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SHORT-RANGE ORDER AND CORRELATION EFFECTS IN SOLID SOLUTIONS

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The results of statistical theory in quasichemical approximation of long- and short-range atomic ordering in ternary substitutional solid solutions $AB_3 + C$ with a face-centered cubic (FCC) lattice $L1_2$ of a Cu_3Au *type suggesting that atoms C are arranged in the sites of both types legal for atoms A and B are given. For particular cases, the formulas of the parameters characterizing short-range ordering depending on the temperature, the alloy composition, the degree of long-range order, and the energy constants are given. The character of their functional dependences is determined, the graphs are constructed. The calculation results correlate with the experimental data published.*

Keywords: statistical theory, quasichemical method, ternary substitutional solid solutions, correlation parameters, long- and short-range order, energy parameters of interatomic interaction.

INTRODUCTION

Physical properties of alloys are predetermined by the chemical nature and concentration of their components, structure, strains, presence of defects, such as heterogeneity of their composition, antiphase boundaries, vacancies, admixture atoms and atomic order, long-, short-range, or local, and such external factors as temperature and pressure [1–12]. At that, atomic orders are formed, altered, and transformed depending on temperature, its increase or decrease, and with the course of time. It is found that short-range atomic order influences electrical, magnetic, galvanomagnetic, thermal, mechanical, and other properties as well as the long-range one. However, the direction of the change in these physical properties may be either the same as at long-range ordering or different, i. e. the opposite one. This causes some peculiarities in functional dependences of various physical characteristics of alloys associated with establishment or decay of short-range ordering.

The addition of various kinds of admixtures to an alloy may lead to some changes in the properties of the latter. Therefore, doping of ordering alloys can be successfully used in the preparation of alloys with predetermined properties.

The aim of this work is to study short-range ordering and clarify the nature of the dependences of short-range order parameters on the temperature, the degree of long-range order, the composition and the energy constants in binary and ternary solid solutions with FCC lattice $L1_2$ of a Cu_3Au type.

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1. LONG-, SHORT-RANGE, AND LOCAL ATOMIC ORDER

Long-range ordering in alloys is characterized by regular alternation of atomic arrangement in crystal lattice sites, when the lattice formed is periodic, and the atoms of each type take specific sites legal for them. Long-range order parameter of alloy AB_3 of the composition a, b is determined by formula

$$\eta = \frac{4}{3}\left(P_A^{(1)} - a\right), \tag{1}$$

where $P_A^{(1)}$ is a priori probability of substitution of the first type site by an atom of type A.

Short-range order can be determined by a parameter characterizing the surrounding of each atom by other atoms of different types. In case of the absence of long-range order for the nearest atomic pairs, it can be determined by formula

$$\sigma = 2P_{AB} - 1 = 2P_A(B)P_B - 1 = 2P_B(A)P_A - 1, \tag{2}$$

where P_{AB} is a posteriori probability of the nearest sites filling, which are equivalent at $\eta = 0$, by atoms A and B, $P_\alpha(\beta)$ is the probability of substitution of a site by atom α, if atom β is in the nearest site (α, $\beta = A$, B). σ may range $0 \le \sigma \le 1$ depending on the temperature.

Short-range order can be characterized by a correlation parameter, which at $\eta = 0$ is equal to

$$\varepsilon = \varepsilon_{AB} = P_{AB} - ab. \tag{3}$$

The values η, σ, and ε are interrelated. In a particular case of stoichiometric alloy with $a = b = 0.5$, in which the sites of each type are completely surrounded by the sites of the second type, this interrelation is determined by a simple formula

$$\sigma = \eta^2 + 4\varepsilon_{AB}, \tag{4}$$

which shows that in case of zero long-range order, the degree of short-range order is determined by correlation, i.e. short-range ordering can be characterized by both parameters σ, and ε.

In experimental studies in literature, for disordered alloys, they sometimes use short-range order parameter γ equal to

$$\gamma = \gamma_{AB} = \pm\left(\frac{P_{AB}}{ab} - 1\right) = \pm\frac{P_A(B) - a}{a} = \pm\frac{P_B(A) - b}{b} = \pm\frac{\varepsilon}{ab}, \tag{5}$$

which in various sources is used under (+) or (–).

Local order is considered for inhomogeneous alloys, when the system contains microdomains (domains or clusters) different in both the composition and the parameters of long- and short-range order. In a particular case, the presence of A–B clusters of two types in the alloy at $\eta = 0$, the parameter of local order is determined by formula [1]

$$\alpha = \gamma_1 + (1 - \gamma_0), \tag{6}$$

where

$$\gamma_1 = \frac{N'a'b'\gamma' + N''a''b''\gamma''}{Nab}, \ \gamma_0 = \frac{N'a'b' + N''a''b''}{Nab}, \tag{7}$$

and values N', a', b', γ', as well as those with two strokes, determine the number of atoms, the concentrations of components *A*, *B*, and the degree of short-range order in a set of clusters of each type; at that,

$$a = a' + a'' ,\ b = b' + b'' \text{ and } a + b = 1 . \tag{8}$$

Clusters may also possess long-range order, which will also vary in clusters of different types. It is also possible that clusters with different long-range orders float in a matrix with short-range order.

