

THERMOACTIVATED STRUCTURE REARRANGEMENTS IN A BINARY Cu_3Au ALLOY UPON DEVIATION FROM STOICHIOMETRIC COMPOSITION

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UDC 539.2

Thermoactivated structure rearrangements at the micro-, meso-, and macroscale levels in a binary Cu_3Au alloy are investigated for the case of deviation from stoichiometry.

INTRODUCTION

The order–disorder phase transition is one of the types of phase transitions occurring in metal alloys in condensed state. Distinguishing features of this transition are a diffuse character of the transformation and a correlation between the short- and long-range ordering of atomic arrangement with the phase symmetry groups, i.e., the distinctive features of the system. Investigation of the origin and fundamental principles of the order–disorder (O–D) transformations in metallic solid substitution solutions were initiated back in early XX century and have been pursued until today. The interest in the O–D phase transition is still profound as this transformation is quite common in metal alloys and strongly affects their properties.

Investigation of atomic arrangement and its effect on alloy properties has a long background history and has been extensively reported in the literature [e.g., 1–22].

The authors of this work are unaware of any studies of the order–disorder processes in condensed systems performed concurrently at the micro-, meso-, and macroscale levels. It is for this reason that we aim at investigation of the process of ordering in a condensed system as a function of its temperature and composition. We believe a binary Cu_3Au alloy to be a reasonable object for investigation in this case as the literature contains a vast body of data on its experimental and theoretical studies [1–22].

Relying on a diffuse character of the process of the O–D transition, it is natural to assume a vacancy diffusion mechanism. It is, however, necessary to take into account that, when we set a vacancy concentration in a model system close to an experimental system, ordering is very fast and intensive. In order to study the process in detail, it is useful to “decelerate” diffusion, prescribing a lower vacancy concentration in the model.

If we start from a disordered state of a system, it becomes possible, using a stochastic Monte Carlo method, to obtain equilibrium configurations of the system with prescribed component concentration in a certain temperature interval.

THE MODEL AND EXPERIMENTAL PROCEDURE

The objects under study were model binary alloys of a Cu–Au system with the following copper content: 70 at. % Cu (Case 1), 75 at. % Cu (Case 2), and 80 at. % Cu (Case 3). These are fcc-alloys, with the stoichiometric

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alloy having an $L1_2$ superstructure in a completely ordered state, and an $A1$ superstructure in a disordered state.

The alloy atoms are in the lattice sites in accordance with the prescribed component concentrations, with the initial state being disordered. The size of the computation grid of a crystal has $36 \times 36 \times 36$ unit fcc-lattice cells, the number of atoms $\sim 2 \cdot 10^5$, and use is made of periodic conditions at the grid boundaries. The temperature is set to be constant and uniform throughout the computation grid. Since during simulations of structural atomic rearrangements a vacancy-induced diffusion mechanism is assumed, so one vacancy is randomly introduced into the alloy, and two coordination spheres, as the most probable, are used to limit the atomic hopping radius.

In a pair-interaction model, the configuration energy of a binary alloy will be given by the following:

$$E = -\sum_{i=1}^{N_s} [N_{AA}^i \phi_{AA}^i + N_{BB}^i \phi_{BB}^i + N_{AB}^i \phi_{AB}^i],$$

where $\phi_{AA}^i, \phi_{BB}^i, \phi_{AB}^i$ are the opposite-sign interaction energies of the atomic pairs AA, BB, AB , respectively, at a distance equal to the radius of the i -th coordination sphere, $N_{AA}^i, N_{BB}^i, N_{AB}^i$ is the number of the respective atom pairs in the i -th coordination sphere, and N_s is the number of interaction spheres taken into consideration.

From the initial disordered state of the system, equilibrium configurations with predetermined component concentrations (Cases 1–3) were obtained using a stochastic Monte Carlo procedure in a certain temperature interval. The state of the alloy was assumed to be equilibrium and stable, if the parameters characterizing the system (energy, ordering parameter, entropy) remained unchanged for as long as necessary, with the system being unable to quit this state without external actions. While the condition of achieving an extremum of some macroscopic characteristic is generally taken as a criterion of equilibrium, in our approach an exact dynamic behavior of the system is replaced by discrete states wherein one step of integration corresponds to one event of atomic self-diffusion following a vacancy mechanism. In each integration step, we calculate the probability of one of atoms in the vicinity of a vacant site occupying this site, bearing in mind that the probability of an atom i hopping into a vacant site j in the lattice exponentially depends on temperature

$$P_{ij} = A \cdot \exp\left(-(\Delta E_{\max} - \Delta E_v^{ij}) / kT\right),$$

where k is the Boltzmann constant, T is the temperature, and A is the normalization factor. The sums of probabilities of hopping for the atoms located at a distance of the first and second coordination spheres from the vacant site is equal to unity, i.e., $\sum_{ij}^n P_{ij} = 1$, where n is the number of atoms located in the first and second coordination spheres from the

vacancy. The value of the energy released (spent) ΔE_v^{ij} is estimated separately for each atom i surrounding the vacancy j in the first and second coordination spheres and is found to be equal to the difference between the energy of the i atom bonding in the position of the vacant site E_k^{ij} and the energy of the i atom bonding before hopping E_n^{ij} , i.e., $\Delta E_v^{ij} = E_k^{ij} - E_n^{ij}$. As a result, a maximum energy is selected from all values of ΔE_v^{ij} and is denoted as ΔE_{\max} .

