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INTERSTITIAL IMPURITIES IN ALLOYS WITH B19 STRUCTURE

A metal having hexagonal B19 structure and introduced interstitial atoms has been considered. The solubility of introduced impurities and the correlation parameters at the substitution of sites and interstitials have been studied, by using the configuration method, and their dependences on the metal composition, temperature, and long-range order degree of the impurity distribution over the sites have been determined. The information about the correlation parameters enables the evaluation of many physical characteristics of alloys. If the correlation parameters are known from experiments, the obtained formulas allow the energy parameters of the alloys to be determined.

Keywords: alloys, solubility, interstitial impurities, correlation parameters, substitutional impurities, B19 structure.

1. Introduction

The study of the solubility of interstitial impurities in a crystalline structure and the corresponding correlation parameters is of significant scientific and practical interest [1–93], because it makes it possible to determine the concentration limits for the existence of homogeneous phases [14–22] and to reveal possibilities for the formation of the short-range [22–30] or local ordering [30–38], which leads to the appearance of nuclei of a new phase [38–44]. It is known that the introduction of interstitial impurities can substantially change the parameters of materials [1–13, 45–

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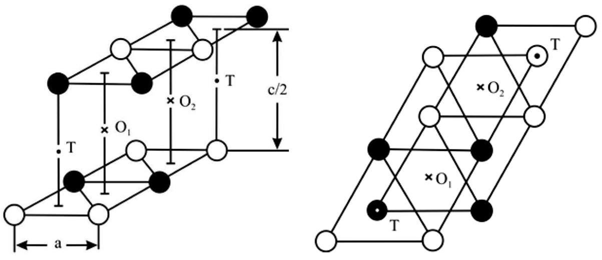
96] and their alloys [14–44]. In particular, such interstitial phases as carbides [30, 44, 63, 65, 66, 76, 79], borides [41], and nitrides [15, 18–20, 25, 26, 29, 47, 58, 60, 66, 74, 75, 78, 81, 84, 87, 89, 90, 92, 93], which are characterized by enhanced hardness, strength, and infusibility, are widely used in practice in instrumental engineering, while constructing metallurgical furnaces, engines of rockets, and so forth.

2. Solubility of Interstitial Impurity

The solubilities of interstitial impurities were mainly studied in alloys with various structures [96, 97], whereas correlations occurring at the substitution of sites and interstices were analyzed for disordered alloys [98]. In this work, we consider a metal with hexagonal B19 structure, with atoms (let us call them C-atoms) being introduced into its interstices. The B19 structure has two types of octahedral interstices (O_1 and O_2) and one type of tetrahedral (T) ones. Figure 1 demonstrates the researched structure in the spatial (Fig. 1, *a*) and projectional (along the C-axis, Fig. 1, *b*) views.

In order to determine the solubility and the correlation properties, it is necessary to calculate the metal free energy F. Here, we use the configuration method, i.e., we account for all changes of atoms A for every interstice. The configuration will be denoted by the index l, which determines the number of nearest atoms around the pore. Then the free energy can be expressed in the following form [98, 99]:

$$F = \sum_{l=0}^{6} (N^l_{O_1} + N^l_{O_2})\upsilon_l - \sum_{l=0}^{4} N^l_{T}\upsilon'_l - \kappa\Theta \times$$
$$\times \Bigg[\sum_{l=0}^{6} Q^l_{O_1} \ln Q^l_{O_1} + \sum_{l=0}^{6} Q^l_{O_2} \ln Q^l_{O_2} + \sum_{l=0}^{4} Q^l_{T} \ln Q^l_{T} -$$
$$- \sum_{l=0}^{6} N^l_{O_1} \ln N^l_{O_1} - \sum_{l=0}^{6} N^l_{O_2} \ln N^l_{O_2} - \sum_{l=0}^{4} N^l_{T} \ln N^l_{T} -$$
$$- \sum_{l=0}^{6} (Q^l_{O_1} - N^l_{O_1}) \ln(Q^l_{O_1} - N^l_{O_1}) -$$
$$- \sum_{l=0}^{6} (Q^l_{O_2} - N^l_{O_2}) \ln(Q^l_{O_2} - N^l_{O_2}) -$$
$$- \sum_{l=0}^{4} (Q^l_{T} - N^l_{T}) \ln(Q^l_{T} - N^l_{T}) \Bigg], \quad (1)$$



a *b*

Fig. 1. Schematic diagrams of the B19 structure: spatial arrangement of components (*a*); projection view along the *C*-axis (*b*). Symbols ● mark first-type sites for atoms A, second-type sites for atoms B (○), octapores (×), and tetrapores (•)

