Computer simulation of the fine structures in A-B alloy

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Abstract

Computer simulation was used to study the fine structures of 2D- square lattice. The temperatures used in the experiment was below the T_C = 770k. Within this range of temperatures, the 2D- square lattice through a chain of successive non- equilibrium configurations which is achieved through the diffusion of atoms into vacant places of lattice .The equilibrium state has been obtained by averaging a number of runs (15-16) million time steps. In equilibrium state of lattice the results showed the existence of different kinds of the fine structures (microdomains, clusters, segregations and antiphase domain boundaries). At a temperatures above T_C, clusters and segregations appear and the concentration of atoms in clusters was 0.5 and in segregation 0.1. Also we noticed the changes in microdomains sizes with temperatures.

Keywords: computer simulation, alloy, diffusion, ordering (disordering process), structure, antiphase domain boundary, microdomain, clusters, segregation.

محاكاة الحاسوب للتراكيب الدقيقة في السبيكة A-B

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الخلاصة

تم استخدام محاكاة الحاسوب لدراسة التراكيب الدقيقة لشبيكة مربعة ثنائية البعد. درجات الحرارة المستخدمة في التجربة اقل T_C = 770k. ضمن هذا المدى من الدرجات الحرارة، تمر الشبيكة المربعة الثنائية البعد بسلسلة متتالية من الاشكال الغير متزنة والتي تحققت من خلال انتشار الذرات في موقع الفراغ للشبيكة. وقد تم الحصول على حالة الاتزان للشبيكة عن طريق حساب متوسط عدد الاشواط (15-16) مليون خطوة زمن . في حالة الاتزان الشبيكة اظهرت النتائج وجود انواع مختلفة من التراكيب الدقيقة (الحجيرة المايكروية ،العناقيد، التمييز وحدود اللا طورية). عند درجات حرارة اعلى من الدرجة الحرجة تظهر العناقيد والتمييز وتركيز الذرات في العناقيد كان 0.5 وفي التمييز كان .0.1. ايصا لاحظنا تغيرات حجم الحجيرات المايكروية مع درجات الحرارة.

كلمات مفتاحية: محاكاة الحاسوب، سبيكة، انتشار، مرتب (عملية غير مرتبة)، تركيب، حدود اللا طورية، الحجيرة المايكروية، العناقيد والتمييز.

Introduction

The fine structure has affected more physical properties and behavior of a material. There are many experimental and theoretical studies for understanding the behavior of the fine structures. The experimental studies depended on the change of the concentration of the material components with the temperature change or the pressure [1-6]. The results of the experimental studies had difficult interpretation because of the existence of several different atomic processes which may occur simultaneously. The theoretical studies depended on the change of vacancies concentrations or the change of the spheres coordination with the temperature change within the lattice [7-8]. The Bragg-Williams used approximation method, they found a relationship between the atoms interaction energies and configuration energy [9]. All previous investigations focused on the final results without passing through the stages of crystallographic structure formation. The computer simulation experiment allowed us to observe these structures and create many facts from successive images of atoms distribution.

We will focus on fine structures growth in lattice which undergo an order-disorder phase transition and discusses the relation of the fine structures sizes with the temperature. In this work two sorts of atoms (A& B) used occupying the square lattice periodically. The number of atoms (A & B) is kept constant in computer experiment. This study use stoichiometric composition (A_3B or AB_3) of AB alloy in computer simulation. We used temperatures below the critical temperature (T_C = 770k), where T_C is the temperature of long-range order disappearing in atomic system of 2D- square lattice.

Computer simulation experiment

We have used the 2D square lattice (rigid lattice) of BCC and FCC crystals, corresponding to the Ising model [10]. The lattice belong to the planes (100) and (111) (in two- dimensional lattice the planes representation in (10) and (11)). The block contains 10000 atoms with periodic boundary condition. We include a single vacancy. In first and second coordination spheres, the interaction between atom-atom and atom-vacancy are equal to zero.

The diffusion process is started after the temperatures change about 0 k. The state of system is changed in fixed time t_n. In this work the number of vacancy jump were the measure of process duration t_n= n,.

$$Q = \exp(-E_v / \kappa T) \qquad \text{- - - - - - - - - - - - - - - (1)}$$

Where Q= Probability.

K = Boltzman's constant .

E_V= activation energy.

T= absolute temperature.

On the other hand, Q may be expressed by the following form:

$$Q = \sum_{k=1}^{4} \sum_{l=1}^{2} p_{kl} \qquad \text{- - - - - - - - - - - - - - - (2)}$$

where p_{kl} = Probability of jump of k-th atom on l-th coordinational sphere in a vaacnt place.

