Solid State Communications 149 (2009) 73–77

Contents lists available at ScienceDirect

Solid State Communications

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

A two dimensional Heusler alloy model

R. Rodríguez-Alba [a], F. Aguilera-Granja [b], J.L. Morán-López [c,*]

[a] Department of Physics and Mathematics, Universidad Autónoma de San Luis Potosí, San Luis Potosí, Mexico

[b] Instute of Physics, Universidad Autónoma de San Luis Potosí, San Luis Potosí, Mexico

[c] Center for Computational Materials, Institute for Computational Engineering and Science, University of Texas at Austin, Austin, TX 78712-0027, United States

ARTICLE INFO

Article history:
Received 6 March 2008
Received in revised form
1 August 2008
Accepted 7 October 2008 by R. Merlin
Available online 19 October 2008

PACS:
75.70.Ak
64.60.De
64.60.Ej

Keywords:
A. Magnetic material
A. Low dimensional systems
A. Heusler alloys
D. Ground states

ABSTRACT

A two dimensional version of a Heusler alloy $X_2Mn_cZ_{1-c}$ is presented. The Hamiltonian includes chemical interactions between nearest neighbors and magnetic interactions between first, second and third neighbors. The ground state phase diagrams at zero magnetic field and their range of stability with regard to the chemical and magnetic interactions are calculated by using the method of linear inequalities. The unit used in the calculation is a five point cluster, which allows describing an ordered alloy with the Mn atoms forming decorated ferromagnetic, antiferromagnetic, superantiferromagnetic and other more complex arrangements. Results for $c = 1/2$ and $3/4$ are presented.

The Heusler alloys, are ternary systems X_2MnZ that have been know since 1903 [1]. These systems have manganese as one of the main components and show a rich variety of magnetic phases, depending on the two other chemical components and on the temperature [2]. These alloys looked very promising for applications since the manganese atom has a magnetic moment close to $4\mu_B$. These ternary systems crystallize with $L2_1$ structure, and in general the X element is a noble or transition metal and the Z element has s and p valence electrons. According to a previous calculation [3] the role of the X atoms is to determine the lattice constant and the Z atoms mediate the interactions between Mn atoms.

There are more complex Heusler alloys in which the element X is also magnetic. Recently these kind of systems have been intensively studied owing to great potential for spintronics [4,5], magnetically driven actuators [6] and shape memory materials [7]. Two of those systems are Co_2MnGa and Ni_2MnGe, in which the magnetic properties of Co and Ni make the alloy more complex but at the same time richer in magneto-electronic behavior. In particular, the Co alloys has a density of states that show half-metallicity. i.e. the majority and minority spin bands show a metallic and semiconductor character. This makes this alloys attractive for applications in spintronics where the capability to inject electrically spin-polarized carriers into unpolarized semiconductors [8–10] is the key element. On the other hand, the Ni alloys are important as magnetic shape memory materials. Here we restrict to Heusler alloys with Mn as its only magnetic component.

This paper has a two-fold motivation. On one hand, a two dimensional model of a Heusler alloy may be more tractable than the three dimensional version and may serve to identify key parameters and recognize interesting features. In addition, due to the complexity of the three-dimensional Heusler alloys, the interplay of magnetism and chemical order, has been addressed only in a reduced number of theoretical studies [11,12]. The simplification to a two-dimensional system, let us study further the chemical and magnetic-order interplay, which rules the properties of these systems. Aware of the development of sophisticated techniques which allow one to deposit multiple chemical elements, it might be possible to grow in the future such two-dimensional systems.

Here, for the first time, we present calculations of the ground states of a two dimensional version of a Heusler alloy within a phenomenological model in which only pairwise interactions,

* Corresponding address: Universidad Politécnica de San Luis Potosí, Iturbide 140 Zona Centro, 78000 San Luis Potosi, Mexico. Tel.: +52 444 8342012; fax: +52 444 8342010.
E-mail address: jlmoran-lopez@upslp.edu.mx (J.L. Morán-López).

0038-1098/$ – see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ssc.2008.10.011

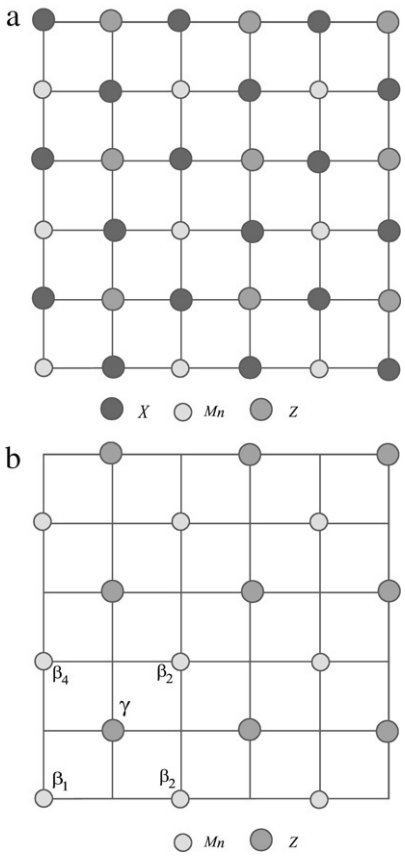

Fig. 1. (a) The two-dimensional Heusler crystalline structure showing the various sublattices occupied by the X, Mn, and Z elements. (b) The decimated lattice containing only the sites occupied by Mn and Z elements. The five-point cluster showing the β_i and the γ sublattices are also displayed.

chemical and magnetic, are included. The chemical interactions between nearest neighbors of type I and J are denoted by $V_{I,J}$. The magnetic interaction between the nth neighbor manganese atoms are denoted by J_n. In Fig. 1(a), we show the two dimensional Heusler lattice model considered here. It is a square lattice in which the four interpenetrating lattices are also square; two of them are occupied by the X atoms, and the other two by the Mn and the Z components.

