $P_m > 0.06$ phase transition occur at increasingly higher temperatures. The critical temperature behavior is presented in Fig. 4. It shows the phase diagram of the system $A_{56.25}B_{43.75}$ as a function of the order parameter.

Energy and magnetization curves were also simulated. Figure 5 shows the fundamental energy (E_0) and the obtained magnetization by spin ($\Theta \to 0$). We see that the fundamental energy per spin presents a linear behavior with S^2, the constant term (2.26 ± 0.1) is close to the average number of expected bonds, assuming a binomial distribution of magnetic atoms in the BCC structure ($zp/2 = 8(0.5625)/2 = 2.25$). The magnetization curve shows saturation close to $S^2 \approx 0.56$ and a fall around $S^2 \approx 0.8 \approx (0.89)^2$, consistent with the phase diagram of Fig. 4.

In Eq. (3) (Ising Hamiltonian), the value of the fundamental energy decreases as increases the number of terms of the sum; Fig. 5, and the above, confirms that the decrease of the order parameter (disorder of the sample) increases the number of magnetic bonds. Then, it is reasonable that the critical temperature must increase as increases the disorder of the sample (decrease of S in Fig. 4).

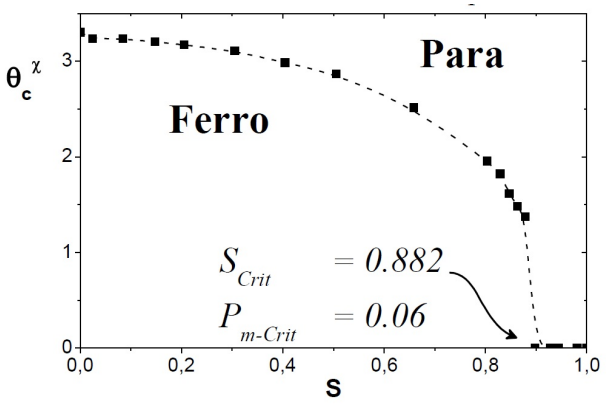

FIGURE 4. Phase diagram of the $A_{56.25}B_{43.75}$ system as a function of order parameter.

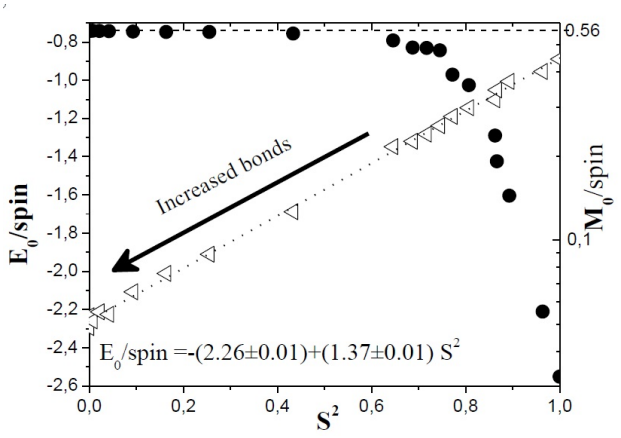

FIGURE 5. Behavior ($\Theta \to 0$) of energy (empty triangles) and magnetization (filled circles) by spin, as a function of S^2.

Initially ($S = 1$) the clusters are isolated (Fig. 1); due to the migration probability (P_m) some magnetic atoms can exchange positions with diluter atoms; so, there are magnetic atoms between clusters, acting as bridges, which provide the interaction between different clusters [1]. It is therefore reasonable to assume that as P_m increase also grows the probability of percolation of magnetic interaction. When the disorder in the sample is such that $P_m > 0.06$ ($S < 0.882$, Fig. 4), the magnetic atoms linked allow percolation of the magnetic interaction in the whole sample, and the phase transition appears.

4. Conclusions

Under spin $1/2$ Ising model disorder induces the appearance of a phase transition from a paramagnetic state (highly ordered samples, $S \sim 1$) to a ferromagnetic state (substitutional disordered samples). Moreover, if the long-range order parameter is less than 0.882 then the phase transition happens. This transition is the result of the increasing of percolation paths as the sample is lest ordered.

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