Solid State Communications 218 (2015) 6–9

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

Ordered states in binary alloys with one magnetic component: A binomial description

R. Rodríguez-Alba [a,1], S.E. Acosta Ortíz [b], J.L. Morán-López [a,2,*]

[a] División de Materiales Avanzados, Instituto Potosino de Investigación Científica y Tenológica, San Luis Potosí, México
[b] Centro de Investigación en Física Aplicada, Aguascalientes, Ags., México

ARTICLE INFO

Article history:
Received 9 February 2015
Received in revised form
16 April 2015
Accepted 17 April 2015
Communicated by R. Merlin
Available online 14 May 2015

Keywords:
A. Magnetic materials
B. Binary alloys with one magnetic component
C. Ground state phases

ABSTRACT

A description of chemically and magnetically ordered states, based on the binomial formalism, is presented. By this method, one can analyze all possible configurations that depend on the crystalline structure and the size of the basic cluster used for the description of the system. The procedure is outlined for a cluster of n sites and its application is illustrated for a 4-point cluster in fcc and bcc lattices. This cluster size is big enough to describe ordered alloys with magnetic atoms forming decorated ferromagnetic, antiferromagnetic, superantiferromagnetic and other more complex arrangements.

The understanding of phase stability, local order, and phase diagrams in magnetic binary alloys, has been the subject of extensive theoretical studies and to a lesser extent, of experimental investigations. The interdependence between chemical order and magnetic interactions in transition metal binary alloys has been reviewed in the past [1–3]. It is well known that the determination of the experimental phase diagrams is a complicated task that involves important metallurgical aspects that are related to the atomic mobility, since the equilibrium atomic distribution is determined by the interplay between the chemical interactions and the magnetic energy associated to the magnetic element. On the other hand, theoretically, the phase diagrams can be calculated to a good accuracy only within phenomenological theories. First principle calculations can be performed mainly to determine the ground state (zero temperature).

To determine the finite temperature phase diagram, on the basis of phenomenological theories, one has to find first the ground state configuration. This is a complicated task, since that state depends on the chemical composition, the interactions included in the Hamiltonian, the crystalline structure, and the geometrical cluster used as a basic unit for the statistical description.

Here, we describe a simple model, based on the binomial formalism, to determine all the different geometrical and magnetic structures in a binary alloy, A_xB_{1-x}, in which one of the components with concentration x, A, carries a magnetic moment. In this treatment we only allow that all the magnetic moments are collinear, in a ferromagnetic ($A_\uparrow$) or antiferromagnetic ($A_\downarrow$) orientation.

The total number of geometrical and magnetic configurations depends on the number of different spices that can occupy the lattice sites, in this case A (up or down) or B, and on the number of cluster sites n. In this particular example, this number is given by $(3)^n$. We use the binomial relation to describe all the configurations

$$[(A_\uparrow + A_\downarrow) + B]^n = \sum_{m=0}^{n} \frac{n!}{(n-m)!m!}(A_\uparrow + A_\downarrow)^m B^{n-m}, \tag{1}$$

with

$$(A_\downarrow + A_\uparrow)^m = \sum_{r=0}^{m} \frac{m!}{(m-r)!r!} A_\uparrow^r A_\downarrow^{m-r}. \tag{2}$$

However, in this case in which we consider only spin up or down orientations for the species A, and due to symmetry reasons not all the configurations are different. Furthermore, the number of non-equivalent configurations depends on the crystallographic lattice under consideration.

We illustrate the method by taking a 4-point cluster. Thus, the total number of states is $3^4 = 81$ and they are described by the relation

$$[(A_\uparrow + A_\downarrow) + B]^4 = (A_\uparrow + A_\downarrow)^4 + 4(A_\uparrow + A_\downarrow)^3 B + 6(A_\uparrow + A_\downarrow)^2 B^2 + 4(A_\uparrow + A_\downarrow)B^3 + B^4 \tag{3}$$

* Corresponding author.
E-mail address: joseluis.moran@ipicyt.edu.mx (J.L. Morán-López).
[1] Permanent address: Departmento de Física y Matemáticas, Universidad Autónoma de San Luis Potosí, San Luis Potosí, México.
[2] On leave from Departamento de Física, Laboratorio Interdisciplinario, Facultad de Ciencias, Universidad Nacional Autónoma de México, México, D.F. Mexico.

http://dx.doi.org/10.1016/j.ssc.2015.04.008
0038-1098/

The various terms correspond to alloys with concentration $x=1$, 0.75, 0.5, 0.25, and 0. The coefficients denote the number of options to accommodate the $A_\uparrow$, $A_\downarrow$ and B atoms in the cluster sites.

