Transactions of the Materials Research Society of Japan. Vol. 20

Reseach of the binary alloy AB atomic structure reconstruction micromechnisms

M.D.Starostenkov, V.V. Evstigneev, O.V. Andruhova, N.V.Lomskikh and A.V.Borisov

General Physics Department, Altai State Technical University, Barnaul, Russia

In present communication we investigate the atomic structure reconstruction under the phase transition order-disorder. Only vacancy mechanism of atoms diffusion on lattice nodal points is considered. It was detected that structural phase transition happen by two-phase region. Order (disorder) process has complex character.

1. INTRODUCTION

The influence of different factors on the atomic structure of binary alloy AB on plane {100} is investigated using methods of computer simulation. Considering crystalographic plane contains 40000 atoms, which stiff bound with the site of the lattice.

The next basic zone with special character of ordering (disordering) were detected in the phase reconstruction process in the crystal: 1) the diffusional zone of total disordered block of the crystal; 2) the diffusional zone within the boundaries of the grain with the order's degree; 3) the diffusional zone in a region of crystal near by boundary between ordered and disordered grains; 4) the diffusional zone of exchange of point defects between two ordered domains, which contains APB.

The achieved alloy equilibrium states were analyzed in all a temperature range of order- disorder change. It is established that structural phase change order-disorder happen by two-phase region. Order (disorder) process has complex character so, here are several critical temperatures and according them, several fields temperature where the alloy has qualitatively different structures.

2. MODEL OF THERMOACTIVATED REGULAR SOLID SOLUTION TRANSFORMATION

The two-dimensional crystal cut in plane (100) (in two-dimensional model (10)) containing 40000 atoms has been simulated with calculation periodic boundary conditions. Atoms of two sorts are occupied the square lattice nodal points, statistical displace-ments and atoms oscilations are absend (lattice is hard). Some nodal points may stay vacant according to vacancy concentration. The concentration of thermal vacancies $C_v = 10^{-4}$ (one vacancy on the periodical block).

Only vacancy mechanism of atomic diffusion on lattice nodal points is introduced. The strainght exchange mechanism of two neighbouring atoms is unliked because it is connected with large lattice distortions and with large activation energies.

The interatomic interaction are described by constants non-equal to zero. Such approach brings about an certain flexibility in our model in parameters variation. Interaction between atoms with two coordinate spheres was taken into account. Interaction energies atom-vacancy was assumed zero. Choice of interaction energies between atoms was carried out in experiments for realization conditions of ordered alloy formation with varies superstructures. Material temperature is a constant on a time and in a space.

Then a initial state of sample (ordered or disordered alloy structure) is generated. The deviation of alloy composition on stoihiometric composition AB is milit. After that the diffusion process is started under the varies alloy temperatures and interaction energies.

System state is changed in fixed time moment. In present communication the number of vacancies jump were the measure of process duration. Probabilites for atom to jump in vacant node are depend on the releasing expending in interchange process energy magnitude and a material temperature. The gain (or the less loss) of energy is more then probabilities have more hight magnitudes. Moreover under the low temperatures the power factor play a general part while growth of temperature were loosen the power influence and jump probabilities for atoms of different sorts are equalized.

Depending on the interaction energies distribution by coordinational spheres the initial alloy structure may be transform during the ordered process into state with varies stable superstructures (chess, labyrinth, layer) [1]. Decay on monoatomic phases are possible too. All that structures are illustrated on fig.1.

We may to see only two types of antiphase domains in ordered alloy with chess superstructure.

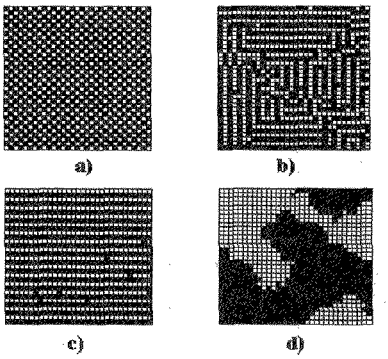

Fig.1. Stable superstructures realizing in ordered process under the varies interatomic energies distribution: chess (a); labyrinth (b); layer (c); decay on mono phases (d).