With the course of time and changes in temperature and composition of alloys, atoms are rearranged and their ordering type and character are reformed. The degree of short-range order may decrease or increase, approaching the equilibrium value, the nature of clustering of the nearest atoms of different or similar types may change: i.e. a tendency to ordering or decay appears with a change in the sign of the short-range order parameter; intermediate state between short- and long-range orders is also possible. These processes may lead to the formation of local order: the appearance of microdomains (domains or clusters) different in the composition and the degree and type of short- and long-range ordering and the emergence of cross-domain boundaries. In the course of the domains' growth, they can absorb, merge, and, as a result, the transition from local to short-range order may occur. These processes determine the appearance of "anomalies" in functional dependences of the alloys' physical properties.

2. EXPERIMENTAL CORRELATION OF SHORT-RANGE ATOMIC ORDERING WITH PHYSICAL PROPERTIES OF THE ALLOYS

Figures 1 and 2 show literature experimental graphs of some physical properties depending on temperature, annealing time, and composition of various binary and ternary alloys manifesting short-range and local ordering [1–14].

The figures demonstrate the diversity of functional dependences of physical properties of the alloys: growth, decline, minimum or maximum extremes, retrograde graphs, the presence of bends, exo- and endo-peaks, which is caused by the development in the process of temperature change or with the course of time of short-range ordering.

With increasing temperature, or in the process of kinetics, short-range order may appear, develop, and further decay; grains (clusters) of a new shape, clusters with different short-range orders, clusters with a superlattice structure, clusters in an intermediate state between long- and short-range order, or clusters with long-range order floating in a matrix with short-range order or disorder may appear.

3. RESULTS OF THE THEORY

In order to solve the problem mentioned, free energy of alloy AB_3 of FCC-structure $L1_2$ with an admixture of component *C* was calculated. The calculation was performed within the quasichemical approximation [15], which allows to determine free energy with an accuracy of order of terms $(w/kT)^3$ (*w* stands for the alloy atoms' mixing energy), takes into account correlation, explains a significant number of experimental facts, and at the same time is simpler than other methods giving similar accuracy. We will take into account pair interaction of the nearest neighboring atoms, considering them independent "molecules". The crystal lattice will be considered geometrically perfect, disregarding its possible distortions. We assume that the parameter of the lattice, and hence the energy of interatomic interaction, are not dependent on the alloy composition. We take into account possible location of atoms of admixture *C* in the sites of both types legal for atoms *A* and *B*.

Free energy of the alloy *F* was calculated using the known formula [16, 17]

$$F = E - kT\ln W, \tag{9}$$

where *E* is the configuration part of the internal energy of the alloy, determined by the sum of the energies of interaction of the nearest atom pairs, *W* is the thermodynamic probability, i. e. the number of energetically distinct configurations of atoms in crystal lattice sites, *k* is the Boltzmann constant, and *T* is the absolute temperature.

