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THE INFLUENCE OF THE DENSITY OF STRUCTURAL PLANAR DEFECTS ON THE STRUCTURAL-PHASE TRANSFORMATIONS IN LOW-STABILITY TETRAGONAL ALLOYS

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Using an ordered face-centered tetragonal alloy with the $L1_0$ superstructure, the effect of density of structural planar defects (antiphase boundaries, APBs) on the thermodynamic stability of alloys is investigated with respect to the structural-phase transformations in a low-stability state of the system. It is shown that the thermodynamic advantage of a long-period relaxational structure compared to the initial structure is ensured already at $T = 0$ K by such relaxational effects as atomic displacements. The structure of the regions of atomic displacements near periodic APBs is the same as that of single APBs: the largest atomic displacements are localized in the vicinity of an APB and rapidly decrease with distance from it, while the size and structure of the regions of these distortions are maintained. It is established that in the ordered fcc tetragonal systems during structural-phase transformations the long-period state is a low-stability state of the system; it is therefore expected that an external action would not only result in a structural-phase transformation but also determine its pathway.

Keywords: low-stability states, phase transformations, structure defects.

It is well-known that low-stability long-period states are experimentally observed in fcc- and hcp-alloys, with the majority of them having an fcc-lattice and a composition in the range from A_3B to AB [1–6]. A CuAu binary alloy with a long-period structure is a classical example of an alloy with a tetragonal face-centered lattice (fct). The influence of the density of periodic antiphase boundaries on the stability towards structural-phase transformations was investigated in fcc-alloys with an A_3B composition in their low-stability states [1–6], therefore we believe it to be useful to investigate a binary alloy particularly with an fcc-lattice and an AB composition.

The main purpose of this work is to study the effect of the density of antiphase boundaries on the stability of fct-alloys towards the structural phase transformations in low-stability states of condensed media.

Let us look at the formation of low-stability long-period structures (LPSs) of a relaxational type [4–30]. Since a classical representative of long-period structures is a binary alloy CuAu with periodic antiphase boundaries (APBs), which determine its long period, we decided to use an alloy of the CuAu type with a basic superstructure $L1_0$ as a model alloy. In a completely ordered state it has an $L1_0$ superstructure and its degree of tetragonality is $c/a = 0.92$. It is for this reason that the study of the features of formation of LPSs and their structure in the alloys with a basic superstructure $L1_0$ is principally important, as also is the influence of APBs on structural-phase transformations in a low-stability tetragonal system. In order to rule out the effects of component re-distribution and the influence of the entropy factor, we are going to perform the investigation at $T = 0$ K. In this case, the energy advantage of an LPS compared to the basic superstructure would be provided by the lattice modulation in the form of atomic displacements only.

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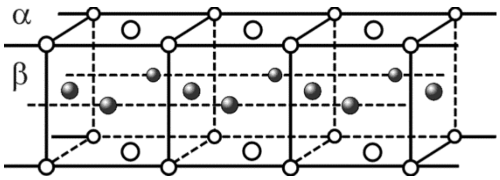

Fig. 1. Lattice of an fct-alloy with the *AB* composition and $L1_0$ superstructure.

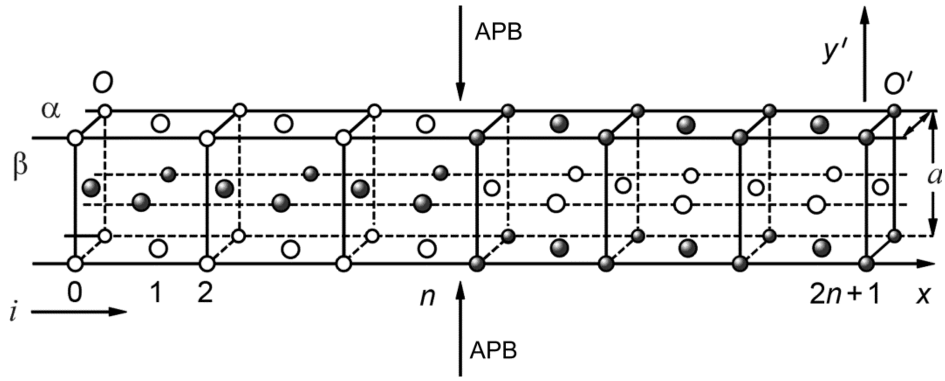

Fig. 2. Schematics of the model system (between the *O*- and *O′*-centers of the adjacent antiphase domains): ○ – atom *A*; ● – atom *B*.