In layer superstructure there are antiphase domains of four types. Their packege give us labyrinth superstructure.

3. THE EQUILIBRIUM STRUCTURES OF THE ORDERED BINARY ALLOY

At the results of the reducing computer experiments we are obtained that there are fifth kinds of equilibrium structures for the alloy with the chess superstructures depending on alloy temperature. Temperature of order-disorder phase transition T is approximate 770K.

Only substitution points defects and small groups of such defects (clusters) take place in the alloy equilibrium state at the temperatures

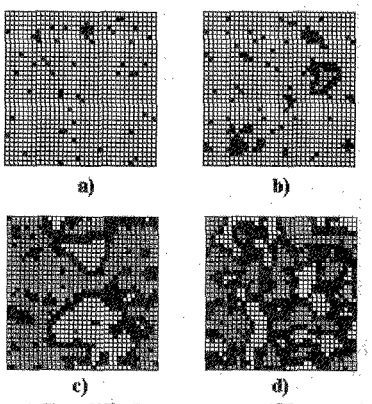

Fig.2.Equilibrium states of binary alloy depen-dining on temperature: a) $T=0,13T_c$; b) $T=0,26T_c$; c) $T=o,42T_c$; d) $T=0,65T_c$.

$0<T<0,26T_c$ (fig.2(a)). The concentration of their defects, number and size of clusters increase.

Except the described defects the nucleated and then disappeared antiphase microdomain are exist in the ordered monodomain at the temperatures $0,26T_c <T<0,4T_c$. The average microdomain size increase with the teemperature growth beginning with microdomain contained 20 and more atoms [2]. Total square occupying by microdomains is smaller then monodomain square. Fig.2(b) illustrate the alloy atomic configuration at the temperature $T = 0,26T_c$.

The situation sharply changes at the temperatures interval $0,4T_c<T<0,52T_c$. The volume fraction of two kinds antiphase domains are equalized on the average at a time. The antiphase boundaries with long length are appeared (fig.2(c)). There are several large domains in the equilibrium state having labyrinth structure. In accordance with anisotropy of APB energies the thermal APB (TAPB) with the orientation {11} dominate in crystal. TAPB with atoms B excess accounts for the greatest part of boundaries length. Since atoms B segregate on the APB than excess of atoms A are disposed inside domains volume as the point defects. In spite of that the shearing APB {01} (SAPB) energy below than the TAPB with atoms A surplus energy the part of last is rise above the first. If only APB {11} with atoms B excess and SAPB {01} existed in alloy than so much number of sort A point defects was bound to exist in crystal. The total energy of this defects (point defects and SAPB {01}) is very much and smaller number of point defects parallel with the substitution some part of SAPB on TAPB with atoms A excess is more energetic profitable. TAPB dual complex energy is smaller then SAPB energy.

The APB depth increases with the temperature growth. Some clusters and disordering microdomain parts are localized on APB where there are also groups or layers from segregated atoms. Such solid solution conduct with APB is conformed to theoretical predictions [3] and experimental dates [2]. It is one may to conclusion that the phase transition connecting with the size reduction of initial domain structure take place.

Ordered phase domains size is quickly reduced with the temperature growth. The microdomains volume fraction increases. Disordered phase zones (phase with short-range order) are appeared approximately at the $T = 0,65T_c$ (fig.2(d)). The ordered phase contains relativity large domains with clusters and microdomains patch; the disordered phase contains microdomains, clusters and segregations of pure alloy components. According to classical determination such alloy is in two-phase zone [2].

The alloy is in state with short-range order at the temperatures interval $T_c < T < 1{,}3T_c$. Under these temperatures the domain contains 100 atoms on the average and less. Obtained in computer experiments alloy structures completely are in agreement with microdomain model: small antiphase domains with thick APB or material layers containing disordered phase clusters or atoms segregations [2]. Such alloys structure is susceptible to temperature. In particular domains size is decrease with the temperature. Domains specific weight increases, layers between it thicken.