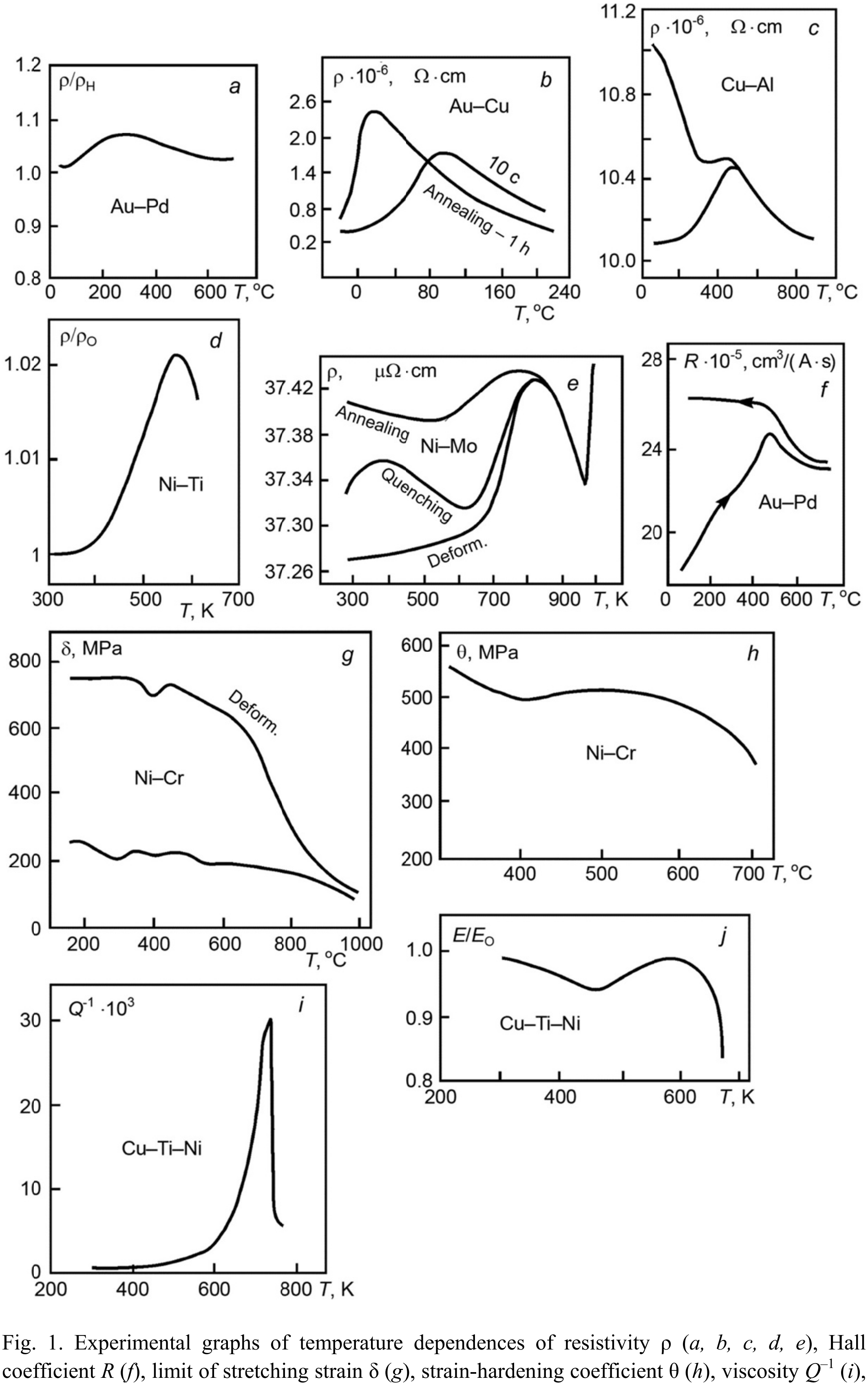

Fig. 1. Experimental graphs of temperature dependences of resistivity ρ (*a, b, c, d, e*), Hall coefficient *R* (*f*), limit of stretching strain δ (*g*), strain-hardening coefficient θ (*h*), viscosity Q^{-1} (*i*), and elasticity modulus *E* (*j*) [1, 4, 5, 7, 9, 10, 12–14].

