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Phase transitions in $Fe_{0.5}Co_{0.5}$ (110) thin films

G. Ramírez-Dámaso[a,*], F.L. Castillo-Alvarado[b], E. Rojas-Hernández[a]

[a] Escuela Superior de Ingeniería y Arquitectura "Unidad Ticomán" del Instituto Politécnico Nacional, Av. Ticomán No. 600, Col. San José Ticomán, Del. G. A. M., C. P. 07330 Ciudad de México, Mexico

[b] Escuela Superior de Física y Matemáticas del Instituto Politécnico Nacional, Edificio 9, Col. San Pedro Zacatenco, C. P. 07738 Ciudad de México, Mexico

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ABSTRACT

In this paper, we present calculations for two second-order phase transitions in (110) $Fe_{0.5}Co_{0.5}$ thin films with 11, 15, and 19 monoatomic layers. The lattice and magnetic transitions are based on thermodynamic equilibrium considerations of the magnetic alloy. The procedure proposed by Valenta and Sukiennicki was applied to calculate the composition x(i), the lattice order parameter t(i), and the magnetic order parameter σ(i) as a function of temperature T. We confirmed that both phase transitions, lattice and magnetic, are of the second order, in accordance with experimental results in the literature. The obtained behavior of these parameters indicates their inhomogeneity due to the boundary conditions on the surfaces of the thin film.

1. Introduction

The order–disorder phenomenon for binary alloys has been studied both theoretically and experimentally by many authors [1–12]. In recent years, two different surface-effect phenomena in thin-film alloys have been studied [4,13–15]: surface disordering and surface melting. The difference between these two phenomena is that melting results in the destruction of the lattice, while disordering preserves the lattice and atoms are exchanged at specific lattice sites [13]. In addition, the surface effects on the ferromagnetic and lattice order–disorder phase transitions in thin films of binary AB_3 type alloys have also been studied. Although the results indicated their simultaneous interdependence [16], not many theoretical studies have been performed. In the present case, we studied a three-dimensional system as a composition of two-dimensional layers. The formulations reported by Hill [17] in the context of small particles can be applied to the film structure when we treat a thin film as a system divided into subsystems equivalent to two-dimensional monoatomic layers (ML) parallel to the surface, lying in a given crystallographic direction [18]. The motivation for this research is to predict that $Fe_{0.5}Co_{0.5}$ (110) thin films, one of the most stable alloys, have a behavior similar to bulk $Fe_{0.5}Co_{0.5}$: when the temperature of the thin films increases, they undergo a second-order phase transition [19,20]. We report that the heat capacity of this alloy experiences a discontinuity near the bulk crystalline temperature phase transition (1002 K) and bulk magnetic temperature phase transition (1254 K).

We describe the phase transition in a thin film of $Fe_{0.5}Co_{0.5}$ (110) alloy using two order parameters: one is the lattice order parameter t(i) and the other is the magnetic order parameter σ(i), where i=1, 2,...,n denotes the position of the 2D monoatomic parallel layers in the alloy thin film. In the thin-film construction, the chemical composition x(i) can be inhomogeneous in the film thickness direction. Taking this fact into account, we obtain the equilibrium values of x(i), t(i), and σ(i) by means of a minimization procedure applied to the Helmholtz free energy of the system with respect to all of these parameters. This procedure was applied to analyze the case of a bcc $Fe_{0.5}Co_{0.5}$ (110) thin film composed of 11, 15, and 19 monoatomic layers (MLs). We studied the properties of $Fe_{0.5}Co_{0.5}$ (110) thin films near the lattice and magnetic order-disorder transition temperatures, and we describe the degree of ordering of the atoms in the lattice and the degree of ordering of the spins of the atoms. The order parameters are quantitative measurements of the lattice order and magnetization order of the sample, respectively. The values t=1 and σ=1 indicate that the sample is completely ordered, while t=0 and σ=0 indicate that the sample is completely disordered.

The need to study FeCo (110) thin films is because nanotechnology is a new branch of scientific research, where ferromagnetic materials have important applications as the fabrication of nanoscale objects, hard drives for data storage or his use in materials for hydrogen storage; there are not enough results about $Fe_{0.5}Co_{0.5}$ thin films with those characteristics.

2. Theory

The main ideas of this study were taken from the work of Sukiennicki [11], who studied the behavior of ferromagnetic thin films

* Corresponding author.
E-mail address: gramirezd@ipn.mx (G. Ramírez-Dámaso).

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with five monolayers of an fcc binary alloy, and Castillo-Alvarado [4], who studied the long-range order parameter of 11 monolayers of an fcc binary alloy. Our main goal in this work is to include the order parameter as a long-range magnetic order parameter in the case of 11, 15, and 19 MLs in order to compare our results with the results of bulk FeCo.