Solution of this problem would allow us not only to illustrate the dependence between the density of periodic APBs (i.e., low-stability long-period states) and stability of the system towards structural-phase transformations, but would also offer a possibility of studying the microstructure of APB regions in a long-period alloy, which is experimentally exceptionally difficult.

SEMI-PHENOMENOLOGICAL DESCRIPTION OF THE LPS FORMATION

Let us consider a model alloy of an equiatomic composition *AB* with a basic superstructure $L1_0$ in a completely ordered state, whose prototype is a CuAu alloy at $T = 0$ K. Clearly, the system's state under the conditions accepted would be entirely determined by its internal energy.

From the lattice geometry (Fig. 1) of this completely ordered alloy it is evident that there are two types of the nodal planes: α (wherein only *A* atoms could be found) and β (with *B* atoms only). These nodal planes are the planes with variable filling.

When considering long-period states, let us assume that the alloy under study consists of equal-dimension antiphase boundaries of the size *M* with an odd number of atomic planes normal to the long period (*x*-direction). Shown in Fig. 2 are the halves of two adjacent antiphase domains. The central atomic plane of the left domain is denoted *O*, and that of the right domain – *O′*, with an arrow showing the APB position. It is necessary and sufficient to include into the model system a set of planes located between the center of the antiphase domain *O* and the APB. Prescribing the number of atomic planes, i.e. *n*, in one half of the domain, we can readily find the size of the respective antiphase domain $M = (2n+1)/2$, which is measured in the parameters of the initial fct-lattice. In other words, we are going to consider a statistically pure state of the system.

It is clear that to find a solution is not difficult in the case of an even number of atomic planes $2n$ in the antiphase domain and its size $M = n$. The only change would be a technical implementation due to the change of the antiphase domain symmetry. For this reason, we are going to omit the case of a long-period state with domains containing an even number of atomic planes, since it would not provide any principally significant information.

For the sake of simplicity, in what follows we are going to assume that in the course of transition into a long-period state every atom would have its individual coordinate in the ***x*** direction of the long period, x_i^k, where k = α, β and i = 0, ..., n. In the two other directions, we assume displacement of the respective atomic planes (see Fig. 2).

In the approximation accepted in this work, according to the symmetry of the system under study, the conditions of the atomic coordinates at its boundaries are given by the following:

$$x_0^k = 0,$$

$$x_{-l}^k = -x_l^k,$$
$$x_{n+i}^k = 2x_M - x_{(n+1)-i}^k,$$

with $i = 1, \ldots, n$ and k, l = α, β, where $l \neq k$.

Let us denote the potential of the central atomic pair interaction, e.g., that between A and B, spaced by distance R, as $V_{AB}(R)$. Then the interactions of atoms in nodes k and d (k, d = α, β) of the nodal planes i and j (see Fig. 2), would be given by

$$w_{ij}^{kd}(R_{ij}^{kd}) = P_i^k P_j^d V_{AA}(R_{ij}^{kd}) + (1 - P_i^k)(1 - P_j^d) V_{BB}(R_{ij}^{kd})$$
$$+ [P_i^k(1 - P_j^d) + (1 - P_i^k) P_j^d] V_{AB}(R_{ij}^{kd}),$$

where P_i^k are the filling numbers for atoms A of nodes k in the nodal plane i.

The interaction energy of an atom located in node k of plane i with the neighborhood up to the Z-neighbor would be given by

$$W_i^k = \frac{1}{2} \sum_{j,d} w_{ij}^{kd}(R_{ij}^{kd}).$$

Summation is performed in a way so that the interacting atoms would enter the Z-neighborhood, with the exception of self-action, in other words for $i = j$ satisfaction of $k = d$ is ruled out.

