THE MICRODOMAIN ROLE IN THE PROCESES OF THE ORDER-DISORDER PHASE TRANSITION. MICRODOMAIN STRUCTURE IN THE SHORT- AND LONG- RANGE ORDERED PHASES

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It was experimentally recognized that under the temperatures higher than the temperature of order-disorder phase transition (ODPT) T_k, the solid solution was in the state, having short - range order of atomic positions at the cell knots of the crystal. The analysis of the difraction pictures showed the existence of the stable microdomain structure under the temperatures, which are slightly higher than T_k. The computer experiment results showed the probable role of the microdomains in the ODPT behavior. The specific points within temperature interval of the order-disorder phase transition were defined including temperatures of the microdomain formations and their merge into one phase having short-range order in the arrangement of atoms. The peculiarities of the alloy microdomain structure and the probable localization of microdomains in the volume were found. Segregations, clusters and microdomains were distributed at the antiphase boundaries from the volume of the long-range ordered phase with the growth of temperature, which lend to their erosion and, as a result, to the transition from antiphase boundaries to the interphase boundaries.

1. Introduction

The problems, connected with order-disorder phase transformation (ODPT) have been investigating for a long time. Until recently the attention was paid advantageously to the grade of alloy ordering and to the means of it's reaching. The displacement of foreign knots by the alloy atoms components – the formation of point defects of substitution (PDS) was traditionally considered as the main mechanism, leading an alloy to disordered state (with the parameter of long-range order $\eta<1$). Main researches, concerning statistic theory of atomic ordering, are based on this theory [1-4]. The parameter of correlation is the single effect of atomic interactions, which taken into account by the statistic theory of atomic ordering. It shows, that the considering volume of solid solution exceeds the value, determined only by the order parameter. However, the problem of local position of atoms, causing the effect of disordering was not analyzed, as a rule, in the limits of statistic theory. To explain all the effects of disordering process was impossible only at the expense of PDS.

But, there are definite theoretical [4-6] and experimental data [7-9], which prove that disordering effect is not caused only by PDS. The other mechanisms, decreasing alloy order, are also important. One of possible disordering mechanisms is the formation of microdomains. Several models of short-range order were suggested. They were based on the conception, that microdomains were local spheres, having maximum sizes 2,5-5 nm and high grade of the atomic order in them ($\eta\geq0,5$). The models were divided into monophase and diphase ones according the all volume, occupied by microdomains. In the fist model, microdomains occupied all the volume and were divided by antiphase boundaries. In the second model, microdomains could be divided by nearly disordered spheres of material or by microdomains with the other type of short-range order in them.

It was experimentally shown, that microdomain structure realized mainly near the temperature of ODPT (T_c) and higher [4]. It is possible that point defects of substitution can unify into microdomains at their accumulation and at temperatures lower than critical one. Separate experimental data indicate on it [10].

FIn real experiment, it is practically impossible to determine the peculiarities of alloy microdomain structure and localization of microdomains in material volume. In this connection, the computer experiment, realizing the processes of ordering and disordering from different initial states, is actual and add reliable information to available data.

2. Methods of experiment holding. Start structures of the material

The simple model [11] of the diffusion of alloy atoms at the knots of the crystal lattice, suggested and approved earlier by the authors, is used in the given research. The model has the

following parameters. There is the dimension and the type of the lattice, the concentration of alloy components and the number of vacancies, the distribution of temperature in the calculated sphere, the energies of atomic pairs bond and the length of interatomic interaction potential (the number of coordination spheres).

The two-dimensional cut of FCC crystal with hard square lattice is considered in the present work. The size of the crystal block was 100x100 atoms and periodical boundary conditions were used. The concentration of alloy components corresponded to stoichiometric composition of AB, equilibrium concentration of thermal vacancies – 10^{-4}. The computer experiment was carried out in the conditions of isothermal annealing – T(x,y,t) = const. The radius of the interatomic interaction varied from two to nine coordinational spheres. The energies of atoms bond of different types in the dependence on the radius of coordinational sphere were chosen in the experiment to make the structure of alloy with the chess position of atoms of different types at the knots of square lattice be energetically profitable at the ordering. The jumps of atoms into a vacant knot from the first two coordinational spheres (L=2) were permitted.