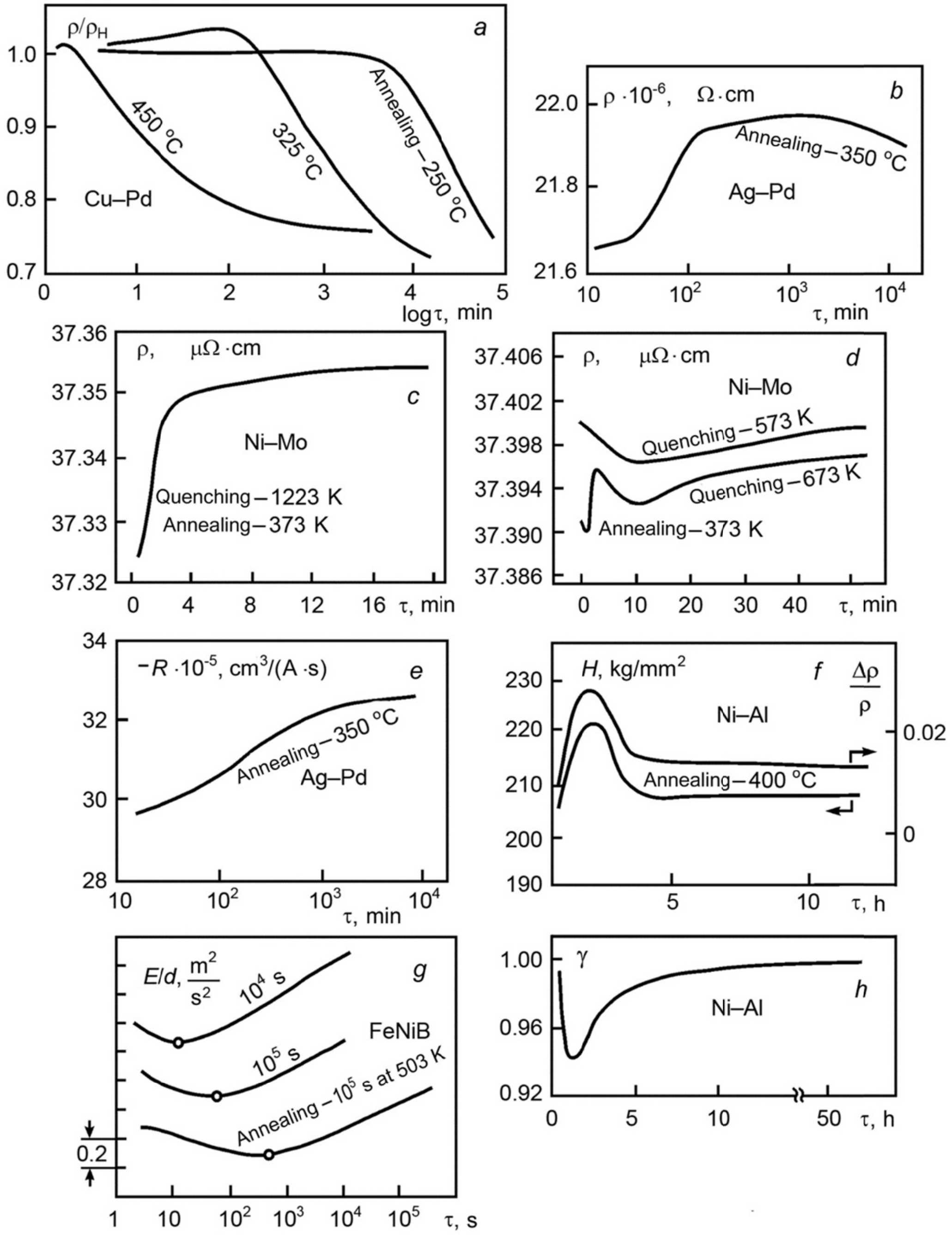

Fig. 2. Experimental graphs of time dependences of resistivity ρ (*a*, *b*, *c*, *d*), Hall coefficient *R* (*e*), microhardness *H* (*f*), elasticity modulus *E*/*d* (*g*) (*d* – density), and short-range order parameter γ (*h*) [1–3, 6, 8, 11, 12].

As a result of the calculation, the formula

$$F = 12N_0\Big[\Big(P_{AA}^{(12)} + P_{AA}^{(22)}\Big)\upsilon_{AA} + \Big(P_{BB}^{(12)} + P_{BB}^{(22)}\Big)\upsilon_{BB} + \Big(P_{CC}^{(12)} + P_{CC}^{(22)}\Big)\upsilon_{CC}$$

$$+\left(P_{AB}^{(12)}+P_{BA}^{(12)}+2P_{AB}^{(22)}\right)\upsilon_{AB}+\left(P_{AC}^{(12)}+P_{CA}^{(12)}+2P_{AC}^{(22)}\right)\upsilon_{AC}+\left(P_{BC}^{(12)}+P_{CB}^{(12)}+2P_{BC}^{(22)}\right)\upsilon_{BC}]$$

$$+12kTN_0\Big[P_{AA}^{(12)}\ln P_{AA}^{(12)}+P_{AA}^{(22)}\ln P_{AA}^{(22)}+P_{BB}^{(12)}\ln P_{BB}^{(12)}+P_{BB}^{(22)}\ln P_{BB}^{(22)}+P_{CC}^{(12)}\ln P_{CC}^{(12)}+P_{CC}^{(22)}\ln P_{CC}^{(22)}$$

$$+P_{AB}^{(12)}\ln P_{AB}^{(12)}+P_{BA}^{(12)}\ln P_{BA}^{(12)}+2P_{AB}^{(22)}\ln P_{AB}^{(22)}+P_{AC}^{(12)}\ln P_{AC}^{(12)}+P_{CA}^{(12)}\ln P_{CA}^{(12)}+2P_{AC}^{(22)}\ln P_{AC}^{(22)} \tag{10}$$

$$+P_{BC}^{(12)}\ln P_{BC}^{(12)}+P_{CB}^{(12)}\ln P_{CB}^{(12)}+2P_{BC}^{(22)}\ln P_{BC}^{(22)}\Big]$$

$$+11kTN_0\Big[P_A^{(1)}\ln P_A^{(1)}+3P_A^{(2)}\ln P_A^{(2)}+P_B^{(1)}\ln P_B^{(1)}+3P_B^{(2)}\ln P_B^{(2)}+P_C^{(1)}\ln P_C^{(1)}+3P_C^{(2)}\ln P_C^{(2)}\Big],$$

is obtained, where $P_{\alpha\beta}^{(ij)}$ represent conditional probabilities of substitution of the sites of type $i, j = 1, 2$ by atoms of type $\alpha, \beta = A, B, C$,