In order to identify the phases (in this case A_3B, AB, AB_3 and phases of pure components) formed in the course of structural changes, use was made of a technique based on determination of the number of bonds of different atoms in the first coordination sphere corresponding to each structure. This means that the structure of phase A_3B is derived for an A kind atom as the number of bonds in the first sphere $A-A$, equal to 4, and $A-B$ equal to 8, and for a B kind atom, the number of bonds $B-B$ is equal to 4 and that of $A-B$ is equal to 8. The structure of phase AB_3 is determined for a B kind atom as the number of bonds in the first sphere $B-B$, equal to 4, and $A-B$ equal to 8, and for an A kind atom the number of bonds $A-B$ is equal to 12. For the phases of pure components, the number of bonds in the first sphere of similar components is equal to the number of atoms in the first coordination sphere, i.e., to 12.

To describe changes in the alloy state, we used the notions of a domain, a cluster, and phase and antiphase boundaries. In what follows, an ordered phase will be characterized by the number, size, and shape of domain structures, the domains being the parts of a crystal ordered as A_3B . Note that domains can have different orientation, and

could be displaced with respect to each other. These domains are antiphase with respect to each other. For instance, in superstructure $L1_2$, there could be four such domains and they would differ in the position of the atom of the second component in a unit cell of the crystal lattice of the superstructure. We are going to assume that a cluster represents a disordered structure and contains atoms of different kinds, in which the number of bonds of atomic pairs in the first coordination sphere does not correspond to the number of pairs of an A_3B ordered phase. The cluster atoms and the point substitution defects make up a disordered phase. The interface between two antiphase domains will be taken as an antiphase boundary, and the region separating the ordered and disordered phases – a phase boundary. A “semi-ordered” phase would include both antiphase and phase boundaries.

To verify the model and the procedure, it is reasonable to make a test comparison of well-studied behavior with the respective dependences obtained within the proposed model and procedure. For this reference, we selected well-known dependences for the long- and short-range ordering parameter on temperature.

It is common knowledge [2, 17, 21], that a measure for the short-range ordering is the ratio of N_n^{AB} (number of atomic pairs A and B , spaced at a distance equal to the radius of the n -th coordination sphere) to the number of pairs of A and B , which could be located at this distance in the case of their totally chaotic arrangement with respect to the lattice sites, i.e.,

$$\sigma_n^{AB} = 1 - \frac{P_n^{AB}}{C_B},$$

where P_n^{AB} is the probability of finding a B kind atom in the n -th coordination sphere, given that there is an A kind atom in the central lattice site.

The long-range ordering degree [2, 17, 21] is proportional to the deviation of $P_A^{(1)}$ (probability that an A atom is located in its sublattice) from C_A (concentration of the A kind atoms in an alloy)

$$\eta = \frac{P_A^{(1)} - C_A}{1 - \nu},$$

where the probability $P_A^{(1)} = \frac{N_A^{(1)}}{N^{(1)}}$ is equal to the ratio of the number of A atoms located in their sites to the total number of sites in the first sublattice, with $\nu = 3/4$.

Free energy is determined as a function of the long-range ordering as

$$F = E - TS(\eta),$$

where T is the temperature, and S is the configurational entropy that is given by

$$S = -\frac{Nk_b}{4} \left[\left(C_B + \frac{3}{4}\eta \right) \ln \left(C_B + \frac{3}{4}\eta \right) + \left(C_A - \frac{3}{4}\eta \right) \ln \left(C_A - \frac{3}{4}\eta \right) \right. \\ \left. + 3 \left(C_B - \frac{1}{4}\eta \right) \ln \left(C_B - \frac{1}{4}\eta \right) + \left(C_A + \frac{1}{4}\eta \right) \ln \left(C_A + \frac{1}{4}\eta \right) \right].$$

RESULTS AND DISCUSSION

A computer simulation experiment was performed to investigate thermoactivated rearrangement of atomic structure of the alloy under study. Three initial blocks of the initial crystal were formed in the first step, wherein one vacancy was introduced, which gave a vacancy concentration of about $0.55 \cdot 10^{-6}$. Then, the temperature and the vacancy