Here, $N^l_{O_1}$, $N^l_{O_2}$, and N^l_{T} are the numbers of C-atoms in the pores O_1, O_2, and T, respectively; $Q^l_{O_1}$, $Q^l_{O_2}$, and Q^l_{T} are the corresponding numbers of those pores in the alloy;

$$\upsilon_1 = l\alpha + (6 - l)\beta, \quad \upsilon'_l = l\alpha' + (4 - l)\beta'$$

are the energies of a C-atom in the octa- and tetrapores, respectively;

$$\alpha = \upsilon_{AC}, \quad \beta = \upsilon_{BC} - \alpha' = \upsilon'_{AC}, \quad \beta' = \upsilon'_{BC}$$

are the energies of interaction between the pairs of nearest indicated atoms; k is the Boltzmann constant; and Θ is the absolute temperature.

From the condition of free energy minimum, we determine the quantities

$$N^l_{O_1} = \frac{DQ^l_{O_1} \exp \frac{\upsilon_l}{\kappa\Theta}}{1 + DQ^l_{O_1} \exp \frac{\upsilon_l}{\kappa\Theta}};$$
$$N^l_{O_2} = \frac{DQ^l_{O_2} \exp \frac{\upsilon_l}{\kappa\Theta}}{1 + DQ^l_{O_2} \exp \frac{\upsilon_l}{\kappa\Theta}}; \quad (2)$$
$$N^l_{T} = \frac{DQ^l_{T} \exp \frac{\upsilon'_l}{\kappa\Theta}}{1 + DQ^l_{T} \exp \frac{\upsilon'_l}{\kappa\Theta}},$$

They satisfy the obvious relation

$$\sum_{l=0}^{6} \left(N^l_{O_1} + N^l_{O_2}\right) + \sum_{l=0}^{4} N^l_{T} = N_C, \quad (3)$$

where N_C is the number of all C-atoms in the alloy. The coefficient D in formula (2) is a factor describing how the function of the system state increases, when an additional atom appears in the system during the process of impurity dissolution. If we put N_C = const when studying the correlation, the coefficient D is determined from condition (3). Formulas (2) are valid for any occupation numbers of interstices with C-atoms.

In the special case of metal A, when, on the one hand, $l = 6$, $\upsilon_l = 6\alpha$, and $Q_\mathrm{O} = N$ for octapores (N is the number of sites in the alloy) and, on the other hand, $l = 4$, $\upsilon'_l = 4\alpha'$, and $Q_\mathrm{T} = 2N$ for tetrapores, instead of nineteen formulas (2), we have only two:

$$N_\mathrm{O} = N\left(1 + \frac{1}{D}\exp\frac{-6\alpha}{\kappa\Theta}\right)^{-1};$$
$$N_\mathrm{T} = 2N\left(1 + \frac{1}{D}\exp\frac{-4\alpha'}{\kappa\Theta}\right)^{-1}. \tag{4}$$

Summing them up, we obtain the component solubility,

$$\nu = \frac{N_\mathrm{O} + N_\mathrm{T}}{3N} = \frac{1}{3}\left[\left(1 + \frac{1}{D}\exp\frac{-6\alpha}{\kappa\Theta}\right)^{-1} + \right.$$
$$\left. + 2\left(1 + \frac{1}{D}\exp\frac{-4\alpha'}{\kappa\Theta}\right)^{-1}\right]. \tag{5}$$

If the C-atoms are located in octapores or tetrapores only, then the solubility should be determined according to the formulas

$$\begin{aligned} \nu_\mathrm{O} &= \frac{N_\mathrm{O}}{N} = \left(1 + \frac{1}{D}\exp\frac{-6\alpha}{\kappa\Theta}\right)^{-1}; \\ \nu_\mathrm{T} &= \frac{N_\mathrm{T}}{2N} = \left(1 + \frac{1}{D}\exp\frac{-4\alpha'}{\kappa\Theta}\right)^{-1}. \end{aligned} \tag{6}$$

In the case of low component concentrations, these formulas become simpler:

$$\nu_\mathrm{O} = D\exp\frac{6\alpha}{\kappa\Theta}; \quad \nu_\mathrm{T} = D\exp\frac{4\alpha'}{\kappa\Theta}, \tag{7}$$

i.e., we obtain a linear dependence of the natural logarithm of the solubility of interstitial atoms on the inverse temperature. Expressions (6) for the dependences of ln ν_O and ln ν_T on $1/\Theta$ are not linear, but monotonic.