The internal energy of an alloy with antiphase boundaries of the size $M = 2n+1$ calculated per single atom could be written as follows:

$$e_1 = \frac{1}{2n+1} \sum_{k=\alpha,\beta} \left[\sum_{i=1}^{n} W_i^k + W_0^k / 2 \right].$$

As an initial state let us take an ordered (fcc-lattice) state obtained by minimizing the internal energy of the alloy per single atom with respect to the lattice parameters a and c for the interaction model selected in this work. As a result, find an equilibrium value of the internal energy per single atom (e_0) and the respective lattice parameters a_0 and c_0.

Then, the thermodynamic possibility of a transition would be characterized by

$$e' = e_1 - e_0,$$

where e_0 is the internal energy per a single atom of the alloy with the basic superstructure $L1_0$. Further, parameter e' would be referred to as the internal energy of an APB per a single atom of the alloy.

After introducing periodic APBs for the given value of n, the equilibrium (relaxed) value of the internal energy of the antiphase boundary per a single atom of the alloy (e) was found by minimizing the value of e' over all $2n+3$ independent variables: a, c, x_M and $2n$ variables of the x_i^k type, where $k = \alpha$, β and $i = 1, ..., n$. Note that along the y coordinate we calculated the lattice parameter a, and along $z - c$. In what follows we are going to assume that that in the course of transition the APB whose coordinate is denoted by x_M can change its position. It should be underlined that the above-mentioned characteristics will be varied so that the internal energy of the resulting LPS could be reduced. The equilibrium state of the alloy with periodic APBs would correspond to the lowest value of the internal energy of the system for the value of the antiphase domain $M = (2n+1)/2$ prescribed in the work. This implies that during transition into the equilibrium state the linear dimensions of the system under study and the individual atomic coordinates were varied in such a way that the total internal energy of the system decreased. As a result, we found the value of the internal APB energy per atom ($\boldsymbol{e}$) and the respective equilibrium values of independent parameters.

RELATIONSHIP BETWEEN THE DENSITY OF PERIODIC ANTIPHASE BOUNDARIES AND SYSTEM'S STABILITY TOWARDS STRUCTURAL-PHASE TRANSFORMATIONS

In our calculations, while writing the energy of atomic interaction with the neighborhood W_i^k, we included into consideration the nearest and next nearest neighbors. In order to approximate the potential of the central pair interaction of atoms, e.g., $V_{AA}(R)$, we used the Morse function

$$V_{AA}(R) = D_{AA}\left\{\exp\left[-2\alpha_{AA}(R - R_{AA}^0)\right] - 2\exp\left[-\alpha_{AA}(R - R_{AA}^0)\right]\right\},$$

where D_{AA} characterizes the energy of dissociation of a pair of atoms A, α_{AA} is the bond 'rigidity', R is the atomic spacing, and R^0_{AA} is the equilibrium value of R for the pair A–A. It is evident that the potential is not a long-range one. One might however expect that in addition to variation in the microscopic lattice characteristics it would determine the thermodynamic possibility of structural-phase transformations in the alloy. We included into consideration the development of 'ionicity' in the course of ordering due to the charge transfer during the distribution of atoms over the lattice sites [4, 5, 10–15]. In order to show this ionicity via the Morse potential, we prescribed anisotropic interactions between the atoms. For the atoms located in the same type nodes (α–α or β–β), the rigidity of the bond α(1) was taken to be different from that of α(2) of the same atoms located in the nodes of different types (α–β or β–α). The potential parameters used in the calculations are close to those reported in [2, 4, 5, 10–15] for the ordered alloy Cu_3Au:

$$D_{AA} = 8.0\cdot10^{-19}\,\text{J},\ R^0_{AA} = 2.95\cdot10^{-10}\,\text{m},$$

$$D_{BB} = 6.5\cdot10^{-19}\,\text{J},\ R^0_{BB} = 2.65\cdot10^{-10}\,\text{m},$$