Among the rich variety of behaviors, it has been found [2], there are alloys in which, in a wide range of temperatures, the X element does not interchange sites with the other components (Pd_2MnIn, Pd_2MnSn). Thus, the element X just provides the skeleton and one can ignore the two sublattices occupied by the X element and decimate these sets of sites. By applying this procedure, we obtain the lattice shown in Fig. 1(b), where we show only the two square interpenetrating lattices occupied by the elements Mn and Z.

In terms of the chemical and magnetic interactions, the total internal energy of the system can be written as

$$E = -\sum_{I,J} N_{I,J} V_{I,J} - \sum_{n}^{3} \sum_{i,j} (\sigma_i \sigma_j)_n J_n, \tag{1}$$

where I and J denote the Mn and Z atoms, σ_i and σ_j are the magnetic spins of Mn with orientation up ($\uparrow$) or down ($\downarrow$), and $n = 1, 2, 3$.

At low temperatures, positive values of $V_1 = V_{MnMn} + V_{ZZ} - 2V_{MnZ}$ drive the alloy to an ordered array while negative ones tend the alloy to separate into two phases. Furthermore, positive (negative) values of J_n favor a ferromagnetic (antiferromagnetic) alignment between the n-th Mn neighbors.

To calculate the ground states that can be attainable with the interactions considered in our Hamiltonian, we take the five-point cluster shown in Fig. 1(b). We denote the sites of the square vertex $\beta_i, i = 1, 2, 3, 4$, and the one in the middle by γ. One can notice that in this cell, the number of first, second, and third neighbors are $z_1 = 4$, $z_2 = 4$, and $z_3 = 2$, respectively. Since each site can be occupied by $Mn_\uparrow$, $Mn_\downarrow$ or Z, the total number of configurations is $3^5 = 243$, however, many of them are degenerate with a multiplicity λ_r. Here, we consider only ordering alloys and by taking into account the symmetry of the cluster one finds that the total number of different configurations reduces to 34. If we denote the probability to find the X_r configuration by x_r, it follows that

$$\sum_{r=1}^{34} \lambda_r x_r = 1. \tag{2}$$

There is a second constraint that has to be observed and involves the nominal concentration of Mn atoms in the binary system

$$\sum_{r=1}^{34} c_r \lambda_r x_r = c \tag{3}$$

where c_r is the concentration of Mn atoms in the cluster r.

Furthermore, this cluster allows to describe ordered arrangements corresponding to the concentrations $c = 1, 7/8, 3/4, 5/8, 1/2, 3/8, 1/4, 1/8$, and 0. In this communication we only report the cases of $c = 1/2$ and $3/4$.

In Fig. 2 we present the different arrangement possible within the five-point cluster in the case of the equiatomic alloy. All the figures represent a complete ordered alloy with the Mn atoms arranged with different magnetic patterns. It is important to notice that in this case there are no pairs of Mn atoms as nearest neighbors. In Fig. 2(a), the Mn atoms order ferromagnetically (F) and the phase is characterized by $J_2 > 0, J_3 > 0$. In Fig. 2(b) the manganese atoms are arranged in alternating diagonals with ferromagnetic and antiferromagnetic coupling (F–AF). This pattern has an equal number of ferromagnetic and antiferromagnetic second and third neighbor pairs. Thus the magnetic contribution to the energy is zero. A superantiferromagnetic (SAF) pattern is shown in Fig. 2(c). This phase has an equal number of ferromagnetic and antiferromagnetic second neighbor pairs and the third neighbor pairs are coupled antiferromagnetically ($J_3 < 0$). Finally, Fig. 2(d), represents the manganese atoms with antiferromagnetic order (AF). This phase is characterized by $J_2 < 0$ and $J_3 > 0$.

Now we proceed to calculate the ground state of the system as a function of the energy parameters. Since E is a linear function of the configurational parameters x_i, all possible ordered states are located inside a convex polyhedron in configurational space. The range of stability with respect to the interaction parameters is given by an hypercone with extreme rays defined by the normals to all phases of the configurational polyhedral converging to the vertex in question [13].

The results for the ground states for the equiatomic system depend on the energy parameters V_{MnZ}, J_2 and J_3. In Fig. 3(a) we show the results in the $V_{12} = V_{MnZ}/J_2$ versus $J_{32} = J_3/J_2$ space and assuming positive values for J_2. The only arrangements possible in this part of the phase space are the ferromagnetic state F, and the superantiferromagnetic state SAF. Since $J_2 > 0$ the states with ferromagnetic arrangements between second nearest neighbors are the ones that are stable. As mentioned above, the SAF is stabilized only by negative values of J_3. In the hatched area the energy is positive; i.e. the magnetic energy does not exceed the negative chemical energy that tends the system to form a segregated alloy.

We show in Fig. 3(b) the phase diagram in the $J_{3V} = J_3/V_{MnZ}$ versus $J_{2V} = J_2/V_{MnZ}$, for the case $V_{MnZ} < 0$. The possible stable states are the ferromagnet F, the antiferromagnet AF, and