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WAGNER INTERACTION COEFFICIENTS OF NITROGEN WITH CHROMIUM AND MOLIBDENUM IN LIQUID NICKEL-BASED ALLOYS

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Abstract. The authors propose a simple theory of thermodynamic properties of liquid nitrogen solutions in alloys of the Fe–Ni–Cr and Fe–Ni–Mo systems. This theory is analogous to the theory for liquid nitrogen solutions in binary alloys of the Fe–Cr and Fe–Ni systems proposed previously by the authors in 2019 and 2021. The theory is based on lattice model of ternary liquid solutions of the Fe–Ni–Cr and Fe–Ni–Mo systems. The model assumes a FCC lattice. Atoms of Fe, Ni, Cr and Mo are deposited in the sites of the lattice. Nitrogen atoms are located in octahedral interstices. The nitrogen atom interacts only with the metal atoms located in the lattice sites neighboring to it. This interaction is pairwise. It is assumed that the energy of this interaction depends neither on composition nor on temperature. It is supposed that the liquid solutions in the Fe–Ni–Cr and Fe–Ni–Mo systems are perfect. Within the framework of the proposed theory, the relation is obtained that expresses the Wagner interaction coefficient between nitrogen and chromium in liquid nickel-based alloys $\varepsilon_N^{\text{Cr}}(\text{Ni})$. The right-hand part of the appropriate formula is a function of the Wagner interaction coefficients between nitrogen and chromium $\varepsilon_N^{\text{Cr}}(\text{Fe})$ and between nitrogen and nickel $\varepsilon_N^{\text{Ni}}(\text{Fe})$ in liquid iron-based alloys. A similar relation is obtained for the Wagner interaction coefficient between nitrogen and molybdenum in liquid nickel-based alloys $\varepsilon_N^{\text{Mo}}(\text{Ni})$. According to the first of these formulas, the value $\varepsilon_N^{\text{Cr}}(\text{Ni}) = -21,9$ at a temperature of 1873 K is calculated. This corresponds to the value of the Langenberg interaction coefficient $e_N^{\text{Cr}}(\text{Ni}) = -0,108$, which coincides with experimental estimate. According to the second formula, the value $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -14,3$ is calculated at a temperature 1873 K. This corresponds to the value of the Langenberg interaction coefficient $e_N^{\text{Cr}}(\text{Ni}) = -0,036$, which is in satisfactory agreement with the experimental estimate $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -15,1$; $e_N^{\text{Cr}}(\text{Ni}) = -0,038$.

Keywords: thermodynamics, solutions, nitrogen, iron, nickel, chromium, molybdenum, activity coefficient, Wagner interaction coefficient, Langenberg interaction coefficient

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ВАГНЕРОВСКИЕ ПАРАМЕТРЫ ВЗАИМОДЕЙСТВИЯ АЗОТА С ХРОМОМ И МОЛИБДЕНОМ В ЖИДКИХ СПЛАВАХ НА ОСНОВЕ НИКЕЛЯ

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Аннотация. Предложена простая теория термодинамических свойств жидких растворов азота в сплавах систем Fe–Ni–Cr и Fe–Ni–Mo, которая аналогична теории для жидких растворов азота в бинарных сплавах систем Fe–Cr и Fe–Ni, представленной авторами ранее (2019 – 2021). Теория основана на решеточной модели трехкомпонентных жидких растворов Fe–Ni–Cr и Fe–Ni–Mo. Предполагается модельная решетка типа ГЦК. В узлах этой решетки располагаются атомы железа, хрома, никеля и молибдена. Атомы азота располагаются в октаэдрических междоузлиях. Атом азота взаимодействует лишь с атомами металлов, находящимися в соседних с этим атомом узлах решетки. Это взаимодействие парное. Предполагается, что энергия этого взаимодействия не зависит ни от состава сплавов, ни от температуры, и что жидкие растворы систем Fe–Ni–Cr и Fe–Ni–Mo являются совершенными. В рамках предложенной теории представлено выражение для вагнеровского параметра взаимодействия азота с хромом в жидких сплавах на основе никеля $\varepsilon_N^{\text{Cr}}(\text{Ni})$. Правая часть соответствующей формулы является функцией вагнеровских параметров взаимодействия азота с хромом $\varepsilon_N^{\text{Cr}}(\text{Fe})$ и азота с никелем $\varepsilon_N^{\text{Ni}}(\text{Fe})$ в жидких сплавах на основе железа. Аналогичное выражение получено для вагнеровского параметра взаимодействия азота с молибденом в жидких сплавах на основе никеля $\varepsilon_N^{\text{Mo}}(\text{Ni})$. По первой из этих формул рассчитано значение $\varepsilon_N^{\text{Cr}}(\text{Ni}) = -21,9$ при температуре 1873 К. Этому соответствует значение лангенберговского параметра взаимодействия $e_N^{\text{Cr}}(\text{Ni}) = -0,108$, что совпадает