We now, specify the lattice under study and restrict to face-centered cubic (fcc) and body-centered cubic (bcc) crystalline structures. In the first case, the four-point cluster forms a regular tetrahedron in which all the sites are nearest neighbors and consists of 6 equal bonds. In the second case, the tetrahedron is irregular, with four bonds shorter than the other two. Thus, each atom has two nearest neighbors and one next-nearest neighbor.

The first term in Eq. (3), corresponds to the situation in which all the four sites are occupied by magnetic atoms. Thus one has to consider the following five arrangements:

$$(A_\uparrow + A_\downarrow)^4 = A_\uparrow^4 + 4A_\uparrow^3 A_\downarrow + 6A_\uparrow^2 A_\downarrow^2 + 4A_\uparrow A_\downarrow^3 + A_\downarrow^4. \quad (4)$$

The sum of the coefficients ($16 = 2^4$) is the total number of ways to occupy the cluster sites with $A_\uparrow$ and $A_\downarrow$. The first and last terms correspond to the cluster occupied by spins pointing in the same orientation; those states are equivalent and therefore degenerated.

In the case of the fcc lattice, from the 16 possible configurations only 3 are different; $A_\uparrow^4$, $A_\uparrow^3 A_\downarrow$, and $A_\uparrow^2 A_\downarrow^2$. The degeneracy for those states is 2, 8, and 6, respectively. These structures are depicted in Fig. 1; the lattice is drawn on the left-hand side and the 4-point cluster on the right. For a better visualization, we show in Fig. 1a a typical tetrahedron in the lattice and identify the atoms with numbers. A simple ferromagnetic arrangement is shown in Fig. 1a. In Fig. 1b we show the case in which one of the magnetic moments in the tetrahedron is oriented in the down direction. This produces a crystal with (100) ferromagnetic planes that alternate with planes that consist of antiferromagnetic arrangements. The case in which two spins point in one direction and the other two in the opposite one correspond to the phases known as AF1 and AF3 [4]. Those are formed by (100) planes with spins in the same direction but opposite between them (AF1) and planes with equal number of up and down spins (AF3). Fig. 1c corresponds to the AF1 phase.

The second term of Eq. (3), corresponds to the case in which one substitutes one magnetic atom by a non-magnetic one, i.e. $x = 3/4$. The various terms are the following:

$$4(A_\uparrow + A_\downarrow)^3 B = 4A_\uparrow^3 B + 12A_\uparrow^2 A_\downarrow B + 12A_\uparrow A_\downarrow^2 B + 4A_\downarrow^3 B. \quad (5)$$

The number of possible configurations sums 32, but the configurations $4A_\uparrow^3 B$ and $4A_\downarrow^3 B$ are equivalent. The same happens with the arrangements $12A_\uparrow^2 A_\downarrow B$ and $12A_\uparrow A_\downarrow^2 B$. Thus, one obtains only two different ordered magnetic phases which are shown in Fig. 2. In Fig. 2a all the magnetic atoms are ferromagnetically aligned and in Fig. 2b the (100) ferromagnetic planes alternate with planes containing the element B and the spin down atoms.

The alloy with equal number of magnetic and non-magnetic elements is described by the third term in Eq. (3).

$$6(A_\uparrow + A_\downarrow)^2 B^2 = 6A_\uparrow^2 B^2 + 12A_\uparrow A_\downarrow B^2 + 6A_\downarrow^2 B^2. \quad (6)$$

Here, despite the fact that the total number of configurations sum 24, only two are different. The crystal consists of alternate (100) planes with magnetic and non-magnetic atoms. In one case all the magnetic atoms point in the same direction (ferromagnetic dysyr) and in the other each plane with magnetic atoms are antiferromagnetically ordered.