If the solubility is described by formula (5), then the manifestation of its extreme properties in the temperature dependence is possible at

$$\frac{\alpha}{\alpha'} = -\exp\frac{2\,(3\alpha - 2\alpha')}{\kappa\Theta}; \tag{8}$$

For that to happen, the energy parameters α and α' must have different signs. In this case, the distributions of C-atoms over the octa- and tetrapores are non-uniform. They can be estimated from the equations

$$\nu_\mathrm{O} + 2\nu_\mathrm{T} = 3c; \quad \frac{\nu_\mathrm{O}\,(1 - \nu_\mathrm{T})}{\nu_\mathrm{T}\,(1 - \nu_\mathrm{O})} = \exp\frac{2\,(3\alpha - 2\alpha')}{\kappa\Theta}, \tag{9}$$

where $c = N_\mathrm{C}/(3N)$. The former equation was obtained from system (4) via excluding the multiplier D, and the latter one is a consequence of condition 3).

By solving the system of equations (9), we get

$$\nu_\mathrm{O} = \frac{\left[\begin{array}{l} 3c\,(1-\varepsilon) - 2 - \varepsilon + \\ + \sqrt{[3c(1-\varepsilon) - 2 - \varepsilon]^2 + 12c\varepsilon\,(1-\varepsilon)} \end{array}\right]}{2\,(1-\varepsilon)},$$
$$\nu_\mathrm{T} = \frac{3}{2}c - \frac{1}{2}\nu_\mathrm{O}, \tag{10}$$

where $\varepsilon = \exp\frac{2(3\alpha - 2\alpha')}{\kappa\Theta}$. In the case $c = 1$, distribution (10) gives $\nu_\mathrm{O} = \nu_\mathrm{T} = 1$, i.e., we have a uniform occupation of all interstices irrespective of the temperature.

At low temperatures, the atomic distribution is determined by the relationship between the energy parameters α and α'. If $3\alpha - 2\alpha' > 0$, then, at the absolute zero temperature, we have

$$\begin{aligned} \nu_\mathrm{O}(0) &= \begin{cases} 3c, & \text{if } 0 \le c \le \dfrac{1}{3}, \\ 1, & \text{if } \dfrac{1}{3} \le c \le 1, \end{cases} \\ \nu_\mathrm{T}(0) &= \begin{cases} 0, & \text{if } 0 \le c \le \dfrac{1}{3}, \\ \dfrac{3}{2}c - \dfrac{1}{2}, & \text{if } \dfrac{1}{3} \le c \le 1, \end{cases} \end{aligned} \tag{11}$$

i.e., the interstitial atoms first occupy the octapores, where they have a deeper potential energy minimum. Only after the octapores turn out occupied, the interstitial atoms begin to occupy the tetrapores. On the other hand, if $3\alpha - 2\alpha' < 0$, then

$$\begin{aligned} \nu_\mathrm{O}(0) &= \begin{cases} 0, & \text{if } 0 \le c \le \dfrac{2}{3}, \\ 3c - 2, & \text{if } \dfrac{2}{3} \le c \le 1, \end{cases} \\ \nu_\mathrm{T}(0) &= \begin{cases} \dfrac{3}{2}c, & \text{if } 0 \le c \le \dfrac{2}{3}, \\ 1, & \text{if } \dfrac{2}{3} \le c \le 1, \end{cases} \end{aligned} \tag{12}$$

i.e., the C-atoms first occupy the tetrapores.

Dependencies (11) and (12) are represented by straight lines in Fig. 2. The curves in this picture

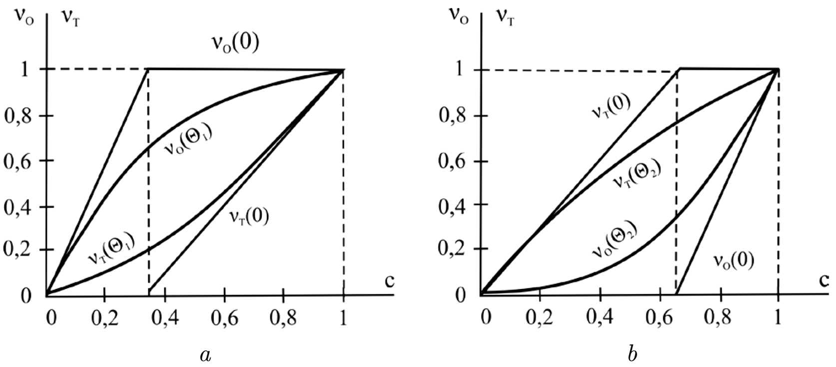


Fig. 2. Dependences of expressions (11), (12), $\nu_{\rm O}(0)$, and $\nu_{\rm T}(0)$ on c calculated in accordance with distribution (10) at the temperatures Θ_1 (a) and Θ_2 (b)

illustrate the dependencies $\nu_{\rm O}(0)$ and $\nu_{\rm T}(0)$ plotted accordingly to distribution (10) at the temperatures

$$\Theta_1 = \frac{4\,(1.5\alpha - \alpha')}{\kappa \ln 10} \qquad \text{(panel } a\text{)}$$

and

$$\Theta_2 = -\frac{4\,(1.5\alpha - \alpha')}{\kappa \ln 10}. \qquad \text{(panel } b\text{)}$$

