Research Article

Thermodynamic and Elastic Properties of Interstitial Alloy FeC with BCC Structure at Zero Pressure

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The analytic expressions for the thermodynamic and elastic quantities such as the mean nearest neighbor distance, the free energy, the isothermal compressibility, the thermal expansion coefficient, the heat capacities at constant volume and at constant pressure, the Young modulus, the bulk modulus, the rigidity modulus, and the elastic constants of binary interstitial alloy with body-centered cubic (BCC) structure, and the small concentration of interstitial atoms (below 5%) are derived by the statistical moment method. The theoretical results are applied to interstitial alloy FeC in the interval of temperature from 100 to 1000 K and in the interval of interstitial atom concentration from 0 to 5%. In special cases, we obtain the thermodynamic quantities of main metal Fe with BCC structure. Our calculated results for some thermodynamic and elastic quantities of main metal Fe and alloy FeC are compared with experiments.

1. Introduction

Thermodynamic and elastic properties of metals and interstitial alloys are specially interested by many theoretical and experimental researchers [1–21]. For example, in [1, 2] the equilibrium vacancy concentration in bcc substitution and interstitial alloys is calculated taking into account thermal redistribution of the interstitial component in different types of interstices. The conditions where this effect gives rise to a decrease or increase in vacancy concentration are formulated. Coatings based on interstitial alloys of transition metals have acquired a wide application range. However, interest in synthesizing coatings from new materials with requisite service properties is limited by the scarceness of data on their melting temperature. In [3], Andryushechkin and Karpman considered the calculation of melting temperature for interstitial alloys of transition metals based on the characteristics of intermolecular interaction. Hirabayashi et al. [4]

attempt to present a survey of the order-disorder transformations in the interstitial alloys of transition metals with hydrogen, deuterium, and oxygen. Special attention is given to the formation of interstitial superstructures, stepwise processes of disordering and property changes attributed to order-disorder. Four groups of interstitial alloys are considered: (1) TO, ZrO, and HfO; (2) VO; (3) VH and VD; and (4) TaH and TaD. Characteristic features of the phase transformations in each group and each system are presented and discussed in comparison with others. In [14], Philibert presents the Morse potential and the Finnis-Sinclair for alloys FeH and FeC. In [15], a type of empirical potential for alloy FeC is developed in calculating defects with high energy. Structural, elastic, and thermal properties of alloy FeC are studied by using the modified embedded atom method (MEAM) in [16].

In this paper, we build the thermodynamic and elastic theory for binary interstitial alloy with bcc structure by the

statistical moment method (SMM) [8–10] and apply the obtained theoretical results to alloy FeC.

2. Content

2.1. Thermodynamic Quantities. The model of interstitial alloy AB with BCC structure in this paper is the same model of interstitial alloy AC in our previous paper [9]. That means in this model, the main atoms A are in body center and peaks of cubic unit cell and the interstitial atoms B are in face centers of cubic unit cell. The cohesive energy u_0 and the crystal parameters k, γ_1, γ_2 , and γ for atoms B, A_1 (atom A in body center), and A_2 (atom A in peaks) in the approximation of three coordination spheres are determined analogously as for atoms C, A_1 , and A_2 in [9]. Note that in the expressions of these quantities there are the cohesive energy and the crystal parameters of atoms A in clean metal A in the approximation of two coordination sphere [8].

The equation of state for interstitial alloy AB with BCC structure at temperature T and pressure P is written in the following form:

$$Pv = -r_1 \left(\frac{1}{6} \frac{\partial u_0}{\partial r_1} + \theta x \coth x \frac{1}{2k} \frac{\partial k}{\partial r_1} \right). \quad (1)$$

At 0 K and zero pressure, this equation has the following form:

$$0 = -r_1 \left(\frac{1}{6} \frac{\partial u_0}{\partial r_1} + \frac{h\omega_0}{4k} \frac{\partial k}{\partial r_1} \right). \quad (2)$$

If we know the form of interaction potential φ_{i0} , equation (2) permits us to determine the nearest neighbor distance $r_{1X}(0,0)$ ($X = B, A, A_1, A_2$) at 0 K and zero pressure. After knowing that, we can determine crystal parameters $k_X(0,0), \gamma_{1X}(0,0), \gamma_{2X}(0,0), \gamma_X(0,0)$ at 0 K and zero pressure. After that, we can calculate the displacements [8–10].

$$y_{0X}(0, T) = \sqrt{\frac{2\gamma_X(0,0)\theta^2}{3k_X^3(0,0)}} A_X(0, T), \quad (3)$$

where $A_X(0, T)$ is determined as in [9]. From that, we derive the nearest neighbor distance $r_{1X}(0, T)$ at temperature T and zero pressure:

$$\begin{aligned} r_{1B}(0, T) &= r_{1B}(0, 0) + y_{A_1}(0, T), r_{1A}(0, T) \\ &= r_{1A}(0, 0) + y_A(0, T), \\ r_{1A_1}(0, T) &\approx r_{1B}(0, T), r_{1A_2}(0, T) = r_{1A_2}(0, 0) + y_B(0, T). \end{aligned} \quad (4)$$