$$D_{AB} = 7.0\cdot10^{-19}\,\text{J},\ R^0_{AB} = 2.76\cdot10^{-10}\,\text{m},$$

$$\alpha1_{AA} = 1.30\cdot10^{10}\,\text{m}^{-1},\ \alpha2_{AA} = 0.85\cdot10^{10}\,\text{m}^{-1},$$

$$\alpha1_{BB} = 1.00\cdot10^{10}\,\text{m}^{-1},\ \alpha2_{BB} = 1.85\cdot10^{10}\,\text{m}^{-1},$$

$$\alpha1_{AB} = 1.05\cdot10^{10}\,\text{m}^{-1},\ \alpha2_{AB} = 1.05\cdot10^{10}\,\text{m}^{-1}.$$

Using the interaction thus selected, we had to find the characteristics of the initial state. To do so, we wrote the internal energy of the fct-alloy with the superstructure $L1_0$. As a result of minimization of the energy of this alloy state with respect to the lattice parameters a and c we found the minimum value of the system's energy per atom (e_0) and obtained the values of the respective lattice parameters a_0 and c_0.

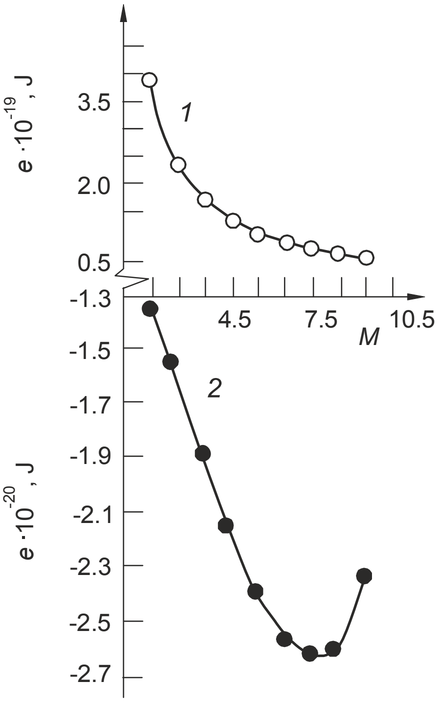

Fig. 3. Dependence of the internal APB energy per atom on the domain size: non-equilibrium APB (curve *1*) and relaxed state (curve *2*).

These characteristics allow us to determine the ordering energies in the nearest (ω1) and next nearest (ω2) neighborhood and, hence, their ratio. For the interaction selected in this work, this ratio is $d = |\omega2/\omega1| < 0.1$. It corresponds to the energy advantage of the superstructure $L1_0$ compared to the alloy state with newly introduced non-relaxed APBs.

For the selected model of interaction for the initial state of the alloy without any periodic APBs (superstructure $L1_0$) we obtained $e_0 = 53.5831\cdot10^{-19}$ J, $a_0 = 3.786$ Å, $c_0 = 3.558$ Å. Thus, the model alloy tetragonality is equal to $c_0/a_0 = 0.948 < 1.0$. The latter suggests within the framework of our model that interaction via an APB would prevent the system energy from decreasing and would result in a partial release of the relaxational energy only.

The selected interaction and value of e_0 allow us to calculate e'. Shown in Fig. 3 is the calculated internal APB energy per atom of the alloy as a function of the size of the antiphase domain $M = (2n+1)/2$. Curve *1* corresponds to the newly introduced non-relaxational APB. These periodic antiphase boundaries, no matter what their density, increase the system's internal energy, which is suggested by the positive sign of e'. Thus, a change in the atomic bonding via the APB being formed increases the 'chemical' fraction of the alloy energy. A long-period structure without any relaxational effects in the form of lattice modulations is therefore disadvantageous for the crystal compared to the initial state of the alloy without APBs. Relaxation of the system via static displacements gives rise to an energy advantage of the final state with the periodic APBs (curve *2*) compared to the initial state. This is indicated by the trend of curve *2* towards the negative values of e. The presence of the minimum in the curve testifies of a predominating realization in the alloy with the interaction selected of a structure with a definite long period. It should be noted that the energy of different-size domains hardly differ in the region of this minimum (about 10^{-22} J). At finite temperatures we would expect the entropy factor $Q = S\cdot T$ (given that the combinatory entropy $S \sim k\cdot\ln\,\Omega$, where the Boltzmann constant $k = 1.38\cdot10^{-22}$ J/K and Ω is the thermodynamic probability) would give rise to an alloy state with different values of M.