$$P_A^{(1)}=a+\frac{3}{4}\eta,\ P_B^{(1)}=b-\frac{3}{4}\eta-\frac{3}{4}\left(P_C^{(1)}-P_C^{(2)}\right),\ P_A^{(2)}=a-\frac{1}{4}\eta,\ P_B^{(2)}=b+\frac{1}{4}\eta+\frac{1}{4}\left(P_C^{(1)}-P_C^{(2)}\right), \tag{11}$$

k is the Boltzmann constant, T is the absolute temperature, and $\upsilon_{\alpha\beta}(\alpha, \beta = A, B, C)$ is the energies of electrochemical interaction of the nearest atom pairs.

As we see, free energy is a function of temperature, a priori and a posteriori probabilities, the alloy composition, and the degree of long-range order, as well as the energy parameters. Free energy is minimal in the state of thermodynamic equilibrium. On condition that free energy is minimal, we can determine the equilibrium values of probabilities $P_{\alpha\beta}^{(ij)}$, which will make it possible to study the correlation parameters of an ordering alloy depending on its composition, temperature, the degree of long-range order, and the energy constants. In a general case, the solution to this problem encounters some mathematical difficulties. The problem was solved for particular cases. Let us write down some results.

A posteriori probabilities $P_A(c),\ P_B(c)$ in case of $\eta = 0$, $c \ll 1$, and $a = 0.25$ are obtained as follows

$$P_A(c)=\left\{1+\left[\frac{\left(1-3\exp\frac{-w_{AB}}{kT}\right)^{1/2}+\left(1+3\exp\frac{-w_{AB}}{kT}\right)}{\left(1+3\exp\frac{-w_{AB}}{kT}\right)+\left(1-\exp\frac{-w_{AB}}{kT}\right)^{1/2}}\right]^{1/2}\exp\frac{w_{BC}-w_{AC}}{2kT}\right\}^{-1},$$

$$\tag{12}$$

$$P_B(c)=\left\{1+\left[\frac{\left(1+3\exp\frac{-w_{AB}}{kT}\right)^{1/2}-\left(1-\exp\frac{-w_{AB}}{kT}\right)}{\left(1-3\exp\frac{-w_{AB}}{kT}\right)+\left(1+3\exp\frac{-w_{AB}}{kT}\right)^{1/2}}\right]^{1/2}\exp\frac{-\left(w_{BC}-w_{AC}\right)}{2kT}\right\}^{-1},$$

where

$$w_{\alpha\beta} = 2\upsilon_{\alpha\beta} - \upsilon_{\alpha\alpha} - \upsilon_{\beta\beta}(\alpha,\ \beta = A,\ B,\ C) \tag{13}$$

are the energies of the atom pairs' *AB*, *AC*, *BC* mixing.

At $a = 0.5$, the formulas for $P_A(c)$, $P_B(c)$ take a simpler form

$$P_A(c) = \frac{\exp\dfrac{w_{AC}}{2kT}}{\exp\dfrac{w_{AC}}{2kT} + \exp\dfrac{w_{BC}}{2kT}},\quad P_B(c) = \frac{\exp\dfrac{w_{BC}}{2kT}}{\exp\dfrac{w_{AC}}{2kT} + \exp\dfrac{w_{BC}}{2kT}}. \tag{14}$$

These conditional probabilities characterize the correlation in the filling of the nearest sites by atoms' pairs *AC* and *BC* depending on the temperature and the energy parameters, i. e. determine short-range ordering or the character of neighborhood (attraction or repulsion) of corresponding pairs of atoms *AC*, *BC*. At that, realization of pairs *AC*, as compared to *BC* ones, is more probable at $w_{AC} > w_{BC} > 0$, and, vice versa, formation of pairs *BC* is more probable at $w_{AC} < w_{BC}$.

Correlation parameters $\varepsilon^{(12)}$, $\varepsilon^{(22)}$ in case of $b = 3a$ and $c \ll 1$ are found in the following form:

$$\varepsilon^{(12)} = \frac{2P_A^{(1)}P_B^{(1)}P_A^{(2)}P_B^{(2)}\left(\exp\dfrac{w_{AB}}{kT} - 1\right)}{\alpha + \left(P_A^{(1)}P_A^{(2)} + P_B^{(1)}P_B^{(2)}\right)\exp\dfrac{w_{AB}}{kT} + P_A^{(1)}P_B^{(2)} + P_A^{(2)}P_B^{(1)}},$$

$$\varepsilon^{(22)} = \frac{2P_A^{(2)2}P_B^{(2)2}\left(\exp\dfrac{w_{AB}}{kT} - 1\right)}{\beta + \left(P_A^{(2)2} + P_B^{(2)2}\right)\exp\dfrac{w_{AB}}{kT} + 2P_A^{(2)}P_B^{(2)}}, \tag{15}$$