It is necessary to consider another special case, namely, a binary alloy with a low concentration of interstitial impurities. In this case, formulas (2) can be simplified:

$$\begin{aligned} N^l_{\rm O_1} &= D Q^l_{\rm O_1} \exp\frac{\upsilon_l}{\kappa\Theta}; \\ N^l_{\rm O_2} &= D Q^l_{\rm O_2} \exp\frac{\upsilon_l}{\kappa\Theta}; \\ N^l_{\rm T} &= D Q^l_{\rm T} \exp\frac{\upsilon'_l}{\kappa\Theta}, \end{aligned} \tag{13}$$

where the parameters $Q^l_{\rm O_1}$, $Q^l_{\rm O_2}$, and $Q^l_{\rm T}$ are determined by the configuration of atoms A around voids:

$$\begin{aligned} Q^l_{\rm O_1} &= \frac{1}{2} N \frac{4!}{i!\,(4-i)!} p_{\rm A}^{(1)i} p_{\rm B}^{(1)(4-i)} \times \\ &\times \frac{2!}{j!\,(2-j)!} p_{\rm A}^{(2)j} p_{\rm B}^{(2)(2-j)}, \\ Q^l_{\rm O_2} &= \frac{1}{2} N \frac{2!}{i!\,(2-i)!} p_{\rm A}^{(1)i} p_{\rm B}^{(1)(2-i)} \times \\ &\times \frac{4!}{j\,(4-j)!} p_{\rm A}^{(2)j} p_{\rm B}^{(2)(4-j)}, \\ Q^l_{\rm T} &= 2N \frac{2!}{i!\,(2-i)!} p_{\rm A}^{(1)i} p_{\rm B}^{(1)(2-i)} \times \\ &\times \frac{2!}{j!\,(2-j)!} p_{\rm A}^{(2)j} p_{\rm B}^{(2)(2-j)}. \end{aligned} \tag{14}$$

Here, $l = i + j$, where i and j are the numbers of A-atoms around an interstice at the of the first- and second-type sites, respectively, and $p^{(1)}_{\rm A}$, $p^{(2)}_{\rm A}$, $p^{(1)}_{\rm B}$, and $p^{(2)}_{\rm B}$ are the probabilities of substituting sites 1 and 2 by atoms A and B, which depend on the composition (a, b) of the binary alloy and the long-range ordering degree η according to the formulas [99]

$$\begin{aligned} p^{(1)}_{\rm A} &= a + \frac{1}{2}\eta; \quad p^{(2)}_{\rm A} = a - \frac{1}{2}\eta; \\ p^{(1)}_{\rm B} &= b - \frac{1}{2}\eta; \quad p^{(2)}_{\rm B} = b + \frac{1}{2}\eta. \end{aligned} \tag{15}$$

Summing up quantities (13) over all configurations and taking Eqs. (14) into account, we get the following formulas for the numbers of C-atoms in the pores $\rm O_1$, $\rm O_2$, and T:

$$\begin{aligned} N^{\rm O_1}_{\rm C} &= \frac{1}{2} N D K^4_1 K^2_2, \\ N^{\rm O_2}_{\rm C} &= \frac{1}{2} N D K^2_1 K^4_2, \\ N^{\rm (T)}_{\rm C} &= 2 N D K'^2_1 K'^2_2, \end{aligned} \tag{16}$$

where

$$\begin{aligned} K_1 &= p^{(1)}_{\rm A} \exp\frac{\alpha}{\kappa\Theta} + p^{(1)}_{\rm B} \exp\frac{\beta}{\kappa\Theta}; \\ K_2 &= p^{(2)}_{\rm A} \exp\frac{\alpha}{\kappa\Theta} + p^{(2)}_{\rm B} \exp\frac{\beta}{\kappa\Theta}; \\ K'{}_1 &= p^{(2)}_{\rm A} \exp\frac{\alpha'}{\kappa\Theta} + p^{(1)}_{\rm B} \exp\frac{\beta'}{\kappa\Theta}; \\ K'_2 &= p^{(2)}_{\rm A} \exp\frac{\alpha'}{\kappa\Theta} + p^{(2)}_{\rm B} \exp\frac{\beta'}{\kappa\Theta}. \end{aligned} \tag{17}$$