The interaction energy between k-th atom and l-th coordinational sphere E_{kl} . The fraction of atoms in a system having maximal energy than E_{kl}, therefor the average energy of any atom can be exppressed in the following terms:

$$D_{kl} = E_{kl} + (E_{max} - (1-b)E_{kl})b \quad \text{- - - - - - - - - - - - (3)}$$

k=1,.., 4, l=1,..,2,

where b= parameter describes the temperature effect on ordering process.

Parameter b can be change from zero to unit.

$$b = 1 - \exp(-\chi T) \quad \text{- - - - - - - - - - - - - - (4)}$$

Where χ = the empirical model constant.

Now the probability p_{kl} defined as:

$$p_{kl} = Q(E_{max} - (1-b)D_{kl}) / A \quad \text{- - - - - - - - - - - - (5)}$$

$$A = \sum_{k=1}^{4} \sum_{l=1}^{2} (E_{max} - (1-b)D_{kl})$$

Where A = normalization constant.

The equations (1-5) are important in this model and belong to [11-15].

The process of ordering was included three stage:

I-initial diffusion (vacancy mechanism). II-Formation and growth of ordered regions-were named domains. III- Fine structures growth in lattice.

The equilibrium state of lattice obtained after 15-16 million time steps.

Results and discussion

The fine structures are generated in the lattice when the lattice undergoes a phase transformations brought about by changing temperature from $0.1T_C$ to 1.3TC.

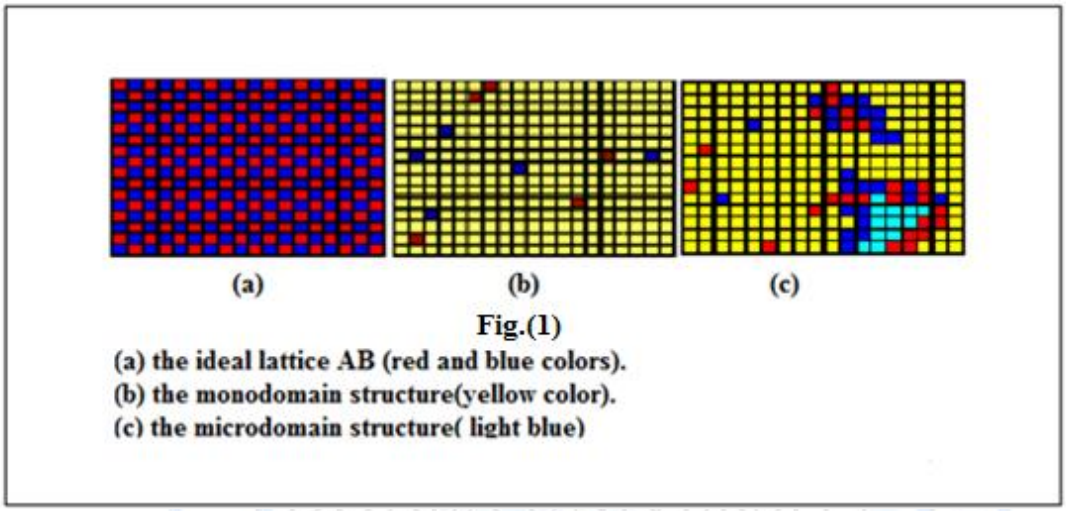


Fig.(1)
(a) the ideal lattice AB (red and blue colors).
(b) the monodomain structure(yellow color).
(c) the microdomain structure(light blue)

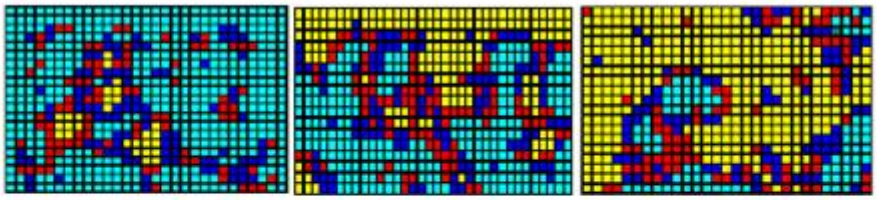
In figure (1a) show the ideal lattice for the used model at T= 0k, which is a big monodomain.

In fig. (1b) the lattice exposure to a temperature of less than $0.1T_C$, a substitution point defect appear inside the momnodomain, so that the long –range order parameter reduced to 0.95.