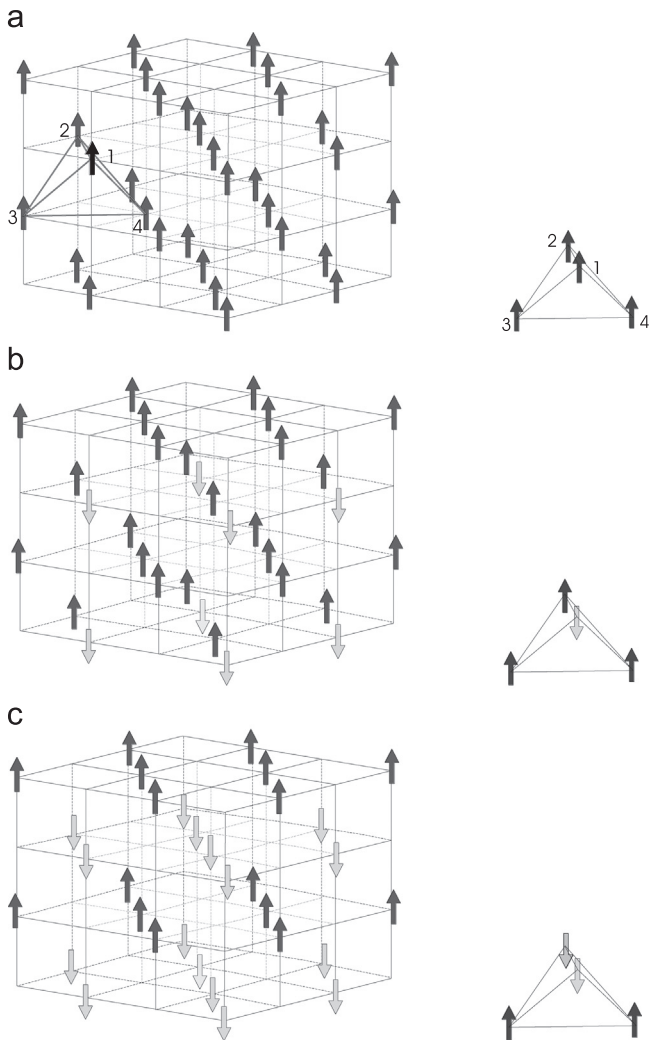

Fig. 1. The fcc crystalline magnetic structures generated by using a regular tetrahedron as a basic set (left figures) and the 4-point cluster occupation (right figures) for a pure magnetic element ($x=1$): (a) ferromagnetic, (b) with one of the four magnetic moments pointing in the opposite direction; (c) when two of the four spins point in the opposite direction. For a better visualization, we show in Fig. 1a a typical tetrahedron in the lattice and identify the atoms with numbers.

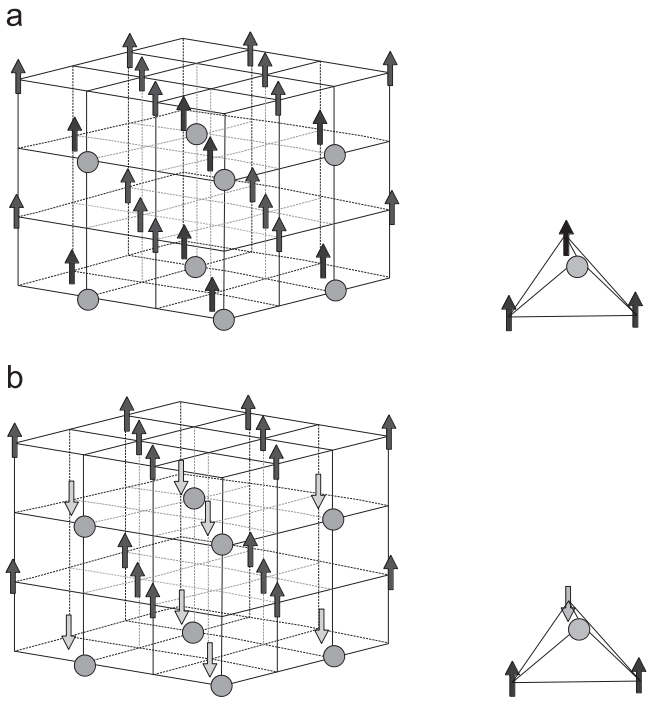

Fig. 2. The two fcc crystalline magnetic structures generated in alloys with $x = 3/4$. On the left (right) we show the lattice (the occupation of the 4-point clusters). (a) The ferromagnetic phase. (b) The phase produced when one of the magnetic moments points in the dawn direction.