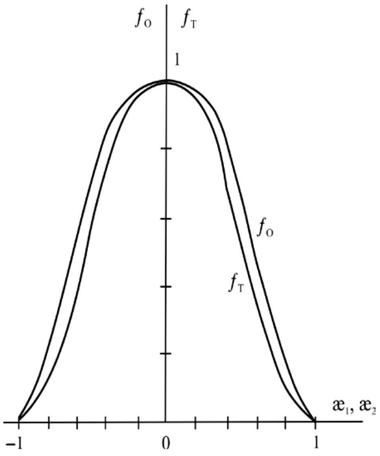


Fig. 3. Influence of the atomic order on the solubility

The impurity solubility, which is determined by the concentration of C-atoms for each of the interstice types, can be obtained from Eqs. (16):

$$\nu_O = \frac{N_C^{(O_1)} + N_C^{(O_2)}}{N} = \frac{1}{2} D K_1^2 K_2^2 \left(K_1^2 + K_2^2\right), \qquad \nu_T = \frac{N_C^{(T)}}{2N} = D K_1'^2 K_2'^2. \tag{18}$$

These formulas together with Eqs. (17) and (15) determine the impurity solubility dependence on the alloy composition, temperature, and order parameters. The former dependence is monotonic for a disordered alloy ($\eta = 0$); the latter one can be extreme at $\eta = 0$, if

$$\frac{\alpha}{\beta} = -\frac{b}{a} \exp \frac{\beta - \alpha}{\kappa \Theta}$$

for the octapores and

$$\frac{\alpha'}{\beta'} = -\frac{b}{a} \exp \frac{\beta' - \alpha'}{\kappa \Theta}$$

for the tetrapores (in this case, the energy parameters α,β and α', β' must be of different signs).

It is convenient to elucidate the influence of the atomic order on the impurity solubility by introducing the relative quantities (Fig. 3)

$$f_O = \nu_O / \left(\nu_O\right)_{\eta=0} = \left(1 - \chi_1^2\right)\left(1 - \chi_1^4\right), \qquad f_T = \nu_T / \left(\nu_T\right)_{\eta=0} = \left(1 - \chi_2^2\right)^2, \tag{19}$$

where

$$\chi_1 = \frac{1}{2} \eta \frac{\exp \frac{\alpha}{\kappa\Theta} - \exp \frac{\beta}{\kappa\Theta}}{a \exp \frac{\alpha}{\kappa\Theta} + b \exp \frac{\beta}{\kappa\Theta}};$$

$$\chi_2 = \frac{1}{2} \eta \frac{\exp \frac{\alpha'}{\kappa\Theta} - \exp \frac{\beta'}{\kappa\Theta}}{a \exp \frac{\alpha'}{\kappa\Theta} + b \exp \frac{\beta'}{\kappa\Theta}}; \tag{20}$$

$$-1 \le \chi_1, \quad \chi_2 < 1.$$

with $-1 \le (\chi_1, \chi_2) < 1$. The behavior of the dependences of the quantities f_O and f_T on η is identical. The ordering reduces the solubility, and the effect is somewhat weaker for the octapores.

If the interstitial impurity is distributed over all interstices, its solubility is determined by the formula

$$\nu = \frac{N_C^{(O_1)} + N_C^{(O_2)} + N_C^{(T)}}{3N} = \frac{1}{6} D \left[K_1^2 K_2^2 \left(K_1^2 + K_2^2\right) + 4 K_1'^2 K_2'^2\right]. \tag{21}$$

The dependence of the solubility on the composition at $\eta = 0$ can be extreme, if the energies α, β or α', β' have different signs. The character of the dependence of ν on η is the same as for the quantities ν_O and ν_T.

Let us determine the correlation parameters for the substitution of sites and interstices when assuming N_C = const. From condition (3) and in view of Eqs. (13), we obtain the coefficient D,

$$D = \frac{6c}{K_1^2 K_2^2 (K_1^2 + K_2^2) + 4 K_1'^2 K_2'^2}. \tag{22}$$

Summing up the quantities $N_{O_1}^l$, $N_{O_2}^l$, and N_T^l [Eqs. (13)] over i or j, we get the number of C-atoms in the indicated pores with the corresponding i-th or j-th, respectively, configuration of A-atoms at the closest to the interstice sites of the same type whatever the occupation of the sites of the other type:

$$N_{O_1}^i = \sum_{j=0}^{2} N_{O_1}^l = \frac{1}{2} D N K_2^2 \frac{4!}{i!(4-i)!} p_A^{(l)i} p_B^{(l)(4-i)} \times \exp \frac{i\alpha + (4-i)\beta}{\kappa\Theta};$$