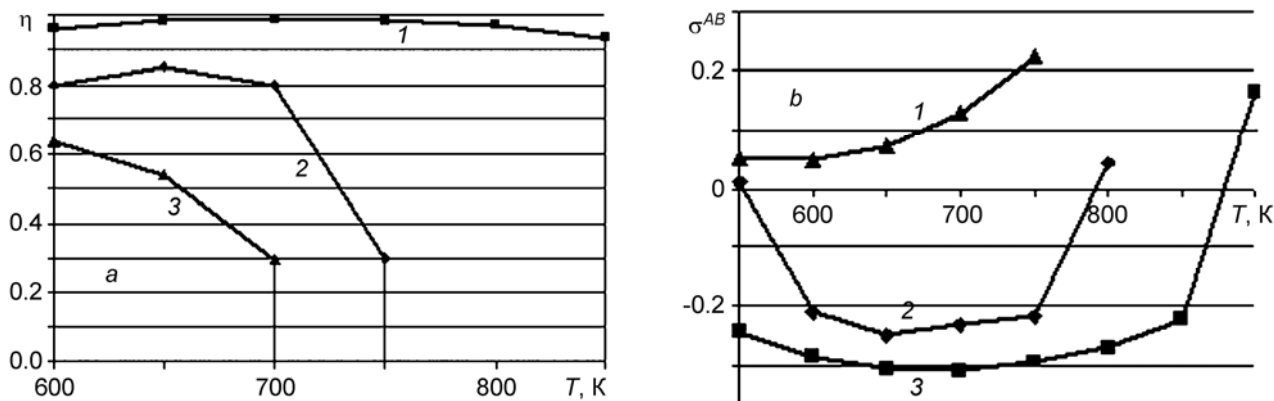


Fig. 1. Temperature dependence: of the long-range ordering parameter in the alloys with 75% Cu (curve 1), 70 at. % Cu (curve 2), and 80 at. % Cu (curve 3) (a) and of the short-range ordering parameter in the alloy with 80% Cu (curve 1), 70 at. % Cu (curve 2), and 75 at. % Cu (curve 3) (b).

mechanism of atomic diffusion were set following the Monte Carlo technique. In so doing, the atomic interaction energy was tabulated with respect to the distance of up to three coordination spheres using the Morse potential function and its parameters from [23, 24]. Thermal activation of the system was performed in a stepwise fashion from $T = 500$ K to $T = 900$ K with a step $\Delta T = 50$ K within 10^8 iterations for each temperature in three calculation grids. At low temperatures, we observed an ordering process, while at elevated temperatures after a certain ordered state, depending on the alloy composition, was achieved, disordering was found to occur.

The specified vacancy concentration, $\sim 5 \cdot 10^{-7}$, is by approximately an order lower than that observed experimentally. The choice of this concentration is dictated by the fact that at concentrations close to experimentally observed ones, the process of thermoactivated structural rearrangement occurs so intensively that it becomes difficult to analyze the ordering process. Since it is the rearrangement that is of major interest for this study, the ordering process in the model was “frozen”.

Behavior of long- and short-range ordering parameters

Figure 1a shows the dependence of the long-range ordering parameter on temperature. It can be readily seen that the most ordered state is observed in a stoichiometric alloy (curve 1), with this ordered state maintained until very high temperatures. On deviation from stoichiometry, a higher ordering degree is exhibited by an alloy with 70 at. % Cu (curve 2) compared to the state of an alloy with 80 at. % Cu (curve 3). Naturally, the temperature of the order–disorder transition is the highest in the stoichiometric alloy.

The behavior of the short-range ordering parameter under temperature variation (Fig. 1b) demonstrates that the highest tendency to surround themselves by the atoms of a different kind (i.e., a tendency to ordering) is manifested in a stoichiometric alloy (curve 3), while upon deviation from stoichiometry this tendency is exhibited only by the alloy with 70 at. % Cu (curve 2). In the alloy with 80 at. % Cu, we observe positive values of the short-range ordering parameter, which testifies to the tendency of Cu atoms to surround themselves by atoms of the same kind. The latter fact suggests that a number of phases of different composition would be formed in this alloy.

Analyzing the temperature dependence of the long-range ordering parameter (Fig. 1), one should pay attention to the following. The shape of the curves $y = y(T)$ is similar to that observed experimentally [7, 16, 22]. The order–disorder transition is a transition of the first kind, as is the case in the experiments. Moreover, it has been found out that, for instance, for a stoichiometric alloy the long-range ordering parameter is close to unity (curve 1) up to the phase transition temperature. It was experimentally shown [7, 16, 22] that the phase transition occurs at $T \sim 660$ K, with the ordering changing in a jump ($\Delta\eta \sim 0.77$).