с экспериментальной оценкой. По второй из формул рассчитано значение $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -14,3$ при температуре 1873 К. Этому соответствует значение лангенберговского параметра взаимодействия $e_N^{\text{Cr}}(\text{Ni}) = -0,036$, что удовлетворительно согласуется с экспериментальной оценкой $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -15,1$; $e_N^{\text{Cr}}(\text{Ni}) = -0,038$.

Ключевые слова: термодинамика, растворы, азот, железо, никель, хром, молибден, коэффициент активности, вагнеровские параметры взаимодействия, лангенберговские параметры взаимодействия

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Nichrome, the heat-resistant alloy, and chromium stainless steel were invented at the beginning of the 20th century, signifying that the addition of chromium as an alloying element in substantial concentrations to iron and nickel passivates the surface of the resulting alloy at normal and high temperatures. Industrial-scale production of nickel-based heat-resistant alloys commenced in the mid-20th century. These alloys are composed of several alloying elements, with chromium being the primary one. Additionally, these alloys typically have a molybdenum content of a few percent.

Molybdenum plays a vital role in the production of corrosion-resistant, nickel-based alloys. Roughly a century ago, corrosion-resistant alloys like Hastelloy A (Ni – 20 % Mo) and Hastelloy B (Ni – 30 % Mo) were developed, with modern grades of Hastelloy featuring up to 30 % Mo. The nitrogen content has a significant impact on the properties of heat-resistant and corrosion-resistant nickel-based alloys.

More than 60 years ago, Schenck H. et al. [1] and Humbert J. et al. [2] conducted experiments to examine the solubility of nitrogen in liquid nickel and its alloys. Ongoing research [3] continues to explore similar studies, necessitating a theoretical explanation based on thermodynamic theory. Such an explanation is vital for estimating the solubility of nitrogen in liquid nickel-based alloys and assessing the potential formation of nitrides in these alloys. This study specifically focuses on the thermodynamics of nitrogen solutions in Fe–Ni–Cr and Fe–Ni–Mo liquid alloys, aiming to determine Wagner interaction coefficients between nitrogen and chromium and nitrogen and molybdenum in nickel-based liquid alloys based on these coefficients in iron-based liquid alloys.

A. Stomakhin was among the pioneering Soviet researchers who investigated the solubility of nitrogen in liquid nickel and nickel-based alloys. This paper is dedicated to honoring the memory of this exceptional researcher and educator.

We start with the Fe–Ni–Cr alloy and denote the concentrations of the solution components Fe–Ni–Cr–N, as c_{Fe} , c_{Ni} , c_{Cr} and c_{N} , respectively, using mole fractions. The fundamental concept explored in this study is the thermodynamic activity of nitrogen within the solution, denoted as a_{N} . The notion of thermodynamic activity was first intro-

duced by Lewis in 1907. In the context of nitrogen solutions, the Lewis definition implies the following equation:

$$a_{\text{N}} = \exp\left(\frac{\mu_{\text{N}} - \mu_{\text{N}}^{\circ}}{RT}\right),$$

where T represents the absolute temperature, R is the universal gas constant, μ_{N} signifies the chemical potential of nitrogen in the solution, μ_{N}° denotes the chemical potential of nitrogen at the standard state and temperature T . The standard state chosen to align with the unit of measurement (UoM) employed for expressing the nitrogen concentration in the solution. For this study, the μ_{N}° value is assumed to be constant. The simplest approach is to assume $\mu_{\text{N}}^{\circ} = 0$, leading to the following definition:

$$a_{\text{N}} = \exp\left(\frac{\mu_{\text{N}}}{RT}\right). \quad (1)$$

This definition, introduced by Guggenheim in the 1930s [4], represent the absolute activity (1). The absolute activity, when $T = \text{const}$, is a dimensionless function depending on the composition of the solution. Its accuracy extends to a certain number of decimal places, determined by an arbitrary constant. Importantly, it remains unaffected by the representation of solution component concentrations and the choice of the standard state. In this study, the activity of nitrogen is determined according to equation (1).