4. STATISTICAL CHARACTERISTICS OF BINARY ALLOY EQUILIBRIUM STATES

The first parameter characterized the phase transition kind is the volume fraction of ordered phase δ_{odr}. The volume fraction of disordered phase is $1-\delta_{odr}$ accordingly. Fig.3 presents the thermal dependencies of ordered (curve 1) and disordered (curve 2) phases. The two phase zone exists at the temperatures $0{,}3T_c$-T_c and order-disorder phase transformed is phase transition of the first kind [3].

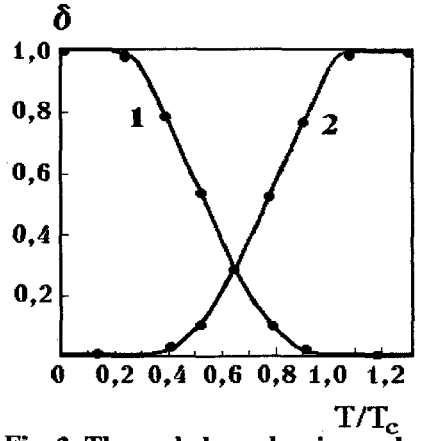

Fig. 3. Thermal dependencies ordered (1) and disordered (2) phases

Fig.4 shows the thermal dependence of long-range parameter $\eta(T/T_c)$ (curve 1) which was calculated only inside ordered phase domains. Curve 1 may be related to the first kind phase transition curves of the second kind with the continuous and all accelerating decrease of order parameter with temperature growth[3]. Nolinear of graph in temperature interval $0{,}65T_c$ - T_c is occurs by existence two phases in alloy under those temperatures. Curves 2 and 3 add transformation picture. Curve 2 gives the dependence of long order parameter $\eta'(T/T_c)$ inside domains and microdomains of ordered phase. There is the point of inflection at T/T_c ~0,31 which exist may be explained the phase with

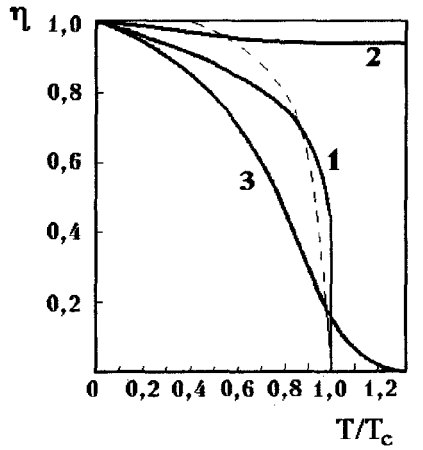

Fig. 4. Thermal dependence of long order parameters.

short-range order appearance. Further size reduction of domain structure with temperature causes to as that order parameter $\eta'(T/T_c)$ is turned a constant value. Curve 3 illustrates the thermal dependence of long-order parameter allowing for domains with long and short order and antiphase boundaries. The dotted curve describes the thermal dependence of long order parameter calculating in BGW approximation [3].

Fig.5 illustrated the thermal dependence of Cowley short-order parameters σ_{AB} in fifth coordinational spheres of equilibrium alloy [4].

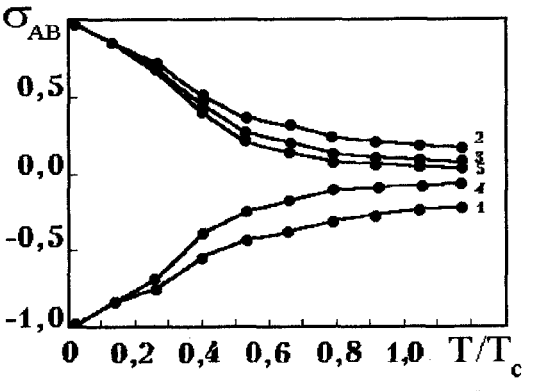

Fig.5. Thermal dependencies Cowley parameters. 1,2,...,5 - coordinational spheres number.