It is noteworthy that different long-period states, i.e., the ones with different densities of antiphase boundaries, provide different internal energy advantage, while the internal energies of the state of a system with antiphase domains of different size hardly differ. At finite temperatures we would expect the entropy factor to favor a state with different values of M in the alloy. The latter implies that at the temperatures other than the absolute zero there will be a certain

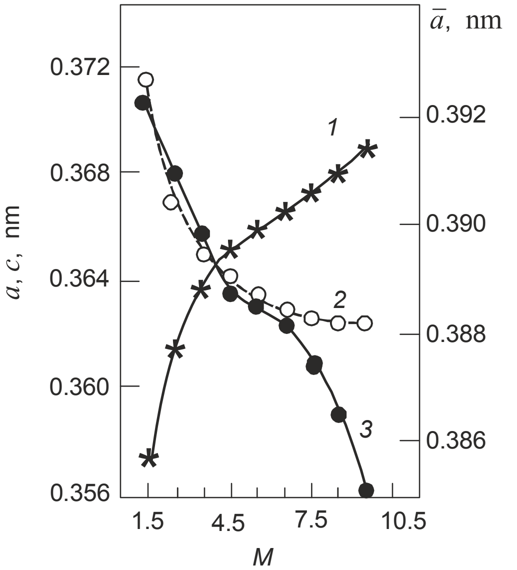

Fig. 4

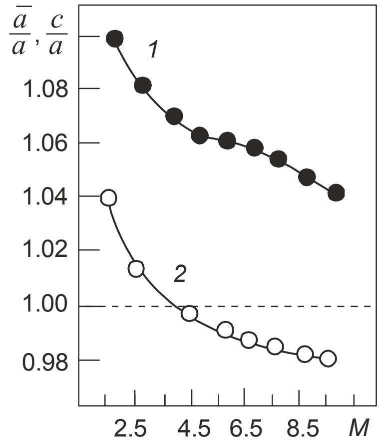

Fig. 5

Fig. 4. Lattice parameters of the final state as a function of the domain size: *a* (curve *1*), *c* (curve *2*), and $\overline{a} = 2x_M/(2n+1)$ (curve *3*).

Fig. 5. Influence of the domain size of the lattice tetragonality of the final state: $\overline{a}/a$ (curve *1*) and c/a (curve *2*).

set of states of the antiphase domain, that is there would appear a certain domain size distribution function with a range of *M* values. This negligible thermodynamic difference between symmetrically different structural states of the system suggests that a transition from a state with a certain long period (density of antiphase boundaries) into a state with a different period (different density of antiphase boundaries) can occur under comparatively small external actions of thermal forces. In this respect, the long-period state is a low-stability state. Clearly, long-period states with different domains differ in their symmetry, while their thermodynamic features are quite similar.

A detailed analysis of the decreased energy of the system revealed that it is the energy of the nearest neighbor bonding in the nodal plane β which decreases (see Fig. 2), the nearest bonding of atoms in the nodes α, β of the nodal planes *i* and *i* + 1, as well as the bonds of the next nearest neighbors located along the *y* axis in the nodal planes *i* (see Fig. 2). The energy of the remaining bonds is increased during transition into a long-period state.