Let us consider a bcc binary alloy $A_{0.5}B_{0.5}$ (Fig. 1) with interaction between the first nearest neighbor atoms, where we suppose that, at low temperatures (near 0 K), all atoms are fixed in the positions shown, with their spins pointing up. We divide this crystallographic structure into two sublattices: the α sublattice consists of the sites in the corners, while the β sublattice consists of the sites in the center of the unit cell..

We introduce eight site probabilities: $P_\alpha^{A\uparrow}$, $P_\alpha^{A\downarrow}$, $P_\beta^{A\uparrow}$, $P_\beta^{A\downarrow}$, $P_\alpha^{B\uparrow}$, $P_\alpha^{B\downarrow}$ $P_\beta^{B\uparrow}$, and $P_\beta^{B\downarrow}$; the group of site probabilities corresponds to the probabilities of finding atoms A or B with spins up (↑), or spins down (↓), at sublattices α or β. These probabilities are normalized as follows:

$$P_\alpha^A(i)+P_\alpha^B(i)=1,\ P_\beta^B(i)+P_\beta^A(i)=1 \tag{1}$$

and:

$$P_\gamma^C(i)=P_\gamma^{C\uparrow}(i)+P_\gamma^{C\downarrow}(\mathrm{i}) \tag{2}$$

The concentration of A atoms in layer i is given as follows:

$$x(i)=P_\alpha^A(i)F_\alpha+P_\beta^A(i)F_\beta \tag{3}$$

The concentration of B atoms in the same layer i is written as follows:

$$y(i)=1-x(i)=P_\alpha^B(i)F_\alpha+P_\beta^B(i)F_\beta \tag{4}$$

We define the crystalline long-range order parameter as follows:

$$t(i)=P_\alpha^A(i)-P_\beta^A(i)=P_\beta^B(i)-P_\alpha^B(i) \tag{5}$$

And the magnetic order parameter as follows:

$$\sigma(i)=\sum_{C,\gamma}F_\gamma x_C P_\gamma^C(i)\sigma_\gamma^C(i) \tag{6}$$

($\gamma=\alpha,\beta$; C=A, B and F_γ denotes the relative number of sites γ; $P_\gamma^C(i)\sigma_\gamma^C(i)=P_\gamma^{C\uparrow}(i)-P_\gamma^{C\downarrow}(\mathrm{i})$).

Using Eqs. (1)–(6), it is possible to write the site probabilities in terms of x(i), t(i), and $\sigma_C^\gamma(i)$ as follows:

$$\begin{aligned}
P_\alpha^{A\uparrow}(i)&=\frac{1}{2}(x(i)+F_\beta t(i))(1+\sigma_A^\alpha(i))\\
P_\alpha^{A\downarrow}(i)&=\frac{1}{2}(x(i)+F_\beta t(i))(1-\sigma_A^\alpha(i))\\
P_\beta^{A\uparrow}(i)&=\frac{1}{2}(x(i)-F_\alpha t(i))(1+\sigma_A^\beta(i))\\
P_\beta^{A\downarrow}(i)&=\frac{1}{2}(x(i)-F_\alpha t(i))(1-\sigma_A^\beta(i))\\
P_\beta^{B\uparrow}(i)&=\frac{1}{2}(1-x(i)+F_\alpha t(i))(1+\sigma_B^\beta(i))\\
P_\beta^{B\downarrow}(i)&=\frac{1}{2}(1-x(i)+F_\alpha t(i))(1-\sigma_B^\beta(i))\\
P_\alpha^{B\uparrow}(i)&=\frac{1}{2}(1-x(i)-F_\beta t(i))(1+\sigma_B^\alpha(i))\\
P_\alpha^{B\downarrow}(i)&=\frac{1}{2}(1-x(i)-F_\beta t(i))(1-\sigma_B^\alpha(i))
\end{aligned} \tag{7}$$

Next we introduce the Helmholtz free energy:

$$\mathrm{F}(x(i),t(i),\sigma(i),\mathrm{T})=\mathrm{U}(x(i),t(i),\sigma(i))-\mathrm{T}\,\mathrm{S}(x(i),t(i),\sigma(i)) \tag{8}$$

where U is the internal energy, T is the temperature, and S is the entropy. In plane i, one atom A in sublattice α has atoms B and A as its first neighbors in sublattice α or β of the plane i, i+1, or i−1. The internal energy (U) consists of two parts connected with the lattice (U_l) and magnetic (U_m) ordering:

$$U=U_l+U_m \tag{9}$$

which are expressed respectively as follows [19]:

$$U_l(x,\ t,\ \sigma)=-\frac{1}{2}N\sum_{CC'}\sum_{\gamma\gamma'}\sum_{\sigma\sigma'}\sum_{ii'}F_\gamma\times[P_\gamma^{C\sigma}(i)r_{\gamma\gamma'}^{ii'}P_{\gamma'}^{C'\sigma'}(i')V_{CC'}^{ii'}] \tag{10}$$