$$N_{O_1}^j = \sum_{i=0}^{4} N_{O_1}^l = \frac{1}{2} D N K_1^4 \frac{2!}{j!(2-j)!} p_A^{(2)j} p_B^{(2)(2-j)} \times \exp \frac{j\alpha + (2-j)\beta}{\kappa\Theta};$$

$$N_{O_2}^i = \sum_{j=0}^{4} N_{O_2}^l = \frac{1}{2} D N K_2^4 \frac{2!}{i!(2-i)!} p_A^{(1)j} p_B^{(1)(2-i)} \times \exp \frac{i\alpha + (2-i)\beta}{\kappa\Theta}; \tag{23}$$

$$N^j_{\mathrm{O}_2} = \sum_{i=0}^{2} N^l_{\mathrm{O}_2} = \frac{1}{2} DNK_1^2 \frac{4!}{j!(4-j)!} p_{\mathrm{A}}^{(2)j} p_{\mathrm{B}}^{(2)(4-j)} \times$$
$$\times \exp\frac{j\alpha + (4-j)\beta}{\kappa\Theta};$$
$$N^i_{\mathrm{T}} = \sum_{j=0}^{2} N^l_{\mathrm{T}} = 2DNK_2'^2 \frac{2!}{i!(2-j)!} p_{\mathrm{A}}^{(1)i} p_{\mathrm{B}}^{(1)(2-i)} \times$$
$$\times \exp\frac{i\alpha' + (2-i)\beta'}{\kappa\Theta};$$
$$N^j_{\mathrm{T}} = \sum_{i=0}^{2} N^l_{\mathrm{T}} = 2DNK_1'^2 \frac{2!}{j!(2-j)!} p_{\mathrm{A}}^{(2)j} p_{\mathrm{B}}^{(2)(2-j)} \times$$
$$\times \exp\frac{j\alpha' + (2-j)\beta'}{\kappa\Theta}.$$

Accordingly, the *a posteriori* and *a priori* probabilities of substituting the nearest pairs of sites and pores with atoms A and C equal

$$p_{\mathrm{AC}}^{(1\mathrm{O}_1)} = \frac{1}{2N}\sum_{i=0}^{4} iN^i_{\mathrm{O}_1} = DK_1^3K_2^2 p_{\mathrm{A}}^{(1)} \exp\frac{\alpha}{\kappa\Theta};$$
$$p_{\mathrm{AC}}^{(1\mathrm{O}_1)^0} = 2p_{\mathrm{A}}^{(1)} N_{\mathrm{C}}^{(\mathrm{O}_1)}/N = DK_1^4K_2^2 p_{\mathrm{A}}^{(1)};$$
$$p_{\mathrm{AC}}^{(2\mathrm{O}_1)} = \frac{1}{N}\sum_{j=0}^{2} jN^j_{\mathrm{O}_1} = DK_1^4K_2 p_{\mathrm{A}}^{(2)} \exp\frac{\alpha}{\kappa\Theta};$$
$$p_{\mathrm{AC}}^{(2\mathrm{O}_1)^0} = 2p_{\mathrm{A}}^{(2)} N_{\mathrm{C}}^{(\mathrm{O}_1)}/N = DK_1^4K_2^2 p_{\mathrm{A}}^{(2)};$$
$$p_{\mathrm{AC}}^{(1\mathrm{O}_2)} = \frac{1}{N}\sum_{i=0}^{2} iN^i_{\mathrm{O}_2} = DK_1K_2^4 p_{\mathrm{A}}^{(1)} \exp\frac{\alpha}{\kappa\Theta};$$
$$p_{\mathrm{AC}}^{(1\mathrm{O}_2)^0} = 2p_{\mathrm{A}}^{(1)} N_{\mathrm{C}}^{(\mathrm{O}_2)}/N = DK_1^2K_2^4 p_{\mathrm{A}}^{(1)};$$
$$p_{\mathrm{AC}}^{(2\mathrm{O}_2)} = \frac{1}{2N}\sum_{j=0}^{4} jN^j_{\mathrm{O}_2} = DK_1^2K_2^3 p_{\mathrm{A}}^{(2)} \exp\frac{\alpha}{\kappa\Theta}; \qquad (24)$$
$$p_{\mathrm{AC}}^{(2\mathrm{O}_2)^0} = 2p_{\mathrm{A}}^{(2)} N_{\mathrm{C}}^{(\mathrm{O}_2)}/N = DK_1^2K_2^4 p_{\mathrm{A}}^{(2)};$$
$$p_{\mathrm{AC}}^{(1\mathrm{T})} = \frac{1}{4N}\sum_{i=0}^{2} iN^i_{\mathrm{T}} = DK_1'K_2'^2 p_{\mathrm{A}}^{(1)} \exp\frac{\alpha'}{\kappa\Theta};$$
$$p_{\mathrm{AC}}^{(1\mathrm{T})^0} = \frac{1}{2} p_{\mathrm{A}}^{(1)} N_{\mathrm{C}}^{(\mathrm{T})}/N = DK_1'^2K_2'^2 p_{\mathrm{A}}^{(1)};$$
$$p_{\mathrm{AC}}^{(2\mathrm{T})} = \frac{1}{4N}\sum_{j=0}^{2} jN^j_{\mathrm{T}} = DK_1'^2K_2' p_{\mathrm{A}}^{(2)} \exp\frac{\alpha'}{\kappa\Theta};$$
$$p_{\mathrm{AC}}^{(2\mathrm{T})^0} = \frac{1}{2} p_{\mathrm{A}}^{(2)} N_{\mathrm{C}}^{(\mathrm{T})}/N = DK_1'^2K_2'^2 p_{\mathrm{A}}^{(2)}.$$