Dependencies has a bend at the T/T_c ~0,26. Under the low temperatures values of σ_{AB} practically do not depend on the coordinational sphere number. With temperatures growth short-order parameters are appeared to zero the

more quickly then high coordinational sphere number.

The next characteristics detected in computer experiment with ideal ordered initial alloy structure. In this case we can say about hereditary domains (order correspond order in initial state) and thermal ones. The numbers of point defects inside two types domains and total defects number in all considered crystal are functions of the total number of the vacancy jumpes K by different temperatures of the alloy. At this experiments is $C_v = 3 * 10^{-4}$. The evolution of the total number of the defects is developed equally independently of the temperature. In early moment the point defects are absent in the alloy then it is a stage of almost lineary increase their number and, finally, stage of the saturation. However the dynamics of change in the point defects number separate by the domain of different types is depend strong on the temperature. When the temperature is low as for example $T=0,2T_c$ a nuclear of the thermal activated domains are not detected practically. And as a consequence the point defects are concentrated in the hereditary domain.

At the case $T=0,35T_c$ a plotes of this functions separately by antiphase domains are an analogoue of a plot of the total number of defects. That is the volume fraction of the thermal domains in crystal at the beginning stage increased and then it is became stable and fluctuated near-by the some equilibrium value during the process of vacancy wandering.

During the first stage the number of the substitution defect within hereditary domain growth process go on, but then conception and fast growth of the thermal domain was brougth to lowering of the number of the substitution defect within hereditary domain owing to its volume decrease. The process of the secondary thermal domains formation numbers a few stages. First the point defects was united into a clusters, then the clusters grow up to the size of the unstable (that is short-existered by this temperature) microdomain and finally the separate microdomains increased to a stable size and formed final domain structure. During the time is flow the value of defects number in two types domains are equalized. That is indicated about equalization of the volume fractions of different types domain. The equilibrium number of substitution defects is depend of the vacancy concentration by the given value of the temperature. This dependence redused to the weak increase of the defects number when the C_v increase.

That was explained by the presence of short-existened defects near-by the vacancy. This defects were destructed soon after they came into being with large probability. Let us note decrease of the relative increase of the defect concentration near by vacancy when the temperature is grow. When the temperature is $0,013T_c$ then $C_n=0.0042$ on the average by the crystal and $C_n = 0.0095$ at the two first coordinational spheres that is 2.26 times as large. If the temperature is $0,13T_c$ then this increase was formed 2.05. When the temperature grow this tendency was saved. Availability near-by the vacancy heigtened concentration of substitution defects explaining above-noted weak increase of this defects in the alloy when the vacancy concentration increase.

5. CONCLUSUON

In present paper results of computer simulation of equilibrium states of ordered alloy with square lattice described. Some parameters of equilibrim states were obtained. It is shown that equilibrium states of the alloy suffer number of qualitative changes with the temperature growth. It is noted the elevated concentration of substitution defects near-by the vacancy. By experiments determine that the order-disorder phase transition arises through two-phase zone. The disordering is realized on structural objects: at low temperatures there are substitution point defects and their clusters in alloy; further microdomains are added; antiphase boundaries are appeared at the approach to the critical temperature. The disordering compound character gives rise to exist several thermal bands in which alloy has varies structures. The simulation showed that the real transition order-disorder have more compound character then the statistical theory of atomic ordering predict.

REFERENCES

1. Grinberg B.A., Syutkina V.I. , New methods of ordered alloys strengthen, Moscow, Metallorgy, 1985.
2. Popov L.E., Koneva H.A., Tereshko I.V., Deformation strengthen of ordered alloys, Moscow, Metallorgy, 1979.
3. Smirnov A.A., Molecular-kinetic theory of metalls, Moscow, Science, 1966.
4. Cowley J.M. Phys. Rev., vol. 138A (1965) 1384