The activity coefficient of nitrogen is determined using the standard equation $\gamma_{\text{N}} = \frac{a_{\text{N}}}{c_{\text{N}}}$. These coefficients were referred to as “rational activity coefficients” by Robinson R. et al. [5]. Considering that $\gamma_{\text{N}} \rightarrow \gamma_{\text{N}}^{\circ}$ at $c_{\text{N}} \rightarrow 0$, $\gamma_{\text{N}}^{\circ}$ represents the rational activity coefficient of nitrogen in an infinitely dilute solution. For Fe–Ni–Cr–N alloys, where $c_{\text{Fe}} \rightarrow 1$ and $T = \text{const}$, it is more convenient to express the coefficient $\gamma_{\text{N}}^{\circ}$ as a function of c_{Ni} and c_{Cr} : $\gamma_{\text{N}}^{\circ} = \gamma_{\text{N}}^{\circ}(c_{\text{Ni}}, c_{\text{Cr}})$. Let us determine the Wagner interaction coefficients [6] that describe the interaction between nitrogen and alloying elements in iron-based liquid alloys:

$$\varepsilon_{\text{N}}^{\text{Ni}}(\text{Fe}) = \frac{\partial \ln \gamma_{\text{N}}^{\circ}(c_{\text{Ni}}; c_{\text{Cr}})}{\partial c_{\text{Ni}}} \text{ at } c_{\text{Fe}} \rightarrow 1;$$

$$\varepsilon_{\text{N}}^{\text{Cr}}(\text{Fe}) = \frac{\partial \ln \gamma_{\text{N}}^{\circ}(c_{\text{Ni}}; c_{\text{Cr}})}{\partial c_{\text{Cr}}} \text{ at } c_{\text{Fe}} \rightarrow 1.$$

Fe–Ni–Cr–N alloys at $c_{\text{Ni}} \rightarrow 1$ and $T = \text{const}$ it is more convenient to express the coefficient $\gamma_{\text{N}}^{\circ}$ as a function of c_{Fe} and c_{Cr} : $\gamma_{\text{N}}^{\circ} = \gamma_{\text{N}}^{\circ}(c_{\text{Fe}}, c_{\text{Cr}})$. Then the Ni–Cr Wagner interaction coefficient in nickel-based liquid alloys is defined as

$$\varepsilon_{\text{N}}^{\text{Cr}}(\text{Ni}) = \frac{\partial \ln \widetilde{\gamma}_{\text{N}}^{\circ}(c_{\text{Fe}}; c_{\text{Cr}})}{\partial c_{\text{Cr}}} \text{ at } c_{\text{Ni}} \rightarrow 1$$

or

$$\varepsilon_{\text{N}}^{\text{Ni}}(\text{Fe}) = \frac{\partial \ln \widetilde{\gamma}_{\text{N}}^{\circ}(1 - c_{\text{Fe}} - c_{\text{Cr}}; c_{\text{Cr}})}{\partial c_{\text{Cr}}} \text{ at } c_{\text{Ni}} \rightarrow 1. \quad (2)$$

In practical metallurgical production, the concentrations of solution components are commonly expressed as wt. %. Therefore, we denote the concentrations of the Fe–Ni–Cr–N solution components as [% Fe], [% Ni], [% Cr] and [% N], respectively. In this context, we will refer to the activity coefficient of nitrogen in the liquid solution $f_{\text{N}} = \frac{a_{\text{N}}}{[\% \text{ N}]}$ “the wt. % activity coefficient”. Let

$\gamma_{\text{N}} \rightarrow f_{\text{N}}^{\circ}$ at $[\% \text{ N}] \rightarrow 0$. f_{N}° is the wt. % the activity coefficient of nitrogen in an infinitely dilute nitrogen solution. Our objective now is to determine the Langenberg interaction coefficient for the nitrogen and alloying elements interaction in iron-based liquid alloys [7]:

$$e_{\text{N}}^{\text{Ni}}(\text{Fe}) = \frac{\partial \lg f_{\text{N}}^{\circ}([\% \text{ Ni}]; [\% \text{ Cr}])}{\partial [\% \text{ Ni}]} \text{ at } [\% \text{ Fe}] \rightarrow 100;$$

$$e_{\text{N}}^{\text{Cr}}(\text{Fe}) = \frac{\partial \lg f_{\text{N}}^{\circ}([\% \text{ Ni}]; [\% \text{ Cr}])}{\partial [\% \text{ Cr}]} \text{ at } [\% \text{ Fe}] \rightarrow 100.$$