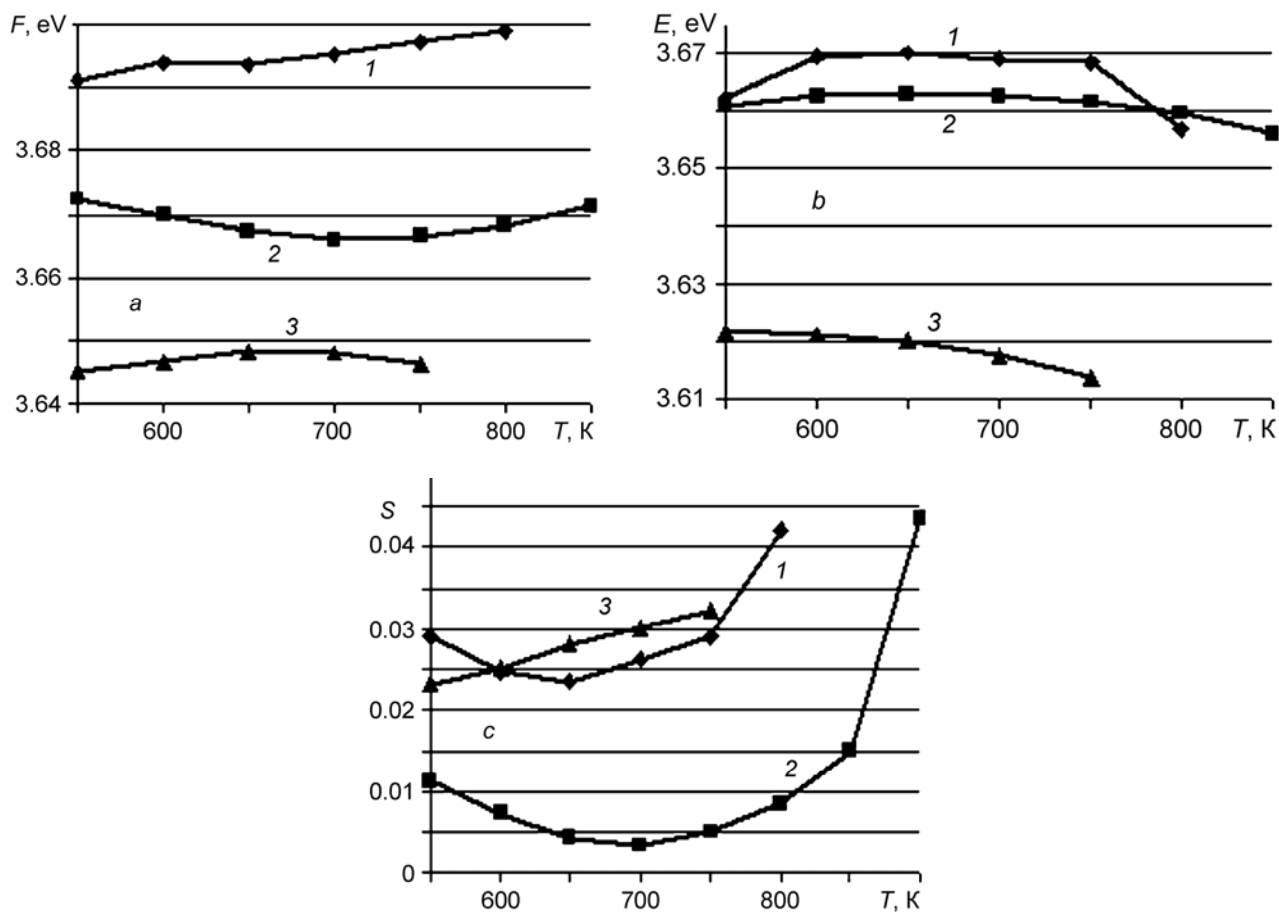


Fig. 2. Temperature dependence of free energy (a), configurational energy (b), and entropy (c) for the alloys of the Cu–Au system with 70 at. % Cu (curve 1), 75 at. % Cu (curve 2) and 80 at. % Cu (curve 3).

Shown in Fig. 2 are the calculated temperature dependences for free energy (a), configurational energy (b), and entropy (c).

It is clearly seen from Fig. 2a that for the stoichiometric alloy the ordered state (curve 2) is thermodynamically more favorable for a phase mixture with the compositions 70 at. % Cu (curve 1) and 80 at. % Cu (curve 3), which is quite reasonable for the Cu–Au system. Thus, the analysis performed as concerns the integral characteristics demonstrates a fairly good performance of the proposed model and investigation procedure.

Peculiarities of the ordering–disordering process of the Cu–Au system in the vicinity of a Cu_3Au composition

The proposed model and investigation procedure allow one to study the ordering–disordering pattern at the microlevel at every temperature and specified alloy composition.

Variation in the alloy component concentration strongly affects the formation of a certain order in the atomic distribution in the crystal, the conditions of implementation of different mechanisms of the order–disorder phase transition, and the formation of transient structures and states in the alloy.

In the case of a stoichiometric alloy, where the concentration of copper is 75 at. % Cu, at the temperature below 500–550 K along with the large domain, antiphase domains of medium and small size are formed (Fig. 3a). The figure shows the structural elements of an ordered, disordered, and “semi-ordered” phases, with the latter being made up by the atoms at the boundaries of their exit onto the surface of a three-dimensional computation grid. Different color shades show the domain structure and the gray color indicates clusters, point substitution defects, their complexes, and