The computer experiment was held according the following scheme: 1) generation of start state of the alloy; 2) starting up of vacancy mechanism of atomic diffusion at the knots of the crystal lattice; 3) the ordering process can break at reaching of equilibrium state by the alloy.

Ideally ordered structure (chess order of atomic position) and disordered structure of solid AB composition were considered as the start configuration of the experiment.

In the dependence on time and temperature, the pictures of atomic distribution at the knots of the crystal lattice and vacancy position were fixed. Then it was restored some characteristics of the developing process and the equilibrium structures of the alloy. There is

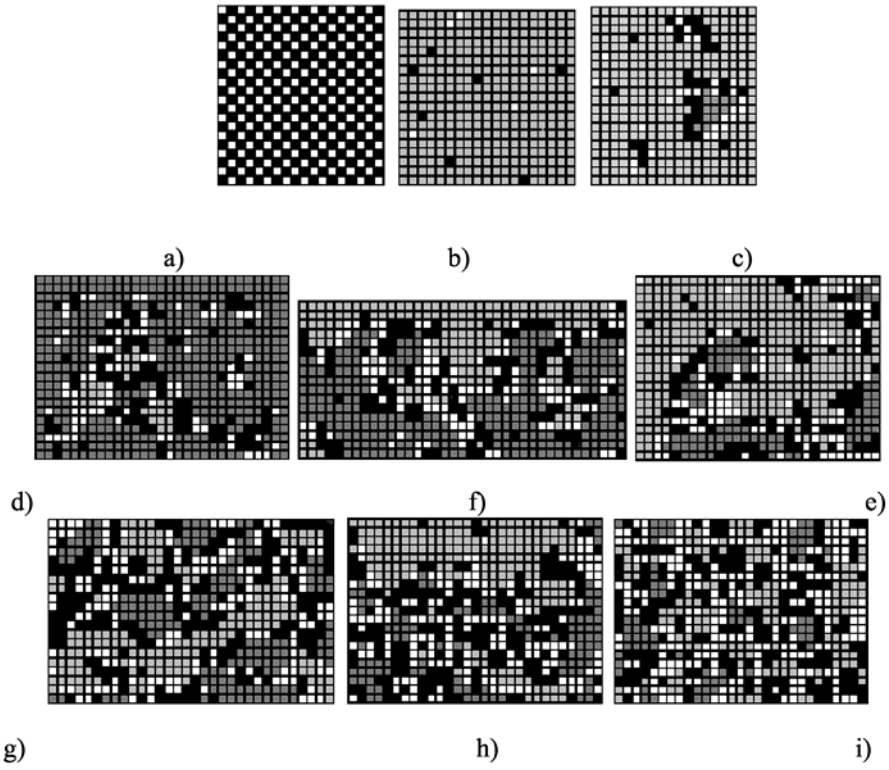

Fig.1. The equilibrium structures of the alloy: the ideal ordered structure (a); monodomain with the point defects (b); microdomains into ordered (c) and disordered (d) phases ($T\sim0,26T_c$); microdomains, clusters and segregations localized on the APB ($T<0,58T_c$) (e, f); fluctuation domains into disordered phase ($0,64T_c\leq T<T_c$) (g, h); structure of the disordered phase under the temperatures higher than T_c (i). Grey and light grey colors show ordered domains and microdomains. Black and white colors demonstrate point defects position and structure of APB, phase with short-range order, clusters and segregation

average energy of the alloy, the entropy, parameters of short-range and long-range order, volume parts of ordered and disordered phases, the number of microdomains and domains and their distribution according sizes, the average size of domains of ordered phase and others.

3. The role of microdomains in ODPT

For the analysis of the contribution of different mechanisms in the process of disordering only equilibrium structures of the alloy, forming in the process of ordering (disordering) are studied. All the realized structures can be divided into five types (Fig.1). The first types are the structures, received at low temperatures of the annealing $T/T_c \leq 0,2$. The equilibrium state is characterized the presence of the ordered monodomain with structural peculiarities in it. At the temperatures lower than $0,026T_c$ only PDS of different types are observed in the domain. The temperature dependence of point defects concentration (C_{PDS}) is shown in Fig.2. It is worse to note, that this dependence grows till the temperature of about $0,32T_c$, then the concentration of point defects decreases, asymptotically approaching to zero asymptotically at temperature $0,8T_c$. The calculations show, that the grade of long-range order does not exceed $0,95 \pm 0,02$ at the moment of the highest concentration of PDS. The concentration of PDS does not exceed 0,03. It means, that the isolated defects (in the limits of the investigated model) can not lead to the considerable disordering of the alloy. Earlier, the possibility of such effect in the statistic theory of the atomic ordering has not been predicted.