For Fe–Ni–Cr–N alloys at $[\% \text{ N}] \rightarrow 100$ and $T = \text{const}$, it is more convenient to express the coefficient f_{N}° as a function of [% Fe] and [% Cr]: $f_{\text{N}}^{\circ} = \widetilde{f}_{\text{N}}^{\circ}([\% \text{ Fe}], [\% \text{ Cr}])$. The N–Cr Langenberg interaction coefficient in nickel-based liquid alloys is defined as follows:

$$e_{\text{N}}^{\text{Cr}}(\text{Ni}) = \frac{\partial \lg \widetilde{f}_{\text{N}}^{\circ}([\% \text{ Fe}]; [\% \text{ Cr}])}{\partial [\% \text{ Cr}]} \text{ at } [\% \text{ Ni}] \rightarrow 100.$$

We will examine the relationship between the Wagner $\varepsilon_i^j(k)$ and Langenberg $e_i^j(k)$ interaction coefficients in alloys based on the k component, where i, j represent the dissolved components. Lupis C. et al. [8] derived the exact ratio, considering the differential invariance of the logarithm of the solution component activity concerning different representations of the concentrations. The ratio is given by:

$$\varepsilon_i^j(k) = 230,3 \frac{A_j}{A_k} e_i^j(k) + \frac{A_k - A_j}{A_k}, \quad (3)$$

where A_j represents the atomic mass of the alloying component j and A_k represents the atomic mass of the base metal.

In the context of this study, component i refers to nitrogen, component j represents chromium or molybdenum, and component k pertains to iron or nickel. The inverse relationship to relation (3) is expressed as [9]:

$$e_i^j(k) = \frac{1}{230,3} \frac{A_k}{A_j} \left[\varepsilon_i^j(k) + \frac{A_k - A_j}{A_k} \right]. \quad (4)$$

The primary objective of this study is to establish analytical relationships between the interaction coefficient $\varepsilon_{\text{N}}^{\text{Cr}}(\text{Ni})$ and the $\varepsilon_{\text{N}}^{\text{Cr}}(\text{Fe})$ and $\varepsilon_{\text{N}}^{\text{Ni}}(\text{Fe})$ coefficients and between the interaction coefficient $\varepsilon_{\text{N}}^{\text{Mo}}(\text{Ni})$ with the $\varepsilon_{\text{N}}^{\text{Mo}}(\text{Fe})$ and $\varepsilon_{\text{N}}^{\text{Ni}}(\text{Fe})$ interaction coefficients. To achieve this, we propose a straightforward model for nitrogen solutions in Fe–Ni–Cr and Fe–Ni–Mo liquid alloys, which serves as a generalization of the model for nitrogen solutions in binary Fe–Cr alloys presented in [10]. The theoretical framework employed in this study utilizes the lattice model of Fe–Ni–Cr and Fe–Ni–Mo solutions, where the lattice structure adheres to the face-centered cubic (FCC) arrangement. Iron, nickel, chromium, and molybdenum atoms are situated at the lattice sites, while nitrogen atoms occupy the octahedral interstices. The interaction between nitrogen and metal atoms occurs exclusively with the neighboring lattice sites, constituting a pair interaction. It is assumed that this interaction energy remains invariant with respect to alloy composition or temperature. Furthermore, the Fe–Ni–Cr and Fe–Ni–Mo liquid solutions are considered to be ideal ternary solutions. We assume that the contribution of positional entropy to the partial entropy of the solution does not rely on the alloy composition or temperature.

