Coordination Spheres Effect On Recomposition Atoms In AB Alloys

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ABSTRACT

This study focused on the variation of the long-range order parameters with temperature for nine coordination spheres. The computer simulation results showed several mechanisms of atoms disordering. These mechanisms are represented in: (Substitution point defect, Clusters and Segregations, Micro domain, Antiphase order and Antiphase boundaries.

As the number of coordination spheres increase, the interatomic interaction increase with a decrease in the ordered phase stability. In the initial stages of the computer simulation two phases in the alloy is found, an ordered phase of long-range order and ordered phase of antiphase domain. In final stages an ordered phase of short –range order is found.

الخلاصة

هذه الدراسة ركزت على تغير مدى الترتيب البعيد مع درجات الحرارة لتسعة محاور كروية. اظهرت نتائج محاكاة الحاسوب مكانيكيات لا ضطراب الذرات. هذه الميكانيكيات ممثلة بنقاط التشوه الاستبدالي، تجمعات ذرات من نفس النوع (**clusters**) ومن ذرات ليست من نفس النوع (**segregations**) ، مايكرودومين ،الترتيب اللا طوري والحدود اللا طوربة.

بزيادة عدد المحاور الكروية يزداد التفاعل ما بين الذرات مع انخفاض استقرارية الطور المرتب. وجد في المراحل البدائية لمحاكاة الحاسوب طورين في السبيكة طور مرتب طويل المدى وطور مرتب للدومين اللا طوري. ووجد في المرحلة النهائية طورمرتب قصيرالمدى.

INTRODUCTION

Alloys phase transformations have attracted great attention of scientific research for their important in technology applications. Therefore many studies in this field appeared experimental and theoretical studies.

Experimental studies [1-5] focused on changing of concentration of the material components with the temperature changes. While the theoretical [6-8] depended on the changing of vacancies concentration within the lattice with the temperature changes. The conclusion of quantum mechanics showing that atoms interaction energies faster than distance between atoms are used [9].

The results of experimental studies have difficult interpretation because of existence several different atomic processes which may occur simultaneously. Also, there were little theoretical studies about it. The computer simulation has a powerful tool to study the growth of lattice, phase separati4on, domain growth, and so on.

In present work we use computer simulation for studying the effect of changing of the coordination spheres of the lattice with temperature and the range of temperatures used in this study is under the critical temperature ($0.1T_C - 1.1T_C$), where $T_C = 900$ k.

MODELLING

A model corresponding to the Ising model [10] is used. Two – dimensions lattice cut from BCC and FCC crystals in planes (10) and (11) is used which its periodical block consists of 10000 atoms. The lattice contains a single vacancy and periodic boundary condition. The number A and B atoms is kept constant. The atomic radius is equal to the distance between two atoms in crystal. The atoms diffusion is produced as result of vacancy mechanism. The interaction between the A and B atoms change with the coordination spheres from 1 to nine.

More details of the model are determined in [11, 12]. The initial configuration for this type of simulation consists of a chain of A and B atoms. The disordering process start after giving the ordered system different values of coordination spheres. The temperature change (100-1000) k. The equilibrium state of system obtained after about 15-16 million time steps. The single vacancy does not affect the equilibrium state. The equilibrium state properties in this model are fluctuation of the ordering energy of alloy and the short- range order appearance.

RESULTS AND DISCUSSIN

Figure 1 and Figure 2 show several mechanisms of atom disordering. These mechanisms are represented in:

1. Substitution point defect.
2. Clusters and Segregations.
3. Micro domains.
4. Antiphase and Antiphase boundaries.

In this experiment (computer simulation) it is found that when the coordination spheres (Z) number is low, the ordering of the lattice will take the shape of the board of the chess as shown in Figure 1. Also its found a mono domain structure with many point substation defects appear at Z=1 as shown in Figure 1a, and that when the coordination spheres Z numbers increase, the

concentration of the substation point defects increase starting from Z=3, as shown in Figures 1b and 1c.

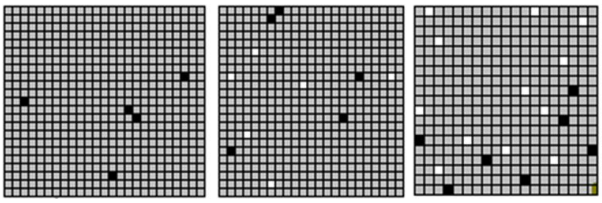

Figure 1: at T= $0.1T_C$ the equilibrium state of an ordered alloy including the substitutional points defects (black squares) at: (a) z=1, (b) z=2 and (c) z=3.

The interatomic interaction depends on the radius of coordination spheres (Z). Therefore the substation point defects at Z=2 and Z=3 tend to form groups of defects.
The degree of the long-range order (η) for the first three coordination spheres have been determined (η=0.92 at Z=1, η=0.89 at Z=2 and η=0.76 at Z=3).
When the number of coordination spheres gradually increases with temperature rise and the interatomic interaction increases, two phases in lattice observed: the first ordered phase represented in antiphase domains with long-range order(domains), as shown in Figure 2a.
The second phase represented in short-rang order (Micro domains, Clusters and Segregations), see Figure 2d.
In Figure 2b, the substitution point defects, with groups of a like atoms (Clusters) and unlike atoms(Segregations). These mechanisms are reduce the long-range order to 0.58. Also we foucs that the main contribution to disorder is from clusters 0.5. Clusters mechanisms can bring the long-range order down to 0.4.
At Z =3 we see new structures known as microdomains, these structure are shown in Figure 2c.