In fig. (1c) the lattice exposure to a temperature above $0.1T_C$, another structure start to appear with increment of substitution point defect and these structures are microdomains, clusters (groups of a like atoms) and segregations (groups of unlike atoms).

Microdomain usually contains 100 atoms or less. The behavior of the microdomains changed with the time in equilibrium state, therefore, they unstable structures.

The structure of microdomain inside the domain represent antiphase microdomain (APM). Also, the boundaries between domains are represented antiphase domain boundaries (APDB).

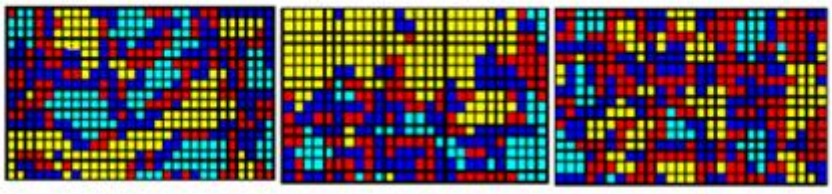


(a) (b) (c)

Fig.(2)

the microdomains,clusters and segregations are localized on the APB ·

In fig.(2a) the lattice exposure to a temperature above $0.2T_C$ antiphase microdomain(APM) and antiphase domain boundaries (APDB) appear. In fig.(2b) and fig.(2c) on lattice exposure to a temperature above $0.3T_C$, antiphase domain boundary(APDB) become more extended because of microdomains, clusters and segregations localization on it and this limit the diffusion of the atoms in the vacancies in the lattice, so we need to increase the temperature of the lattice to more than $0.3T_C$.



(a) (b) (c)

Fig.(3)

(a), (b) and (c) the structures of disorderd phase below the critical temperature.

yellow and light blue colors show ordered domains and microdomains, dark blue and red colors show point defects and structures(clusters and segregations) into APB.

In fig.(3a) and fig.(3b) lattice exposure to a temperature above $0.6T_C$ domain fluctuation starts inside the antiphase domain boundary(APDB). Where these fluctuations destroy the

large domains and small new domains appear. The long-range order parameter decrease to 0.59. This stage represent the beginning of the growth of the short–range order parameter.

At a temperature above $0.72T_C$,the domains destruction increase the number of microdomains, clusters and segregations. For this reason the long-range order decrease to 0.48, as in figure (3c). At the end of each stage during the simulation , we calculated the concentration of atoms (in relative unit) inside domains, microdomains, clusters and segregations . These calculations are plotted vs temperature, as in fig.(4).

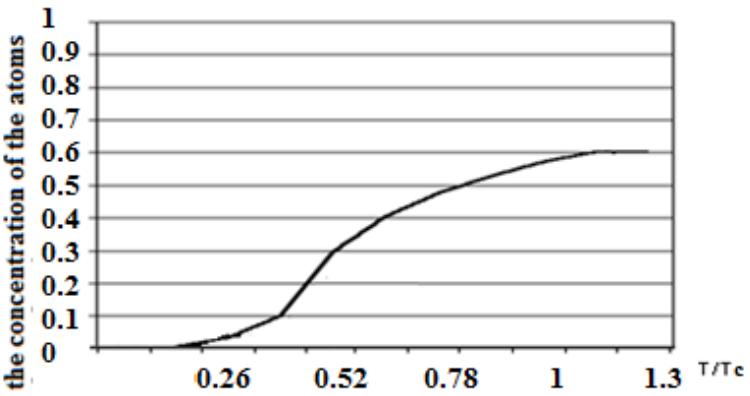


Fig.(4) the concentration of the atoms in clusters, segregatinos and microdomains. dependencies on temperature .

At temperature above T_C, microdomains disappear and clustres are formed. The concentration of atoms in the clusters and segregations reach to 0.6. The concentration of atoms in the segregations is 0.1 and that in the clusters is 0.5, so that the clusters are the main contributor to the disordering, For this reason the long-range order decrease son the long-range order decrease to less 0.30.

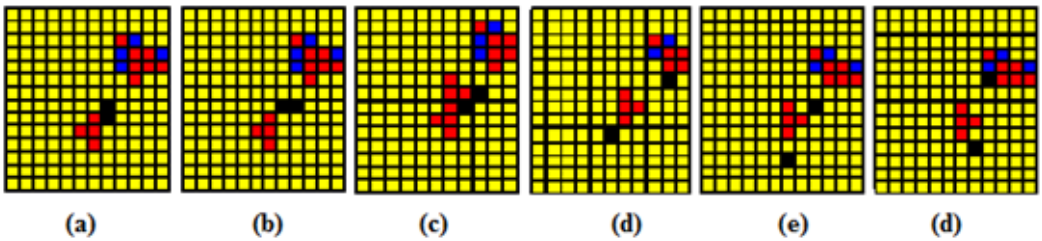


Fig. (5)

the segregations are fluctuation with simulation time in the equilibrium state of the alloy .