A similar model, based on classical statistical mechanics principles, is presented in [11; 12]. The model as applied to the Fe–Cr–Ni–N system is reduced to

$$\gamma_{\text{N}}^{\circ} = \left\{ 1 - \frac{1}{\delta} \left[\varepsilon_{\text{N}}^{\text{Ni}}(\text{Fe}) c_{\text{Ni}} + \varepsilon_{\text{N}}^{\text{Cr}}(\text{Fe}) c_{\text{Cr}} \right] \right\}^{-\delta},$$

where δ represents the number of FCC lattice sites adjacent to the octahedral interstices ($\delta = 6$); $\gamma_{\text{N}}^{\circ}$ is the nitrogen activity coefficient in an infinitely diluted nitrogen solution normalized as follows: $\gamma_{\text{N}}^{\circ} = 1$ at $c_{\text{Fe}} \rightarrow 1$. Therefore

$$\ln \gamma_{\text{N}}^{\circ}(1 - c_{\text{Fe}} - c_{\text{Cr}}, c_{\text{Cr}}) = -\delta \ln \left\{ 1 - \frac{1}{\delta} \left[\varepsilon_{\text{N}}^{\text{Ni}}(\text{Fe}) (1 - c_{\text{Fe}} - c_{\text{Cr}}) + \varepsilon_{\text{N}}^{\text{Cr}}(\text{Fe}) c_{\text{Cr}} \right] \right\}. \quad (5)$$

It follows from (2) and (5):

$$\varepsilon_{\text{N}}^{\text{Cr}}(\text{Ni}) = \delta \frac{\varepsilon_{\text{N}}^{\text{Cr}}(\text{Fe}) - \varepsilon_{\text{N}}^{\text{Ni}}(\text{Fe})}{\delta - \varepsilon_{\text{N}}^{\text{Ni}}(\text{Fe})}.$$

The final equation is:

$$\varepsilon_N^{\text{Cr}}(\text{Ni}) = 6 \frac{\varepsilon_N^{\text{Cr}}(\text{Fe}) - \varepsilon_N^{\text{Ni}}(\text{Fe})}{6 - \varepsilon_N^{\text{Ni}}(\text{Fe})}. \quad (6)$$

The definitions and models for the Fe–Ni–Mo–N system are similar, leading to a final equation that is also similar to equation (6):

$$\varepsilon_N^{\text{Mo}}(\text{Ni}) = 6 \frac{\varepsilon_N^{\text{Mo}}(\text{Fe}) - \varepsilon_N^{\text{Ni}}(\text{Fe})}{6 - \varepsilon_N^{\text{Ni}}(\text{Fe})}. \quad (7)$$

To utilize equation (6), we also require the Wagner interaction coefficients $\varepsilon_N^{\text{Cr}}(\text{Fe})$ and $\varepsilon_N^{\text{Ni}}(\text{Fe})$ in iron-based alloys. We have considered the most reliable experimental studies on nitrogen solubility in Fe–Cr liquid alloys that estimate of the Langenberg interaction coefficient at $T = 1873$ K: $e_N^{\text{Cr}}(\text{Fe}) = -0.045$ [13] and $e_N^{\text{Cr}}(\text{Fe}) = -0.047$ [14]. Another recommended value is $e_N^{\text{Cr}}(\text{Fe}) = -0.046$ as suggested by Linchevsky B. et al. [15]. According to equation (3), this corresponds to the Wagner interaction coefficient $\varepsilon_N^{\text{Cr}}(\text{Fe}) = -9.8$.

Papers [14; 16] report the Langenberg interaction coefficient $e_N^{\text{Ni}}(\text{Fe}) = 0.011$. According to equation (3), this value corresponds to $\varepsilon_N^{\text{Ni}}(\text{Fe}) = 2.6$.

By substituting $\varepsilon_N^{\text{Cr}}(\text{Fe}) = -9.8$ and $\varepsilon_N^{\text{Ni}}(\text{Fe}) = 2.6$, into the right-hand side of equation (6), we can obtain the analytical value of the N–Cr Wagner interaction coefficient in liquid nickel-based alloys $\varepsilon_N^{\text{Cr}}(\text{Ni}) = -21.9$ at $T = 1873$ K. According to equation (4), this value corresponds to the Langenberg interaction coefficient $e_N^{\text{Cr}}(\text{Ni}) = -0.108$. This result is consistent with the experimental values reported by Surovoy Yu. et al. [16].