where

$$\alpha = \left[\left(P_B^{(2)} - P_A^{(1)}\right)^2\exp\frac{2w_{AB}}{kT} + 2\left(P_A^{(1)}P_B^{(1)} + P_A^{(2)}P_B^{(2)}\right)\exp\frac{w_{AB}}{kT} + \left(P_A^{(1)} - P_A^{(2)}\right)^2\right]^{1/2},$$

$$\beta = \left[\left(P_A^{(2)} - P_B^{(2)}\right)^2\exp\frac{2w_{AB}}{kT} + 4P_A^{(2)}P_B^{(2)}\exp\frac{w_{AB}}{kT}\right]^{1/2}. \tag{16}$$

Taking into account equations (11), these formulas determine the dependence of correlation parameters for pairs of the nearest atoms *AB* of ternary alloy *A*–*B*–*C* ($c \ll 1$) on the temperature, the concentration of component *C*, the degree of long-range order η, and the energy constants w_{AB}, $w_{BC} - w_{AC}$. Equations (15) at $c = 0$ coincide with the corresponding formulas for a binary alloy [18].

In a disordered binary alloy, correlation parameters are equal to each other:

$$\varepsilon = \varepsilon^{(12)} = \varepsilon^{(22)} = \frac{2a^2b^2\left(\exp\frac{w_{AB}}{kT} - 1\right)}{\left[(a-b)^2\exp\frac{2w_{AB}}{kT} + 4ab\exp\frac{w_{AB}}{kT}\right]^{1/2} + \left(a^2+b^2\right)\exp\frac{w_{AB}}{kT} + 2}. \quad (17)$$

If the temperature is so high that $w_{AB}/kT \ll 1$, then, expanding equation (17) in a series with respect to a small quantity w_{AB}/kT, we obtain the formula for the correlation parameter ε of the disordered alloy

$$\varepsilon = a^2b^2\frac{w_{AB}}{kT}, \quad (18)$$

which shows, that the dependence of ε on the inverse temperature is linear, while the dependence of ε on the alloy composition is parabolic with an extremum at $a = b$ (maximum at $w_{AB} > 0$ and minimum at $w_{AB} < 0$).

Due to the bulkiness of formulas (12), (16), and (17), they were analyzed by numerical methods.

Formulas (12)–(17) obtained for a posteriori probabilities and correlation parameters make it possible to study changes in short-range order in a binary alloy upon adding an admixture of the third component.

The character of concentration dependence of parameters γ_{AC}, γ_{BC} in the substitution of the nearest sites of the lattice by a pair of atoms *AC*, *BC* in a ternary alloy, obtained by adding the third component *C* to binary alloy *AB* of equiatomic composition $a = b$ at $kT \gg w_{\alpha\beta}$ ($\alpha, \beta = A, B, C$), is determined by the following formula:

$$\gamma_{AC} = a\frac{w_0}{2kT} + ac\frac{w}{kT}, \quad \gamma_{BC} = -a\frac{w_0}{2kT} + ac\frac{w}{kT}, \quad (19)$$

where

$$w_0 = w_{AC} - w_{BC}, \ w = -w_{AB} + 2w_{AC} + 2w_{BC}. \quad (20)$$

In accordance with formulas (19), the concentration dependences $\gamma_{AC}(c)$ and $\gamma_{BC}(c)$ can be monotonous or extreme, depending on the ratio between energy parameters w_0 and w (20).

In a particular case of $b = 3a$ at $kT \gg w_{\alpha\beta}$ ($\alpha, \beta = A, B, C$), the parameter γ_{AB} takes the following form:

$$\gamma_{AB} = \left(w_1 + w_2c + w_3c^2\right)\frac{1}{kT}, \quad (21)$$

where

$$w_1 = \frac{3}{16}w_{AB}, \ w_2 = \frac{1}{2}\left(\frac{3}{4}w_{AB} - \frac{1}{2}w_{AC} + w_{BC}\right), \ w_3 = \frac{1}{2}\left(\frac{3}{4}w_{AB} - \frac{1}{2}w_{AC} - 3w_{BC}\right). \quad (22)$$

A parabolic dependence of the short-range order parameter γ_{AB} on the concentration of admixture *C* was obtained, which also can be extreme depending on the numerical values of energies w_i ($i = 1, 2, 3$) (22).