The segregation structure has a role in the disorder process through its fluctuation in the lattice which increase atomic distribution in addition to the vacancy mechanism, as in figure (5). There are many theories that describe the segregation mechanisms in complex system as mentioned in the reference[16].

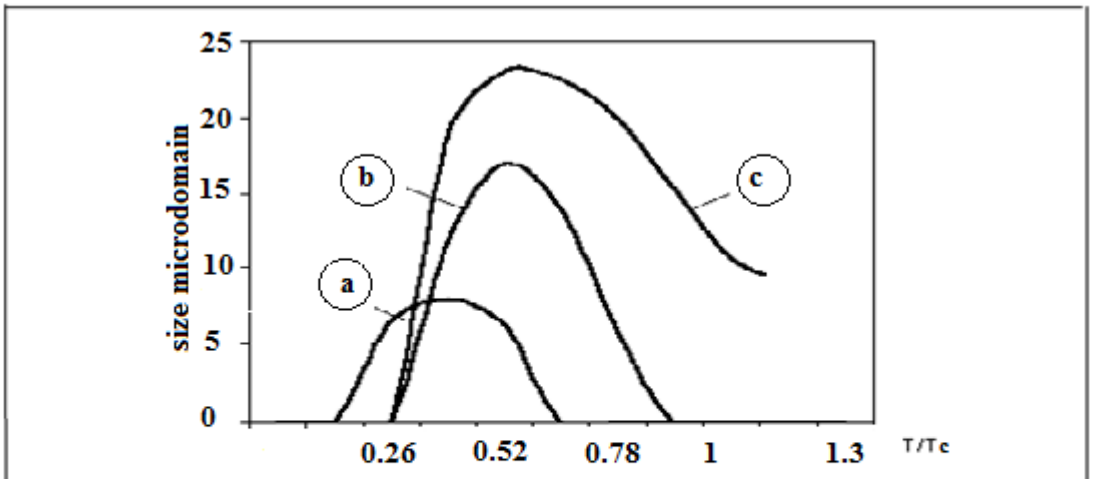


Fig.(6) the microdomains size dependencies on temperature.

(a) the microdomains sizes inside domains.

(b) the microdomains sizes in antiphase boundaries.

(c) the microdomains size in the short-range order stage.

Figure (6), shows the variation of the microdomains size (in relative unit) with temperatures in equilibrium state. The structure of a microdomain situated inside an ordered domain represents antiphase order and the maximum microdomain size is obtained at a temperature

of $0.4T_C$. The maximum microdomain size in the (APDB) is obtained at a temperature of $0.58T_C$. The disorder process proceeds as temperature increases. Some evidences exist that disordering proceeds more in the neighborhood of domain boundary than inside the domain, therefore decrease the domain size. So point defects can be found inside microdomains. As a rule, if small microdomains exist inside the domain, the order parameter will be at least 0.90. The fluctuation of microdomains inside the domain during disordering proceeds causing domain destruction and probably clusters will be formed from this destruction. The maximum microdomain size at this stage is obtained at a temperature of $0.66T_C$. At a temperature near T_C, the lattice disordering seems to have a more transition than lattice having ordered parameter ($T < T_C$). What distinguishes this stage is the appearance of short-range order and the lattice loss of ordered phase stability. The results are agree with Schwartz and Cohen [17], they found the probabilities to form clusters, segregations and short-range order of a binary AB alloy with N atoms. Fenske and Lott [18], used neutron diffraction to study the phase transitions in Fe_{50} Pt_{50} alloy as a function of annealing temperature at $T \ll T_C$ and $T \sim T_C$. And the current study results goes parallel with calculations of diffusion in FCC. binary alloys using the fly Kinetic Monte Carlo [19].

Conclusion

The appearance of fine structures in the lattice leads to a reduction in the long-range order parameters and the same time leads to a growth the short-range order parameters. The number and size of fine structures increases with the rise in temperature under T_C and at temperature near T_C the microdomain size of the short-range order start decrease. At temperature above T_C appear only clusters and segregations.

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