Estimating the true interaction coefficient $e_N^{\text{Cr}}(\text{Ni})$ poses significant challenges. Here are some experimental values of this coefficient at $T = 1873$ K obtained from nitrogen solubility measurements in Ni–Cr melts: -0.13 [2]; -0.11 (at $T = 1823$ K) [17]; -0.098 [18]; -0.108 [16]; -0.093 [19]; -0.0766 [20]; -0.0952 (at $T = 1823$ K) [21]. The arithmetic mean of these values is $e_N^{\text{Cr}}(\text{Ni}) = -0.102$. Monographs [15; 22] suggest $\varepsilon_N^{\text{Cr}}(\text{Ni}) = -0.1$ at $T = 1873$ K.

Previously, we presented an alternative theory [9] to estimate the $\varepsilon_N^{\text{Cr}}(\text{Ni})$ Wagner interaction coefficient. Let us express Sievert's law [23] for the solubility of nitrogen in Fe–Cr liquid alloys as follows:

$$[\% \text{ N}]^* = K'_N \sqrt{\frac{P_{\text{N}_2}}{P_0}},$$

where P_{N_2} represents the partial pressure of the nitrogen gas phase; P_0 is the standard pressure ($P_0 = 1 \text{ atm} \approx 0.101 \text{ MPa}$); K'_N is Sievert's law constant for the solubility of nitrogen in Ni–Cr liquid alloys. Let $K'_N(\text{Ni})$ at $c_{\text{Ni}} = 1$

and $K'_N = K'_N(\text{Cr})$ at $c_{\text{Cr}} = 1$. According to the theory presented in [9]

$$\varepsilon_N^{\text{Cr}}(\text{Ni}) = 6 \left(1 - \sqrt{\frac{A_{\text{Cr}} K'_N(\text{Cr})}{A_{\text{Ni}} K'_N(\text{Ni})}} \right). \quad (8)$$

As mentioned in [9], equations (8) and (4) yield the following N–Cr Langenberg interaction coefficient in liquid nickel alloys $e_N^{\text{Cr}}(\text{Ni}) = -0.105$ at $T = 1873$ K.

Therefore, according to [9], the interaction coefficient $e_N^{\text{Cr}}(\text{Ni})$ at $T = 1873$ K is -0.105 , and according to the theory proposed in this paper, $e_N^{\text{Cr}}(\text{Ni}) = -0.108$. These values are very close, considering the experimental uncertainty. A similar conclusion is reached when comparing this result with the averaged experimental value $e_N^{\text{Cr}}(\text{Ni}) = -0.102$.

It should be noted that theory [9] and equation (8) cannot estimate the N–Mo Wagner interaction coefficients in liquid nickel-based alloys due to the high melting point of molybdenum (approximately 2888 K [24]).

To use equation (7) for estimating the $\varepsilon_N^{\text{Mo}}(\text{Ni})$ coefficient, we need to know the Wagner interaction coefficient $\varepsilon_N^{\text{Mo}}(\text{Fe})$ in iron-based alloys. Here are the Langenberg interaction coefficient values at $T = 1873$ K, reported in reputable studies on nitrogen solubility in Fe–Mo liquid alloys: $e_N^{\text{Mo}}(\text{Fe}) = -0.011$ [13] and $e_N^{\text{Mo}}(\text{Fe}) = -0.013$ [25]. The arithmetic mean of these values is $e_N^{\text{Mo}}(\text{Fe}) = -0.012$. According to equation (3), this value corresponds to the Wagner interaction coefficient $\varepsilon_N^{\text{Mo}}(\text{Fe}) = -5.5$.

Let us substitute $\varepsilon_N^{\text{Mo}}(\text{Fe}) = -5.5$ and $\varepsilon_N^{\text{Ni}}(\text{Fe}) = 2.6$ in equation (7). Then we obtain the analytical N–Mo interaction Wagner interaction coefficient in liquid nickel-based alloys at $T = 1873$ K: $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -14.3$. Equation (4) yields the theoretical value of the Langenberg interaction coefficient $e_N^{\text{Mo}}(\text{Ni}) = -0.036$.

Let us consider the $e_N^{\text{Mo}}(\text{Ni})$ and $\varepsilon_N^{\text{Mo}}(\text{Ni})$ interaction coefficients at $T = 1873$ K. Stomakhin A. et al. [17] applied the Sievert method [23] to study the solubility of nitrogen in Ni–Mo liquid alloys at $T = 1823$ K. They reported the experimental value of the Langenberg interaction coefficient $e_N^{\text{Mo}}(\text{Ni}) = -0.04$. According to equation (3), the Wagner interaction coefficient $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -15.9$ at $T = 1823$ K.