Clusters and segregations appear in the alloy beginning from the temperature of about $0,13T_c$. They are evidently main mechanisms of decreasing of long-range order. At least, the concentration of atoms, situated in the clusters and segregations near the critical temperatures T_c, comes to 0,6. Relatively small part (C_{segr} ~ 0,1) is related to segregations of atoms. The clusters make main contribution to the disordering ($C_{cl.}$ ~ 0,5). This mechanism can provide the decreasing of order to 0,4. Of course, this value is maximum one. The appearance of the segregations and clusters at low temperatures is stipulated by the decreasing of the energies of point defects at their junction. The distribution of atoms in them restore the lost regular bonds at the first and the second coordination spheres, increasing the parameter of pair correlation. The point defects do not make positive contribution to the parameter of pair correlation.

The increasing of temperature (to $0,2T_c$ – $0,35T_c$) leads to the appearance of new structural formations – microdomains. Microdomains are ordered domains, where the number of atoms does not increase 100-110. This criterion is stipulated by the alloy structure at the temperatures higher than T_c. Microdomains are non-stable, they born and disappear, forming clusters at the clapping. But their presence is a typical detail. At the temperatures $0,26\text{-}0,28T_c$, the formation of small “islands” of the phases with short-range order (structural unification of clusters, segregations and microdomains) is observed in the equilibrium alloy structure (Fig.1(d)).

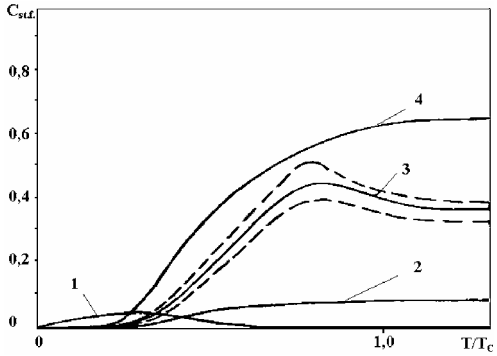

Fig.2. The temperature dependencies of the atoms concentration in the different structural formations. The curve 1 shows the concentration of the point defects. The curve 2 shows the concentration of the atoms in the segregations. Curve 3 shows the concentration of the atoms in the microdomains. Curve 4 shows the concentration of the atoms in clusters, segregations and microdomains

At the increasing of temperature ($0,35T_c \leq T < 0,42T_c$), microdomains, reaching critical size, grow and two or more antiphase domains form in the alloy. Domenization of the equilibrium structure of the material with the formation of extensive antiphase boundaries (APB) takes place. At these temperatures, the structure of the APB has no peculiarities, they are “pure”. The following increasing of the experimental temperature ($0,42T_c \leq T < 0,65T_c$) leads to the increasing of the number of antiphase domains and to the decreasing of their sizes. The domain structure of the alloy becomes shallow. The structural peculiarities – clusters, segregations and microdomains – appear to be localized at the APB, the phase with short-range order “precipitate” in the environment of the antiphase boundaries.

Then, the influence of temperature growth is observed in the effect of the APB "washing" and their gradual transition in the disordered phase with short-range order; the interphase boundaries appear; the ordered domains gradually transform into microdomains. At the temperatures higher than T_c, the alloy has only the phase with short-range order, which is sensible to temperature. The microdomains becomes shallow with the further growth of temperature.

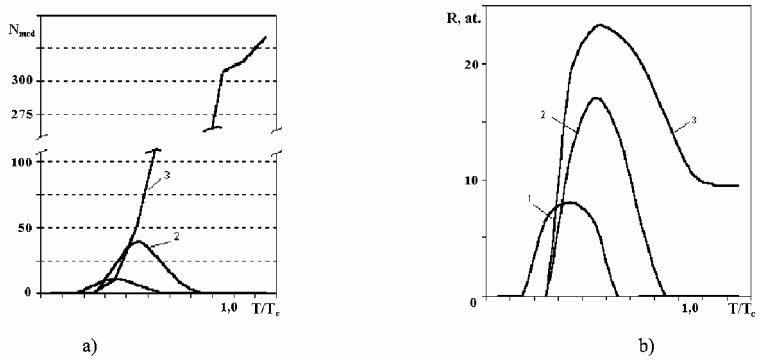

Fig.3. The temperature dependencies of microdomains number (a) and their average size (b). Curve 1 illustrates the microdomains inside ordered antiphase domains. Curve 2 shows the microdomains at the antiphase boundaries. Curve 3 shows microdomains in the phase with short-range order