The differences between these possibilities determine the correlation parameters.

The correlation parameters for the pairs of atoms B and C can be calculated in a similar way. As a result, we obtain

$$\varepsilon^{(1\mathrm{O}_1)} = \varepsilon_{\mathrm{AC}}^{(1\mathrm{O}_1)} = -\varepsilon_{\mathrm{BC}}^{(1\mathrm{O}_1)} =$$
$$= DK_1^3K_2^2 p_{\mathrm{A}}^{(1)} p_{\mathrm{B}}^{(1)} \left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right);$$
$$\varepsilon^{(2\mathrm{O}_1)} = \varepsilon_{\mathrm{AC}}^{(2\mathrm{O}_1)} = -\varepsilon_{\mathrm{BC}}^{(2\mathrm{O}_1)} =$$
$$= DK_1^4K_2 p_{\mathrm{A}}^{(2)} p_{\mathrm{B}}^{(2)} \left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right);$$
$$\varepsilon^{(1\mathrm{O}_2)} = \varepsilon_{\mathrm{AC}}^{(1\mathrm{O}_2)} = -\varepsilon_{\mathrm{BC}}^{(1\mathrm{O}_2)} =$$
$$= DK_1K_2^4 p_{\mathrm{A}}^{(1)} p_{\mathrm{B}}^{(1)} \left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right); \qquad (25)$$
$$\varepsilon^{(2\mathrm{O}_2)} = \varepsilon_{\mathrm{AC}}^{(2\mathrm{O}_2)} = -\varepsilon_{\mathrm{BC}}^{(2\mathrm{O}_2)} =$$
$$= DK_1^2K_2^3 p_{\mathrm{A}}^{(2)} p_{\mathrm{B}}^{(2)} \left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right);$$
$$\varepsilon^{(1\mathrm{T})} = \varepsilon_{\mathrm{AC}}^{(1\mathrm{T})} = -\varepsilon_{\mathrm{BC}}^{(1\mathrm{T})} =$$
$$= DK_1'K_2'^2 p_{\mathrm{A}}^{(1)} p_{\mathrm{B}}^{(1)} \left(\exp\frac{\alpha'}{\kappa\Theta} - \exp\frac{\beta'}{\kappa\Theta}\right);$$
$$\varepsilon^{(2\mathrm{T})} = \varepsilon_{\mathrm{AC}}^{(2\mathrm{T})} = -\varepsilon_{\mathrm{BC}}^{(2\mathrm{T})} =$$
$$= DK_1'^2\mathrm{K}_2' p_{\mathrm{A}}^{(2)} p_{\mathrm{B}}^{(2)} \left(\exp\frac{\alpha'}{\kappa\Theta} - \exp\frac{\beta'}{\kappa\Theta}\right).$$

The obtained formulas, taking Eqs. (23), (17), and (15) into account, determine the dependence of the correlation parameters on the alloy composition, temperature, and long-range order degree. The knowledge of the latter makes it possible to determine whether the short-range ordering or the stratification of atoms takes place in the alloy.

The correlation parameters for the octa- and tetrapores can be of different signs, e.g., if $\alpha > \beta$ and $\alpha' < \beta'$. This means that the C-atoms will be primarily accumulated at the octahedral interstices. For a disordered alloy, i.e., if $\eta = 0$,

$$K = K_1 = K_2 = a\exp\frac{\alpha}{\kappa\Theta} + b\exp\frac{\beta}{\kappa\Theta},$$
$$K' = K_1' = K_2' = a\exp\frac{\alpha'}{\kappa\Theta} + b\exp\frac{\beta'}{\kappa\Theta},$$

only two correlation parameters, for pores O and T, survive:

$$\varepsilon^{(\mathrm{O})} = 3abcK^5 \left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right) / (K^6 + 2K'^4); \qquad (26)$$
$$\varepsilon^{(\mathrm{T})} = 3abcK'^3 \left(\exp\frac{\alpha'}{\kappa\Theta} - \exp\frac{\beta'}{\kappa\Theta}\right) / (K^6 + 2K'^4).$$