In the study [9], we proposed an analytical equation to convert the Wagner interaction coefficient for the interaction between nitrogen and alloying metal from temperature T_0 to temperature T . For the $\varepsilon_N^{\text{Mo}}$ interaction coefficient and $\delta = 6$, this equation can be expressed as:

$$\varepsilon_N^{\text{Mo}}(T) = 6 \left\{ 1 - \left[1 - \frac{1}{6} \varepsilon_N^{\text{Mo}}(T_0) \right]^{\frac{T_0}{T}} \right\}. \quad (9)$$

By substituting the values $T_0 = 1823$ K, $T = 1873$ K, $\varepsilon_N^{\text{Mo}}(1823) = -15.9$ into equation (9), we obtain $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -15.1$ at $T = 1873$ K. It corresponds to the N–Mo Langenberg interaction coefficient in nickel-based liquid alloys $e_N^{\text{Mo}}(\text{Ni}) = -0.038$ (equation (4)). The theoretical value $e_N^{\text{Mo}}(\text{Ni}) = -0.036$, (equation (7)) agrees well with the experimental value [17].

With these analytical results, we can verify the experiments. The most plausible N–Cr interaction coefficient in liquid nickel-based alloys is $e_N^{\text{Cr}}(\text{Ni}) = -0.108$ at $T = 1873$ K. This value was obtained by Surovoy Yu. et al. [16] who measured the nitrogen solubility using the Sievers method. This coincides with the conclusions presented in [9].

The most plausible N–Mo interaction coefficient in liquid nickel-based alloys is $e_N^{\text{Mo}}(\text{Ni}) = 0.04$ at $T = 1823$ K. It was obtained by Stomakhin A. et al. [17] who measured the nitrogen solubility using the Sievers method. If we convert this value by equation (9) to $T = 1873$ K, the result is $e_N^{\text{Mo}}(\text{Ni}) = -0.038$.

The most plausible experimental values of the Wagner interaction coefficients for nitrogen in liquid nickel at $T = 1873$ K seem to be $\varepsilon_N^{\text{Cr}}(\text{Ni}) = -21.9$; $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -15.1$. The analytical values of these parameters are $\varepsilon_N^{\text{Cr}}(\text{Ni}) = -21.9$; $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -14.3$.

It is indeed noteworthy that both chromium and molybdenum belong to the same group in the Periodic Table, specifically group VI (chromium subgroup). Molybdenum serves as the closest chemical analog to chromium. This helps explain the applicability of the theoretical model to both Fe–Ni–Cr–N and Fe–Ni–Mo–N systems.

Furthermore, it is important to highlight the continued interest and research in the thermodynamics of nitrogen solutions in pure Cr, Mn, Fe, and Ni metals and alloys (refer to [3; 20; 21; 26–30]).

CONCLUSIONS

In our proposed analytical model of the structure and interatomic interaction for nitrogen solutions in Fe–Ni–Cr and Fe–Ni–Mo liquid alloys, we have developed equations (6) and (7) to calculate the Wagner interaction coefficients $\varepsilon_N^{\text{Cr}}(\text{Ni})$ and $\varepsilon_N^{\text{Mo}}(\text{Ni})$ for nitrogen in nickel-based liquid alloys based on the corresponding $\varepsilon_N^{\text{Cr}}(\text{Fe})$ and $\varepsilon_N^{\text{Mo}}(\text{Fe})$ coefficients in iron-based liquid alloys.

We obtained analytical values for the nitrogen interaction coefficients in liquid nickel-based alloys at $T = 1873$ K: $\varepsilon_N^{\text{Cr}}(\text{Ni}) = -21.9$; $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -14.3$; $e_N^{\text{Cr}}(\text{Ni}) = -0.108$; $e_N^{\text{Mo}}(\text{Ni}) = -0.036$.

The most plausible experimental values for the nitrogen interaction coefficients in liquid nickel-based alloys

at $T = 1873$ K are: $e_N^{\text{Cr}}(\text{Ni}) = -0.108$; $e_N^{\text{Mo}}(\text{Ni}) = -0.038$; $\varepsilon_N^{\text{Cr}}(\text{Ni}) = -21.9$; $\varepsilon_N^{\text{Mo}}(\text{Ni}) = -15.1$.

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