Fig. 3 shows calculated graphs of short-range order parameters, constructed according to formulas (14)–(22) depending on the temperature, the parameter of long-range order, and the concentrations for the following data:

a – $c = 0$, $\eta = 0$, $w_{AB} = 0.0125$ eV, $a = 0.2, 0.3$ (curves *1* and *2*);
b – $c = 0$, $\eta = 0$, $kT \gg w_{AB}$;
c – $a = 0.5$, $c \ll 1$, $\eta = 0$, $w_{AC} - w_{BC} = 0.08$ eV;
d – $b = 3a$, $c = 0.05$, $w_{AB}/kT = 1.22$, $(w_{BC} - w_{AC})/kT = 0.01$;

$e - b = 3a$, $c = 0, 0.05, 0.1$ (curves *1*, *2*, *3*), $w_{AB}/kT = 1.114$, $(w_{BC} - w_{AC})/kT = -0.018$;

$$\left.\begin{array}{l} f - a = b,\ kT >> w_{AB}, w_{BC},\ w_0 = 0.4,\ w = 0.8 \text{ (solid curves)}, \\ w_0 = 0.4,\ w = 0.2 \text{ (dashed curves)}, \\ g - a = b,\ kT >> w_{AB}, w_{AC}, w_{BC},\ w_0 = 0.4,\ w = -0.8 \text{ (solid curves)}, \\ w_0 = 0.4,\ w = -0.2 \text{ (dashed curves)}, \\ h - b = 3a,\ kT >> w_{AB}, w_{AC}, w_{BC},\ w_1 = 0.015,\ w_2 = -0.045,\ w_3 = -0.145, \end{array}\right\} ,\ kT, \qquad (23)$$

$kT = 0.08$ and 0.16 (curves *1* and *2*), eV.

CONCLUSIONS

Thus, the statistical theory developed with the use of quasichemical method made it possible to establish the dependence of short-range order parameters on the temperature, the alloy composition, the degree of long-range order, and the range of energy constants for ternary FCC-substitutional alloy $AB_3 + C$.

The calculated values of conditional probabilities $P_{\alpha\beta}$ or $P_\alpha(\beta)$, correlation parameters $\varepsilon_{\alpha\beta}^{(ij)}$ or $\varepsilon_{\alpha\beta}$, and short-range order parameters $\gamma_{\alpha\beta}$, depending on the temperature, the alloy composition, and the energy constants, determine the character of mutual arrangement of the nearest atoms, which can be such that in some cases, there will be a tendency to approximation of atoms of different types, which facilitates the process of ordering, while in other cases, on the contrary, there will be a tendency to mutual approximation of atoms of similar types, which facilitates the beginning of the process of decay into phases of different compositions. In the process of temperature change, or with the course of time, or with changing concentrations of components in the entire alloy or in its phases, reorientation of the arrangements of different types of atoms and the character of their mutual approximation may occur. Such processes will affect physical properties of solid solutions. At that, one can regulate the process of short-range ordering of atoms by the appropriate heat treatment or selection of the concentration of admixture *C* and thereby achieve the formation of certain physical properties required from the alloy.

The calculations conducted and the graphs constructed show the whole variety of the functional dependences of values $P_\alpha(\beta)$, $\varepsilon_{\alpha\beta}^{(ij)}$, $\varepsilon_{\alpha\beta}$, and $\gamma_{\alpha\beta}$ determining short-range ordering. Here we deal with increase, decrease, minimum or maximum extremes, sign change, i.e. changing tendencies of ordering and decay. The same variety of the graphs' forms is observed in the experiments. Retrograde character of functional dependences is usually caused by the presence and re-formation of local order, which has not been studied in the present investigation.

The remarkable thing is that knowing the energies of pair interaction of atoms $\upsilon_{\alpha\beta}$ (for example, from independent experiments for binary alloys *AB*, *AC*, *BC*), one can predetermine functional dependences of short-range order parameters with the help of the obtained formulas or calculate the right amount of admixture *C* of a certain type to regulate the process of short-range ordering and thus achieve the formation of certain physical properties in the alloy.

If the short-range order parameters are known from the experiments, then the obtained formulas make it possible to determine the energy parameters $\upsilon_{\alpha\beta}$ of interatomic interactions, which represents a separate academic interest.

The obtained formulas of all the values characterizing short-range ordering can be used to study scattering of different types of waves by crystals, including the intensity of incoherent scattering of X-rays in the alloy and the influence of substitutional admixture on the changes in the intensity of X-ray scattering, as well as to study resistivity and heat capacity of ordering alloys, etc. [19–21].