$$U_m(x,\ t,\ \sigma)=-\frac{1}{2}N\sum_{CC'}\sum_{\gamma\gamma'}\sum_{\sigma\sigma'}\sum_{ii'}F_\gamma\times[P_\gamma^{C\sigma}(i)r_{\gamma\gamma'}^{ii'}P_{\gamma'}^{C'\sigma'}(i')J_{CC'}^{ii'}\sigma\sigma'] \tag{11}$$

where N is the total number of atoms, i, i′= 1,...,n, $\gamma,\ \gamma'=\alpha,\beta,\sigma,\sigma'=\uparrow,\downarrow$ (spin up or spin down) and C,C′=A, B.

Energy $V_{CC'}^{ii'}$ in Eq. (10) describes the interaction between two nearest neighboring atoms C and C' in the sense of the Bragg-Williams approximation [4] in the same plane or between two consecutive planes. In a similar manner, the magnetic part of the energy can be characterized by $J_{CC'}^{ii'}\sigma\sigma'$ in Eq. (11), which describes the magnetic interaction of the two nearest neighboring atoms C and C' in the same layer or between two consecutive layers. The explicit form of the internal energy becomes as follows:

$$U(x,\ t,\ \sigma)=-\frac{1}{2}N\sum_{CC'}\sum_{\gamma\gamma'}\sum_{\sigma\sigma'}\sum_{ii'}F_\gamma\times[P_\gamma^{C\sigma}(i)r_{\gamma\gamma'}^{ii'}P_{\gamma'}^{C'\sigma'}(i')(V_{CC'}^{ii'}+J_{CC'}^{ii'}\sigma_C^\gamma(i)\sigma_{C'}^{\gamma'}(i'))] \tag{12}$$

The entropy term (Bragg-Williams approximation) is calculated in the usual manner as follows [4]:

$$S(x,\ t,\ \sigma)=-k_BN^2\sum_{C,\gamma,\sigma,i}P_\gamma^{C\sigma}(i)\ln P_\gamma^{C\sigma}(i) \tag{13}$$

where $P_\gamma^{C\sigma}(i)$ are the probabilities expressed by Eq. (7) and k_B is Boltzmann's constant.

In Fig. 2(a), we present consecutive planes (plane i and plane i+1) parallel to (110), and in Fig. 2(b), we show the number of nearest neighbors of plane i. The given site α is surrounded by the number of nearest neighbor β sites, which is $r_{\alpha\beta}$(i)=4. Similarly, $r_{\beta\alpha}$(i)=4, $r_{\alpha\alpha}$(i)=0, and $r_{\beta\beta}$(i)=0. We obtain the number of nearest neighbors between consecutive planes from Fig. 2(a): $r_{\alpha\beta}(i\pm1)=2$, $r_{\beta\alpha}(i\pm1)=2$, $r_{\alpha\alpha}(i\pm1)=0$, and $r_{\beta\beta}(i\pm1)=0$. The magnetic interaction is defined by three parameters, whose values are similar to those given by Morán-López [3], for the ferromagnetic case (in absolute temperature units): J_{AA}=394 and J_{BB}=498; we propose instead $J_{AB}=J_{BA}=2.41(J_{AA}+J_{BB})$, $V_{AA}=1.16J_{AA}$, $V_{BB}=1.4J_{BB}$, and $V_{AB}=V_{BA}=0.56J_{AB}$..

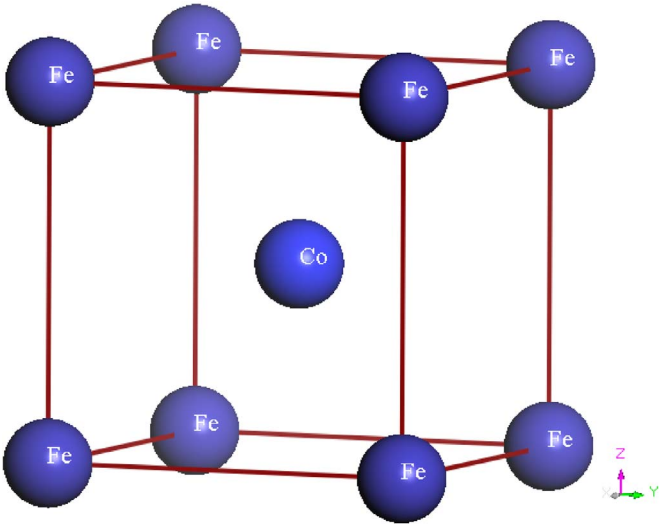

Fig. 1. Crystallographic structure of the bcc $Fe_{0.5}Co_{0.5}$ alloy.