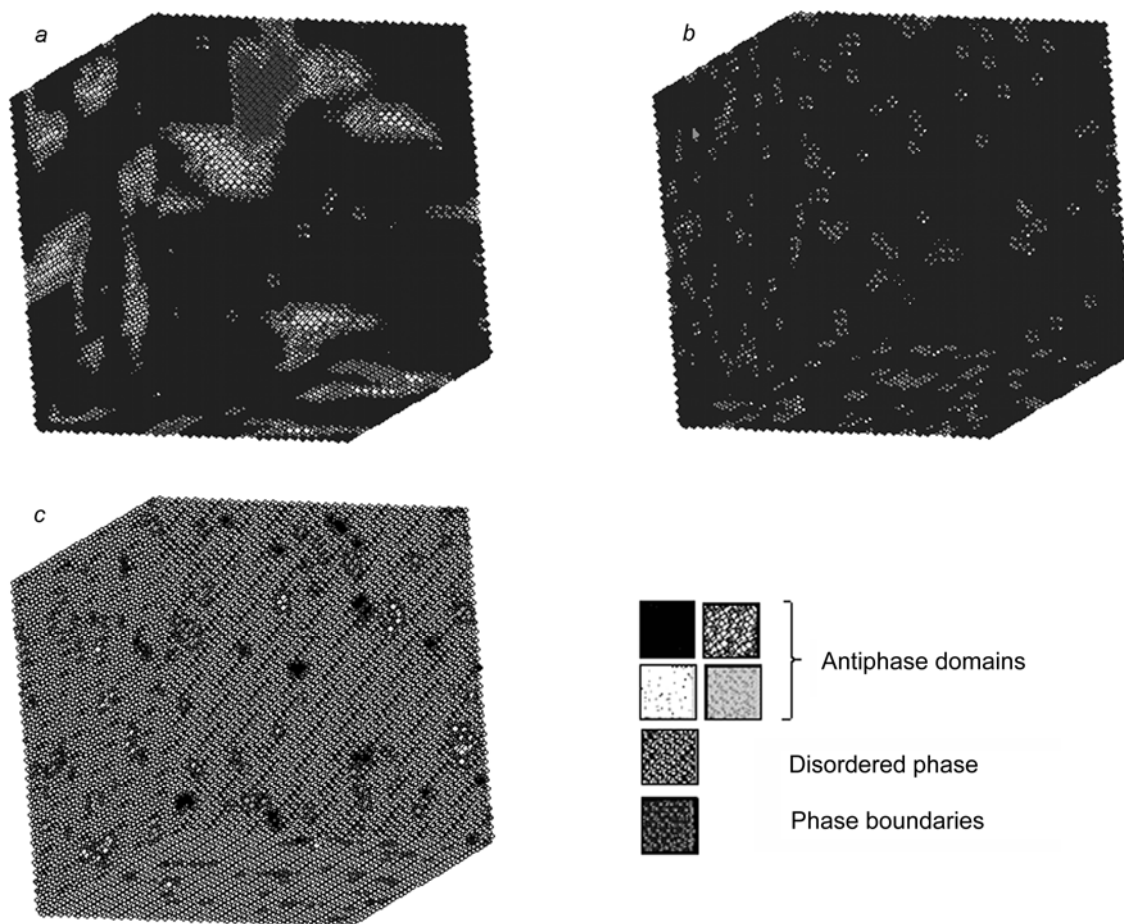


Fig. 3. Distribution of structural elements of the ordered and disordered phases, and boundary atoms forming a “semi-ordered” phase in the alloyed Cu_3Au at $T = 550$ (a), 750 (b) and 900 K (c).

phase and antiphase boundaries. Note that the domains are surrounded by a thin layer of antiphase boundaries that, migrating, introduce a large contribution into the process of atomic ordering. There is a tendency for large domains to absorb their antiphase neighbors, and the volume of small and medium size domains tends to increase. Flat domains are the first to be smeared, while the large domains of regularly round shape are found to be most stable. Structural transformation occurs largely due to antiphase boundary migration and increased volume of the ordered phase due to absorption of segregated domains. As the temperature is further increased up to $600\text{--}850$ K, single-domain structure is found to sustain with formation of a small fraction of a disordered phase. The peculiarities of the process of disordering are associated with the formation of a flow of point defects and their complexes. At the temperature $T = 900$ K, the alloy is completely disordered and we observe a very slight process of formation of microdomains, the nuclei of a new phase.

In the alloy with 70 at. % Cu the fraction of clusters is decreased from the minimum value 40% by another 15–20% due to the formation of a “semi-ordered” phase (made up by antiphase boundaries). The alloy possesses only intra-domain long-range order, with the process of ordering occurring similarly to the case of the stoichiometric composition, but with a higher fraction of the “semi-ordered” phase. Enlargement of domains occurs due to their growth by addition of atoms from the phase boundary between the domains or due to segregations made up by microdomains. The main interaction between two domains occurs via phase boundaries, with a wide phase boundary being formed between two domains, which is rearranged into one of the larger antiphase domains and absorbs the latter. The domains thus formed have a higher density of substitution point defects and microclusters with comparatively large regions of the ordered phase. In the course of ordering at comparatively low temperatures, the phase boundaries rearrange quite fast to form