The dependences of the quantities $\varepsilon^{(O)}$ and $\varepsilon^{(T)}$ on the composition are extreme and asymmetric. The maxima in those dependences take place at the following compositions:

$$a_* = \left(\exp\frac{\alpha - \beta}{2\kappa\Theta} + 1\right)^{-1} \quad \text{for } \varepsilon^{(\mathrm{O})}$$

and

$$a_* = \left(\exp\frac{\alpha' - \beta'}{\kappa\Theta} + 1\right)^{-1} \quad \text{for } \varepsilon^{(\mathrm{T})}.$$

As the temperature grows, the asymmetry of the concentration dependences decreases, and, at very high temperatures, the values of a_* become close to the stoichiometric one, $a_* \approx \frac{1}{2}$. At high temperatures, formulas (26) become simpler:

$$\varepsilon^{(\mathrm{O})} = abc\frac{\alpha - \beta}{\kappa\Theta}, \quad \varepsilon^{(\mathrm{T})} = abc\frac{\alpha' - \beta'}{\kappa\Theta}. \qquad (27)$$

Finally, let us write down formulas for the correlation parameters in the case where the atoms are distributed over only octapores or tetrapores. In the former case, $c = N_C/N$ and $D = 2s[K_1K_2(K_1^2 + K_2^2)]^{-1}$ so that

$$\varepsilon^{(1\mathrm{O}_1)} = 2cp_{\mathrm{A}}^{(1)}p_{\mathrm{B}}^{(1)}\left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right) K_1/(K_1^2 + K_2^2);$$
$$\varepsilon^{(2\mathrm{O}_1)} = 2cp_{\mathrm{A}}^{(2)}p_{\mathrm{B}}^{(2)}\left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right) \times$$
$$\times K_1^2/K_2(K_1^2 + K_2^2); \qquad (28)$$
$$\varepsilon^{(1\mathrm{O}_2)} = 2cp_{\mathrm{A}}^{(1)}p_{\mathrm{B}}^{(1)}\left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right) \times$$
$$\times K_2^2/K_1(K_1^2 + K_2^2);$$
$$\varepsilon^{(2\mathrm{O}_2)} = 2cp_{\mathrm{A}}^{(2)}p_{\mathrm{B}}^{(2)}\left(\exp\frac{\alpha}{\kappa\Theta} - \exp\frac{\beta}{\kappa\Theta}\right) K_2/(K_1^2 + K_2^2);$$

In the latter case, $c = N_C/2N$ and $D = c(K_1' + K_2')^{-2}$ so that

$$\varepsilon^{(1\mathrm{T})} = cp_{\mathrm{A}}^{(1)}p_{\mathrm{B}}^{(1)}\left(\exp\frac{\alpha'}{\kappa\Theta} - \exp\frac{\beta'}{\kappa\Theta}\right) / K_1', \qquad (29)$$
$$\varepsilon^{(2\mathrm{T})} = cp_{\mathrm{A}}^{(2)}p_{\mathrm{B}}^{(2)}\left(\exp\frac{\alpha'}{\kappa\Theta} - \exp\frac{\beta'}{\kappa\Theta}\right) / K_2'.$$

3. Conclusions

Knowing the values of correlation parameters (25) [or (29)] and (28) makes it possible to estimate a lot of physical parameters of alloys. If the correlation parameters are known from experiments, the formulas derived above allow the determination of the energy parameters of alloys, which is of high scientific importance.

Owing to the results of calculations presented in this work, the alloys corresponding to the B19 structure can be used as a working body in modern hydrogen accumulators, where they absorb and store hydrogen due to the diffusion of interstitial atoms into the bulk of their crystalline structure.

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ДОМІШКИ ВПРОВАДЖЕННЯ У СПЛАВАХ ЗІ СТРУКТУРОЮ B19

У роботі розглянуто метал з гексагональною структурою B19, в міжвузля якого впроваджуються атоми. Методом конфігурацій вивчено розчинність впроваджених домішок та параметри кореляції у заміщенні вузлів і міжвузлів, знайдено їх залежність від складу металу, температури та ступеня дальнього порядку у вузлах. Знання параметрів кореляції дозволяє оцінити багато фізичних характеристик сплавів. Якщо ж параметри кореляції відомі з експериментів, отримані формули дозволяють визначити енергетичні параметри сплавів, що має наукову цінність.

Ключові слова: сплави, розчинність, домішки впровадження, параметри кореляції, домішки заміщення, структура B19.