4. The structure of microdomains and their localization in the material

The structure of the microdomains, situated inside the ordered domains, represent an antiphase order related to surrounding material, separated by the micro antiphase boundary (micro APB).

Point defects can take place inside microdomains, but small microdomains are perfect, as a rule ($\eta \geq 0{,}98$). Micro APB, separating microdomains from surrounding ordered solid solution, are "pure" enough. The part of such structural formations, as clusters, micro-segregations, situated on them is insignificant. The width of such APB is small, because fluctuational microdomains form instead of clusters. The long-range order parameter η on them is high enough (not lower 0,85).

Let us further analyze the localization of microdomains in the volume of the investigating material.

Fig.3(a) shows temperature dependencies of the microdomains number inside the domains of the ordered phase (the size of more than 100 atoms)(the curve 1), at the APB (the curve 2) and in the phase with short-range order (the curve 3). With the growth of temperature, the number of microdomains inside big domains increases till reaching the temperature $0{,}36T_c$, and then decreases. Such behavior of the curve (1) is stipulated by the domenization of the alloy structure and the presence of extensive the APB with the structural peculiarities on them ($0{,}38T_c$ – $0{,}71T_c$) in the equilibrium structure of the alloy and appearing of the phase with short-range order (beginning from the temperature $0{,}28T_c$). The break at the temperature $0{,}39T_c$ is stipulated by the sharp increasing of boundaries length and, consequently, by the increasing of microdomains number, "sticking" to the APB. The influence of the phase with short-range order is insignificant at this stage, it is localized at the APB.

The number of microdomains near the APB grows till the temperature $0{,}58T_c$. It is worse to note, that the number of microdomains in the phase with short-range order at this temperature is the same, as at APB. It means, that the numbers of atoms in the phases with short- and long-range order in diphase systems become equal. The increasing of temperature leads to bigger shallowing of the alloy domain structure and the increasing of domains number in the phase with short-range order in the localization of atoms. The number of microdomains at APB and in the domains of ordered phase decreases, asymptotically approaching to zero at the temperatures near the $0{,}9T_c$.

Fig.3(b) demonstrates the changing of the microdomains of average size inside the ordered domains (the curve 1), at the APB (the curve 2) and in the phase with short-range order (the curve 3) with the growth of annealing temperature. The average sizes of microdomains inside the antiphase domains, at the APB and in the disordered phase reach maximum values at the temperatures equal to $0{,}41T_c$, $0{,}48T_c$ and $0{,}66T_c$ correspondingly. The behavior of the curves and shear of its peaks relatively each other along the temperature axis illustrate the contribution of different mechanisms of the disordering into formation of the equilibrium structure of the alloy. The difference in half-width of dependence graphs of the microdomains average size demonstrates

temperature spheres of the existence of the ordered domains, the APB and the phase with short-range order.

There are some differences of opinions, concerning statistic theory of ordering, working with average integral parameters, and microdomain models. Statistic theory, taking into account at least pair correlations, give the value of order parameter in partially disordered alloy always bigger than zero. Such effect appears only at the formation of clusters from point defects, situated in antiphase positions. Evidently, microdomains is the only way of realization of such configuration.

5. Conclusion

In the limits of the computer experiment, it is established, that there are several mechanisms, leading the alloy to the disordered state: point defects, clusters and segregations, microdomains and APB. Clusters and microdomains intertransform easily at the accident wandering of vacancies. With the growth of temperature, the disordering realizes in the result of localization at APB of clusters, segregations and microdomains. These mechanisms can not be considered separately. The structure of model alloy at the temperatures near T_c fully corresponds to the notions of microdomain model: small antiphase domains with thick layers of APB or layers of the material, containing disordered clusters or clusters with the prevailing of one of alloy components. Such correlation of the simulation results and the formed notions is a good acknowledge of the correctness of the chosen approach and it's realization.

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