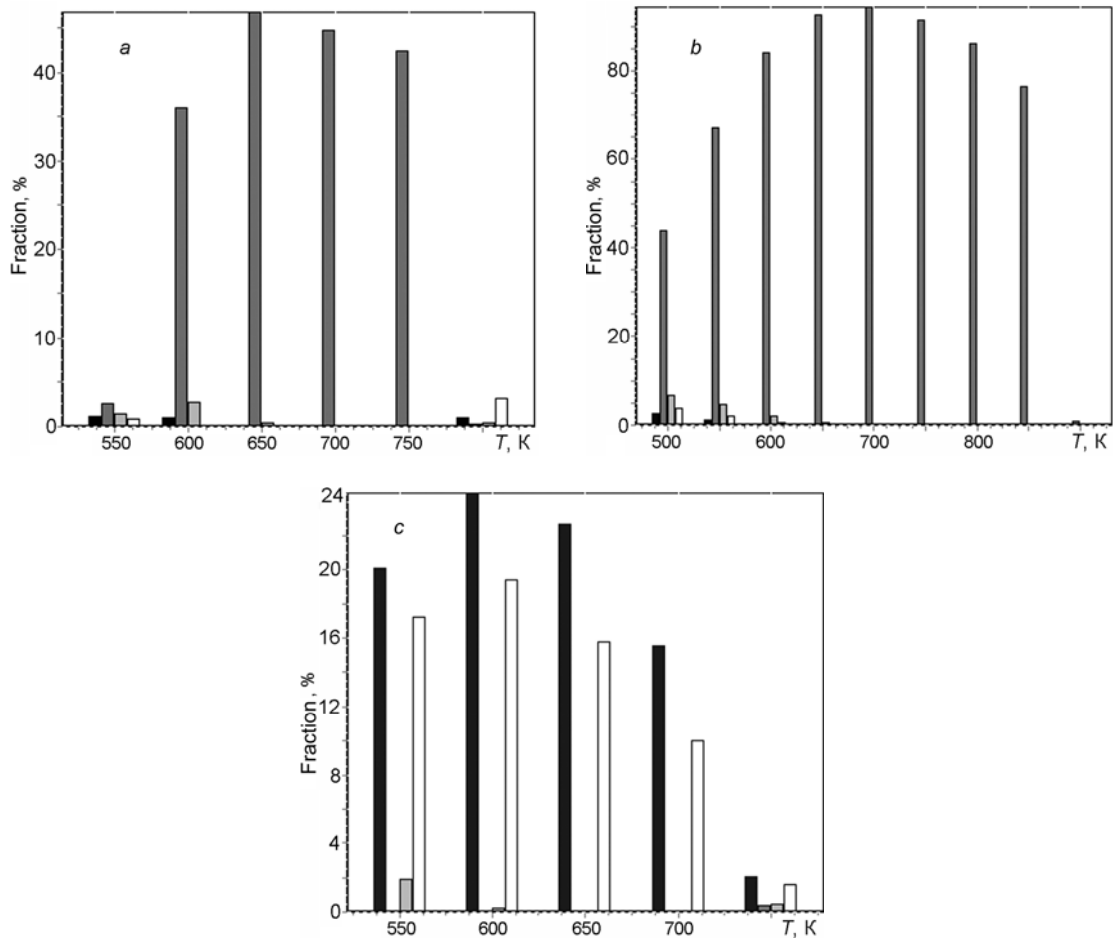


Fig. 4. Distribution of atoms over antiphase domains as a function of temperature in a binary alloy close to the composition of Cu_3Au : 70 at. % Cu (a), 75 at. % Cu (b), and 80 at. % Cu (c). The four antiphase domains are shown by different color shades.

an ordered inhomogeneous region. During disordering with increasing the temperature, the phase boundaries also rearrange fast to form a disordered phase.

In the alloy with 80 at. % Cu, the disordered phase accounts for about 55% at $T = 600$ K, the remaining part of the system is largely made up by two relatively large domains (about 20%), with small-size segregations formed at the phase boundaries. As the temperature is increased, the disordered phase fraction is observed to increase, the process of disordering is switched on, small and medium domains annihilate, and the two large ones are destroyed. Both near the boundary and inside the domain, defects and their complexes are found to form. The main interaction occurs at the phase boundary between the ordered and disordered phases. The phase boundary has a maze structure that in the course of disordering with increasing temperature intrudes into the ordered region. It should be noted that within the entire temperature range under study, pure Cu (up to ~3%) is observed to precipitate.

Phase structure analysis

In the course of thermal activation, peculiar kinetic behavior of the alloy domain structure is manifested, which makes it possible to perform structural analysis of the ordered, disordered, and “semi-ordered” phases, the latter containing antiphase and phase boundaries.