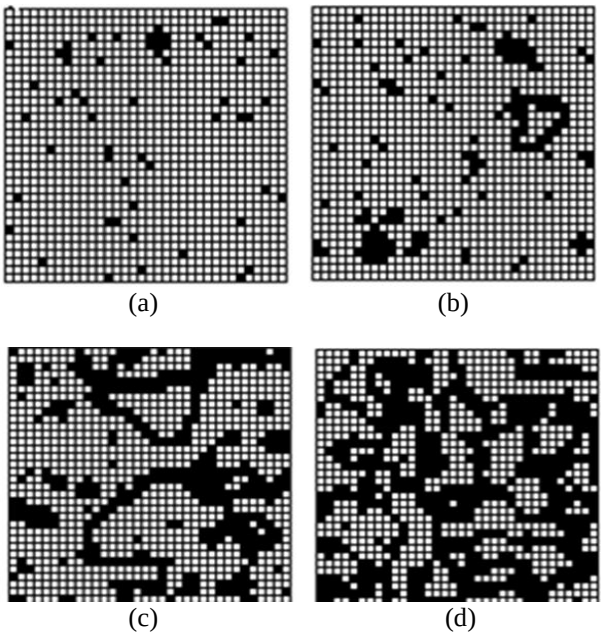

Figure 2: at T= $0.2T_C$ we can see the equilibrium state of an ordered alloy at: (a) z=1, (b) z=3, (c) z=4 and (d) z=6. The white area in the structure (domain) and the dark area the (antiphase domain boundaries).

In equilibrium state the behavior of the micro domains changed with the time, therefore, they unstable structures. These micro domains can occupy the entire volume of the domain and are separated from another by antiphase domain boundaries. If small micro domains exist inside the domain, the long–rang parameter will be less than 0.9. The structure of micro domains usually contains 100 atoms or less.
There is a possibility of finding a substitution point defects inside the micro domains Figure 2d. At temperatures below the critical temperature we observed a fluctuation of the micro domains inside domains. these fluctuations destroy the domains and probably forming clusters sites.
Figure 3 shows that the microdomains, clusters and segregations are increasing with temperatures. Because of these mechanisms, the long-range parameter decrease to 0.41.

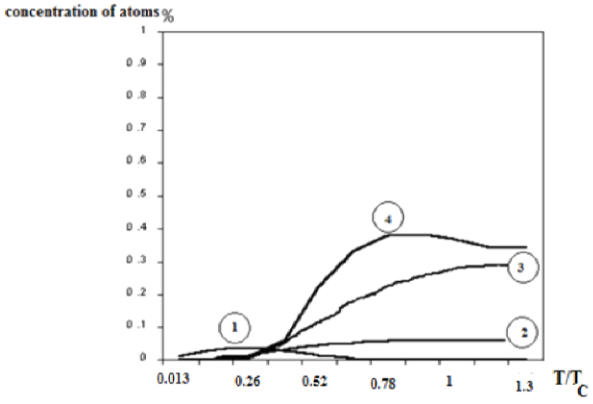

Figure 3: show the relationship between the concentration of the atoms in the different structures obtained and different temperatures. 1. The concentration of the atoms in substitutional point defects. 2. The concentration of the atoms in segregations. 3. The concentration of the atoms in clusters. 4. The concentration of the atoms in micro-domains.

At the first three coordination spheres the antiphase domain boundaries thickness contain few atomic layers causing small lattice disordering compared with the high numbers of coordination spheres. The long-range order behavior depend on the range of the temperatures that were chosen, and in the current study annealing temperatures (100–1000)K, below the critical temperature is chosen, Figure 4.

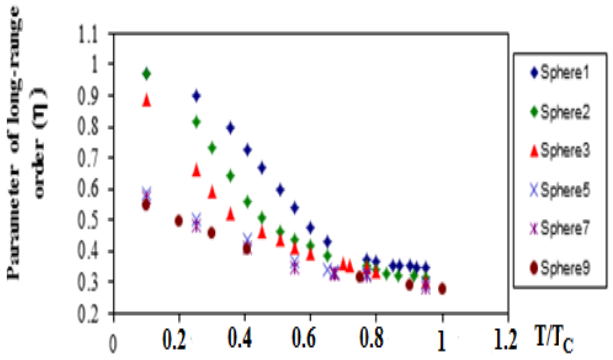

Figure 4: Long-range order parameter vs annealing temperature for the different coordination spheres

The ordered phase have a stability that depend on the domain and antiphase domain boundaries, the ordered phase stability decrease with an increase of the interatomic interaction. At z = 6, 7, 8, 9 the ordered phase stability rapidly decreases with an increase in the temperatures. Therefore the probability of existence of the short –range order phase becomes more.

At a temperature near T_C, the Clusters and Segregations remain in the lattice. The results goes parallel with Lindsey and Fultz [13].

They observed the ordering develops at low lattice coordination numbers with the vacancy trapping increases at the antiphase domain boundaries. Iveronova and Katselson [14] used x-ray diffraction to study many solid solutions metals and they found the long-range order parameters gradually decrease with increase in number of the coordination sphere.

CONCLUSIONS

The variation of the coordination spheres with temperature of AB alloy shows several mechanism of atoms disordering. These mechanisms are represented in point substitution defects, micro-domains, antiphase boundaries, clusters and segregations. It is found that an increase in the number of the coordination spheres leads to a decrease of the long-range order parameters and growth of the shot-range parameters. Accordingly, the correlation effects (three and four partial correlation) appear with the increment of interatomic interaction.

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