It should be noted that the formation in crystals of local polyatomic systems with short- and long-range ordering and their influence on the properties of crystals continue to attract the attention of scientists. For example, in [22–28], super-localization of atoms in single-crystals Ni_3Ge was studied, atomic ordering of solid solutions containing interstitial atoms was investigated; strengthening of heterogeneous FCC-alloys by particles with the superstructure $L1_2$ was evaluated, the generation of interstitial atoms in FCC-crystals was studied, the peculiarities of the formation of microstructures in Al_2O_3 alloys were investigated; general approach to the modeling of polyatomic systems was

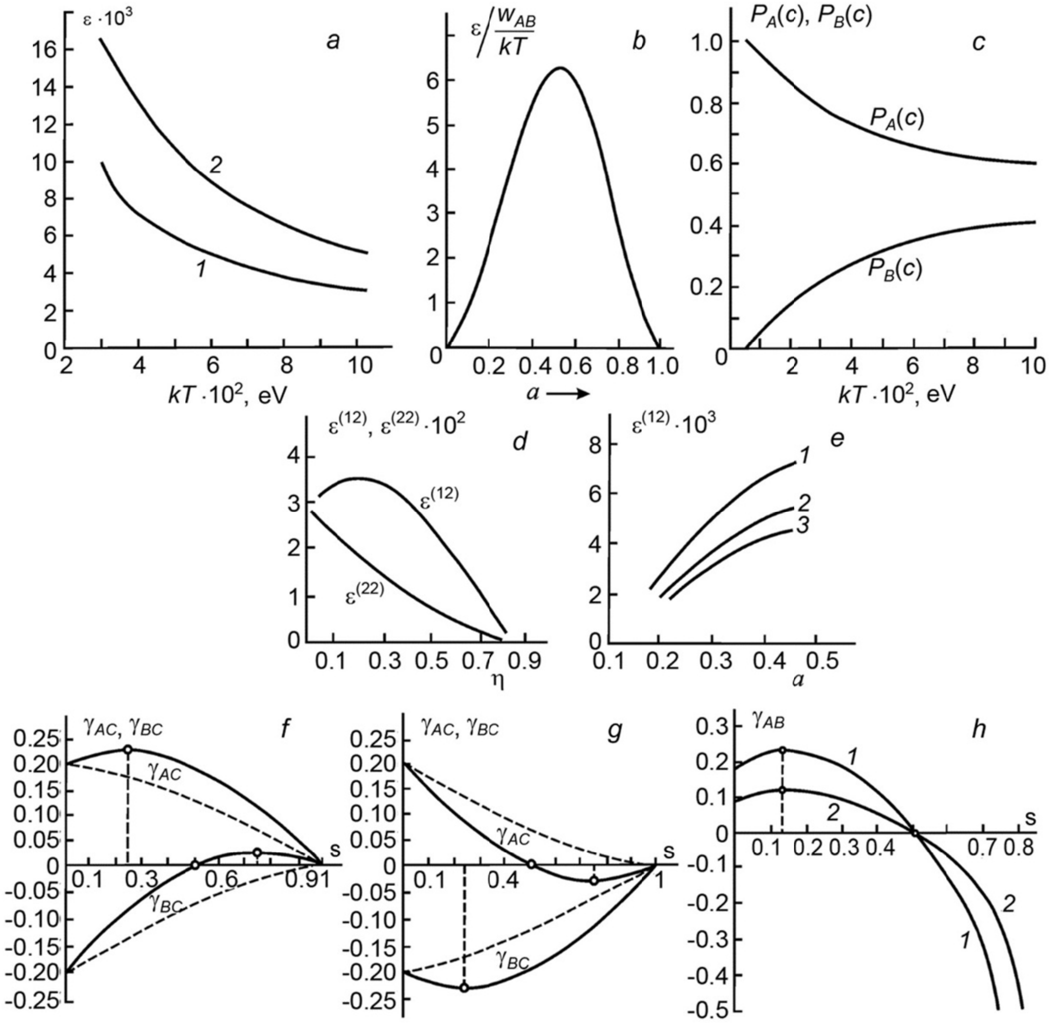

Fig. 3. Calculated graphs of short-range order parameters depending on the temperature, the degree of long-range order, and the concentrations for the data indicated in (23): *a* – temperature dependence of the correlation parameter ε according to formula (17), *b* – the dependence of the correlation parameter ε on the concentration *a* according to formula (18), *c* – temperature dependence of a posteriori probabilities $P_A(c)$ and $P_B(c)$ according to formulas (14), *d* – the dependences of the correlation parameters $\varepsilon^{(12)}$ and $\varepsilon^{(22)}$ on the degree of long-range order η according to formulas (11), (15), and (16), *e* – the dependence of the correlation parameter $\varepsilon^{(12)}$ on the concentration *a* according to formulas (11), (15), (16), *f* and *g* – the dependences of the short-range order parameters γ_{AC} and γ_{BC} on the concentration *c* according to formulas (19), (20), *h* – the dependence of the short-range order parameter γ_{AB} on the concentration *c* according to formulas (21), (22).

developed; the parameters of submicrocrystal structure of copper with an admixture of aluminum were determined. At that, these processes manifest themselves under the influence of such external factors as electromagnetic field, mechanical force (press molding), and temperature change (roast).

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