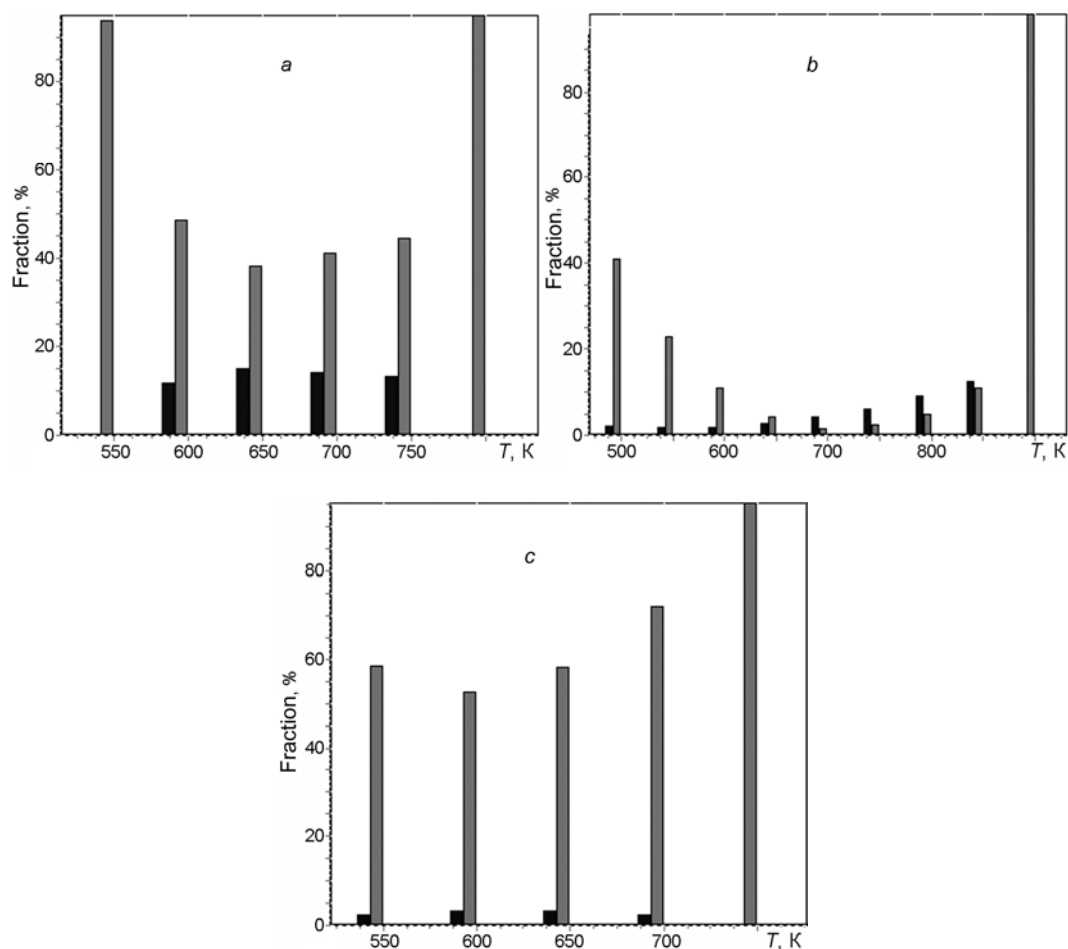


Fig. 5. Distribution of atoms over clusters and “semi-ordered” phase in the alloy with a composition close to that of Cu_3Au : 70 at. % Cu (a), 75 at. % Cu (b), and 80 at. % Cu (c). The fraction of antiphase and phase boundaries forming the “semi-ordered” phase (dark bars) and clusters (light bars).

In the alloy under study, four equivalent sublattices are displaced with respect to each other by the antiphase vector, thus four types of domains are formed, with the respective distribution over these domains shown in Fig. 4. In the alloy of the stoichiometric composition at $T = 500$ K, all four types of domains are observed to form, with one predominating. The size of the larger domain is increasing with the temperature, while smaller domains decrease in their size. At the phase transition temperature of the order–disorder transition, $T = 700$ K, the alloy exhibits single-domain structure (about 95% of the volume), while with further increase in temperature the domain is smeared. Similar changes in the domain structure have been noted in a binary alloy with 70 at. % Cu: at the temperature $T = 650$ K there is only one single domain left, whose maximum size accounts for 47% of the volume. In the case of a composition with 80% Cu, the structure is broken into two types of domains occupying (at $T = 600$ K) 24 and 20% of the volume, respectively. In all of the cases of the temperature increasing above critical, the domains are observed to disintegrate. It is readily seen that these results correlate well with the data on the short- and long-range ordering given in Fig. 1. In particular, the increase in the degree of short-range ordering is associated with the increase in the size of the single-domain region. The temperature at which the long-range ordering parameter achieves its maximum value corresponds to that at which the single-domain structure occupies the maximum volume.

Figure 5 shows the distribution of atoms over the structure of the disordered and “semi-ordered” phases, the latter containing phase and antiphase boundaries. The fraction of atoms belonging to the domain boundary appears to be