Let us consider the antiphase domain structure as a function of its size, i.e., density of antiphase boundaries. Shown in Fig. 4 are dependences of the lattice parameters *a* (curve *1*), *c* (curve *2*) and $\overline{a} = 2x_M/(2n+1)$ (curve *3*) on the domain size. It is evident that as the domain size *M* increases (density of antiphase boundaries decreases), the equilibrium values of the lattice parameters *c*, *a* and $\overline{a}$ tend to those in the initial structure, i.e., towards c_0 and a_0. An essential fact is that this tendency is downwards, while that of *a* – upwards. Having constructed the dependences of the ratios $\overline{a}/a$ and c/a on *M*. which are shown in Fig. 5 in curves *1* and *2*, we can readily note a change of tetragonality in the course of transition into a long-period state. While in the initial state $c_0/a_0 = 0.948$, in the equilibrium long-period state for $M = 7.5$, for instance, $c/a = 0.9873$ and $\overline{a}/a = 1.031$. This implies that the lattice in the course of this transition tends to reduce tetragonality in the direction normal to the long period and to increase it along this period. In addition, from the relation between $\overline{a}$ and a_0 it becomes evident that the lattice undergoes a general expansion along the long period during transition into a long-period state as it was experimentally observed in CuAuII [29]. When *M* increases, the relative elongation is decreased. For instance, for $M = 7.5$ it is equal to ~2.3%.

It should be underlined that for $M = 1.5$ the ratio of the lattice axes are $c/a = 1.040$ and $\overline{a}/a = 1.098$, while for $M = 7.5$ $c/a = 0.987$ and $\overline{a}/a = 1.031$. When the size of the antiphase domain changes the lattice undergoes strong

TABLE 1. Calculated Atomic Coordinates

Number of plane i	Atom in node α	Coordinate x_i^{α}	Coordinate x_i^{β}	Atom in node β
1	*A*	1.93	1.93	B
2	*A*	3.86	3.86	*B*
3	*A*	5.79	5.79	*B*
4	*A*	7.72	7.72	*B*
5	*A*	9.66	9.66	*B*
6	*A*	11. 59	11.60	*B*
7	*A*	13.48	13.57	*B*

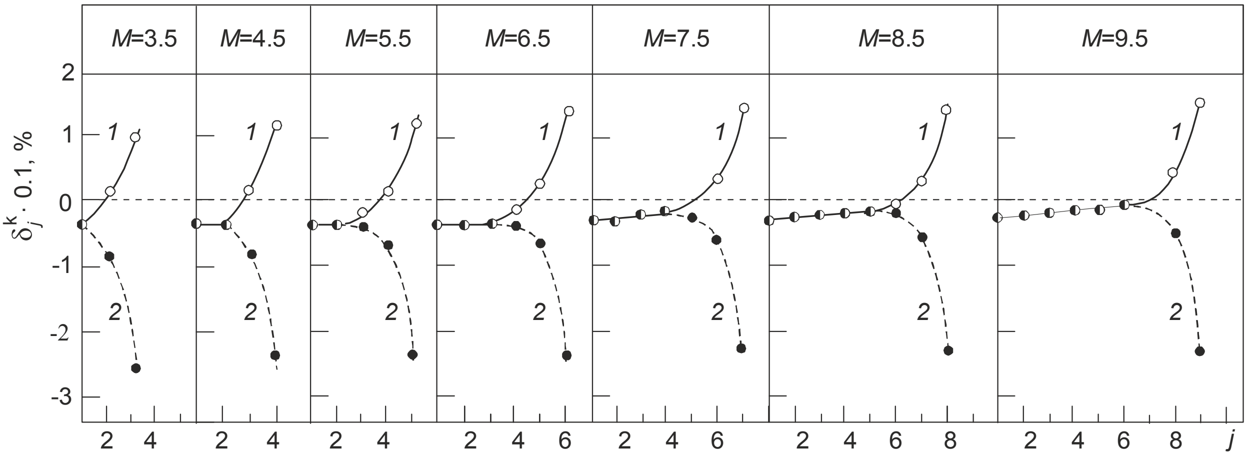

Fig. 6. Changes in δ and δ(*j*) under variation of the domain size: Nodal planes β (curve *1*) and α (curve *2*).

deformation. This might be essential for the state of the alloy with different values of *M* (mixed state) at finite temperatures. On the one hand, the thermodynamics of this mixed state is quite clear. On the other, the adjacent position of the antiphase domains of different length requires their sufficient accommodation, otherwise resulting in strong elastic stresses due their size difference. The latter would either make the occurrence of the mixed state difficult or give rise to large elastic stresses developed at slow accommodation rates.