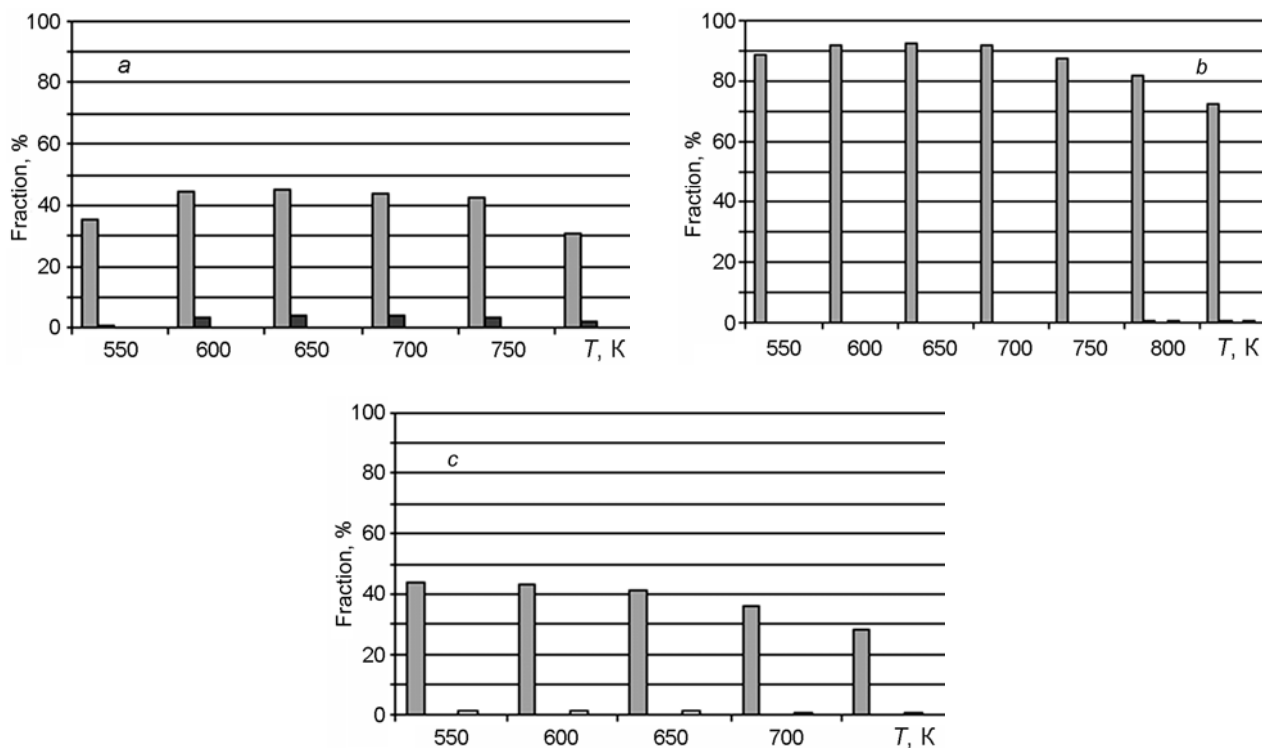


Fig. 6. Distribution of fractions of the phases A_3B , AB , AB_3 , B and A as a function of temperature in the alloys of compositions close to that of Cu_3Au : 70 at. % Cu (9a), 75 at. % Cu (b), and 80 at. % Cu (c): Cu_3Au (gray bars), CuAu (dark bars), and pure Cu (light bars).

the largest for the alloy with 70 at. % Cu (Case1) in the temperature interval from 600 to 750 K, within which the short-range ordering is maintained negative (Fig. 1b).

In the alloy of the stoichiometric composition, near the critical temperature $T = 700$ K the fraction of the boundary atoms of the “semi-ordered” phase exceeds that of disordered. As the temperature is still further increased, the process of disordering involves more mechanisms such as those associated with faceting of the antiphase boundaries and elongation and thickening of the boundaries, which proceeds until complete disordering of the alloy at the temperature above 850 K. In all of the alloys under study the volume of clusters in the disordered phase at the temperature of the order–disorder transition is small, and as the temperature increases their fraction begins to grow, achieving a maximum at the temperatures above the phase transition temperatures. A change in the “semi-ordered” phase distribution strongly depends on the alloy component concentration. The effect of the phase and antiphase boundaries is the largest in the alloy with 70 at. % Cu. In the stoichiometric alloy, faceting and grain-boundary migration start near the temperature of the order–disorder transition. In the alloy with lower concentration of gold, the disordered phase predominates, the volume of phase boundaries is as low as 3%, and their influence is negligible.

A structural analysis of the phases A_3B , AB , AB_3 , A , B formed during thermal activation of the alloy allowed us to construct bar diagrams of the distribution of their fractions (see Fig. 6).

For the alloy of the stoichiometric composition, the phase fraction with superstructure $L1_2$ predominates at the temperature below the phase transition temperature, but begins to decrease approaching the disordering temperature. For the alloy with 70 at. % Cu, the fraction of superstructure $L1_2$ reaches maximum (about 45%) within the temperature range from 600 to 750 K, with the increase in concentration of gold resulting in precipitation of the CuAu phase (nearly 5%). At the concentration of 80 at. % Cu, within the temperature interval 550–750 K precipitation of pure Cu (up to 2%) is found to occur as well as the presence of atom aggregates corresponding to superstructure $L1_2$ (reaches 44%), with the remaining part of the crystal identified as a disordered phase, which is in conformity with [25]. In the alloy of

the stoichiometric composition, precipitation of structural phases is negligible and occurs at comparatively low temperatures.

SUMMARY

The investigation performed in this work has demonstrated the efficiency of the (vacancy-based) diffusion model of structural rearrangement of the ordering systems. The model thus constructed and the use of the Monte Carlo method gave a number of plausible results. Primarily, this enabled us to follow the pattern of the process of ordering of a binary alloy as a function of temperature and composition in detail. Furthermore, the process has been examined at the micro-, meso-, and macrolevels.

As a result, it has been found out that the major mechanism in the early stage of ordering is the process of antiphase domain formation. In the alloy of a stoichiometric composition, the fraction of atoms making up the antiphase domains reaches 90%, while upon deviation from stoichiometry by ± 5 at. % this fraction is below 50%.

The mechanism of structural transformations strongly depends on mesostructural peculiarities (domain structure, shape and size, length and width of antiphase boundaries, etc.). In the alloy of a stoichiometric composition, the fraction of clusters is small, and the major role is played by the mechanisms of absorption of smaller domains by the larger ones, and antiphase boundary migration, with the intradomain ordering sustained.

Upon deviation of Cu_3Au from stoichiometry towards smaller fraction of copper (70 at. % Cu), the fraction of the atoms belonging to the phase boundaries considerably increases (up to 50%), which testifies to the absence of homogeneity of the domain region. In this alloy, the mechanism of structural transformations is associated primarily with fluctuation of the phase and antiphase boundaries; larger domains absorb smaller ones (same as in the alloy of a stoichiometric composition) but without sustaining the intradomain ordering.

Upon deviation of Cu_3Au from stoichiometry towards larger fraction of copper (80 at. %), the fraction of atoms belonging to the disordered phase is found to be the largest (up to 55%). The domain structure is characterized by small domains whose maximum size is as low as $\sim 23\%$ of the volume of the system. The mechanism of structural transformations in this alloy is primarily associated with smearing of the domain structures of the disordered phase.

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