Attention now should be drawn to the fine structure of the alloy in the vicinity of the antiphase boundary. Table 1 presents the atomic coordinates in a half of a domain with $M = 7.5$. It is evident that near the APB ‘small” atoms *A* are shifted from the APB, while ‘large’ atoms *B* – are shifted towards it. This is consistent with the atomic coordination observed experimentally in CuAuII [29].

Having constructed the curves for the relation between projections of interatomic spacings onto orientation of the long period to their average value

$$\delta_j^k = \frac{(x_i^k - x_{i-1}^k) - \bar{a}/2}{\bar{a}/2} \cdot 100\%$$

for different antiphase domain dimensions, we can readily find out that the maximum displacements are localized near the APB, which qualitatively agrees with the experimental behavior of the alloy CuAuII observed in [31–32]. Shown in Fig. 6 are the results obtained from the measurements of the domain. Curves *1* correspond to the nodal planes β, and curves *2* – to the nodal planes α. It should be noted that the region of local structure variations covers approximately two adjacent atomic planes nearest to the APB. The distortions measure about 1–3% on the atomic plane nearest to the boundary and are practically absent in the next nearest plane. Variation in the domain size, i.e., APB density, causes no changes in the size of the region of distortions or appreciable changes of their magnitude.

An analysis of Fig. 6 clearly shows that the dimensions of the disturbed region are maintained when *M* increases (APB density decreases) and are found to be about 2–3 interatomic spacings. Along the $\boldsymbol{x}$ direction, the linear dimesnions of the region of disturbances are symmetrical with respect to the plane nearest to the APB and normal to the $\boldsymbol{x}$ direction. It seems useful to compare the structure of the disturbed region of a periodic antiphase boundary with that of a single APB. In [33–36] the authors present the results of their calculations of the 1/2 <110>{100} APBs in completely ordered Cu–Au alloys to an approximation of the interatomic pair potential including interactions of every atom in all three coordination spheres. We revealed that the disturbances disappear already in the third plane from the APB. Comparing this to a periodic APB, we may conclude that the dimensions of the regions of disturbances of single and periodic APBs are nearly the same.

Thus, it should be emphasized that disturbance of interatomic spacings falls within the region of 2–3 interatomic bonds.

The dependences on the structure of the region of disturbances in a single APB obtained independently [33–36] are in a good agreement with the respective data on a periodic APB. Comparing this to a periodic APB, we can make a conclusion on the constancy of the regions of disturbances in the case of single or periodic APBs.

SUMMARY

It has been shown that the density of planar structural defects (in this case antiphase boundaries) exerts an essential influence on the structural-phase transformations in tetragonal alloys in their low-stability state. The thermodynamic advantage of long-period relaxational structures compared to the initial superstructure is ensured at the temperature as low as $T = 0$ K by the relaxational effects such as atomic displacements.

It should be emphasized that different long-period states (i.e., the states with different density of APBs) provide a different internal energy advantage for the system, with the internal energies of the system's states with different APB density are nearly the same. At finite temperatures one might expect a mixed state in the system due to the entropy factor. The latter, in its turn, implies that at the temperatures different from zero there will be a certain set of states, i.e., there will be a certain function of state distribution with a range of values. The above-mentioned slight thermodynamic difference of the symmetrically different structural states suggests that a transition from a state with a single long period (one APB density) into a state with a different period (different APB density) can occur at comparatively small action of thermal forces.

Comparing the dimensions and structure of the regions of disturbances in the vicinity of single and periodic antiphase boundaries, we can conclude that they remain practically invariable both in the case of single and periodic antiphase boundaries. It has to be emphasized that the disturbance of interatomic spacings is generally observed within 2–3 interatomic bonds in the vicinity of an antiphase boundary.

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