Then, we calculate the mean nearest neighbor distance in interstitial alloy AB by the expressions as follows [8–10]:

$$\begin{aligned} \overline{r_{1A}(0, T)} &= \overline{r_{1A}(0, 0)} + \overline{y(0, T)}, \\ \overline{r_{1A}(0, 0)} &= (1 - c_B)r_{1A}(0, 0) + c_B r'_{1A}(0, 0), r'_{1A}(0, 0) \\ &= \sqrt{3}r_{1B}(0, 0), \\ \overline{y(0, T)} &= (1 - 7c_B)y_A(0, T) + c_By_B(0, T) \\ &\quad + 2c_By_{A_1}(0, T) + 4c_By_{A_2}(0, T), \end{aligned} \quad (5)$$

where $\overline{r_{1A}(0, T)} \equiv a_{AB}(0, T)$ is the mean nearest neighbor distance between atoms A in interstitial alloy AB at zero pressure and temperature T , $\overline{r_{1A}(0, 0)}$ is the mean nearest neighbor distance between atoms A in interstitial alloy AB at zero pressure, 0 K, $r_{1A}(0, 0)$ is the nearest neighbor distance between atoms A in clean metal A at zero pressure, 0 K, $r'_{1A}(0, 0)$ is the nearest neighbor distance between atoms A in the zone containing the interstitial atom B at zero pressure and 0 K, and c_B is the concentration of interstitial atoms B.

The free energy of alloy AB with BCC structure and the condition $c_B \ll c_A$ has the following form:

$$\begin{aligned} \psi_{AB} &= (1 - 7c_B)\psi_A + c_B\psi_B + 2c_B\psi_{A_1} + 4c_B\psi_{A_2} - TS_c, \\ \psi_X &\approx \frac{1}{2} \cdot N \cdot u_{0X} + \psi_{0X} + 3N \left\{ \frac{\theta^2}{k_X^2} \left[\gamma_{2X}X_X^2 - \frac{2\gamma_{1X}}{3} \left(1 + \frac{X_X}{2} \right) \right] \right. \\ &\quad + \frac{2\theta^3}{k_X^4} \left[\frac{4}{3}\gamma_{2X}^2 X_X \left(1 + \frac{X_X}{2} \right) - 2(\gamma_{1X}^2 + 2\gamma_{1X}\gamma_{2X}) \right. \\ &\quad \left. \left. \cdot \left(1 + \frac{X_X}{2} \right) (1 + X_X) \right] \right\}, \end{aligned}$$

$$\psi_{0X} = 3N\theta \left[x_X + \ln(1 - e^{-2x_X}) \right], X_X \equiv x_X \coth x_X, \quad (6)$$

where ψ_X is the free energy of atom X, ψ_{AB} is the free energy of interstitial alloy AB, S_c is the configuration entropy of interstitial alloy AB.

The isothermal compressibility of interstitial alloy AB has the following form:

$$\begin{aligned} \chi_{TAB} &= \frac{(a_{AB}/a_{0AB})^3}{\sqrt{3}/4a_{AB}1/3N(\partial^2\psi_{AB}/\partial a_{AB}^2)_T}, \\ \left(\frac{\partial^2\psi_{AB}}{\partial a_{AB}^2} \right)_T &\approx (1 - 7c_B) \left(\frac{\partial^2\psi_A}{\partial r_{1A}^2} \right)_T + c_B \left(\frac{\partial^2\psi_B}{\partial r_{1B}^2} \right)_T \\ &\quad + 2c_B \left(\frac{\partial^2\psi_{A_1}}{\partial r_{1A_1}^2} \right)_T + 4c_B \left(\frac{\partial^2\psi_{A_2}}{\partial r_{1A_2}^2} \right)_T, \\ \frac{1}{3N} \left(\frac{\partial^2\psi_X}{\partial r_{1X}^2} \right)_T &= \frac{1}{6} \frac{\partial^2 u_{0X}}{\partial r_{1X}^2} + \frac{h\omega_X}{4k_X} \left[\frac{\partial^2 k_X}{\partial r_{1X}^2} - \frac{1}{2k_X} \left(\frac{\partial k_X}{\partial r_{1X}} \right)^2 \right]. \end{aligned} \quad (7)$$

The thermal expansion coefficient of interstitial alloy AB has the following form:

$$\begin{aligned}\alpha_{TAB} &= -\frac{k_B \chi_{TAB}}{3} \left(\frac{a_{0AB}}{a_{AB}} \right)^2 \frac{a_{AB}}{3V_{AB}} \frac{\partial^2 \psi_{AB}}{\partial \theta \partial a_{AB}}, V_{AB} = N v_{AB} = N \frac{4a_{AB}^3}{3\sqrt{3}}, \\ \frac{\partial^2 \psi_{AB}}{\partial \theta \partial a_{AB}} &\approx (1 - 7c_B) \frac{\partial^2 \psi_A}{\partial \theta \partial r_{1A}} + c_B \frac{\partial^2 \psi_B}{\partial \theta \partial r_{1B}} + 2c_B \frac{\partial^2 \psi_{A_1}}{\partial \theta \partial r_{1A_1}} + 4c_B \frac{\partial^2 \psi_{A_2}}{\partial \theta \partial r_{1A_2}}, \\ \frac{1}{3N} \frac{\partial^2 \psi_X}{\partial \theta \partial r_{1X}} &= \frac{1}{2k_X} \frac{\partial k_X}{\partial r_{1X}} Y_X^2 + \frac{2\theta^2}{k_X^2} \left[\frac{\gamma_{1X}}{3k_X} \frac{\partial k_X}{\partial r_{1X}} (2 + X_X Y_X^2) \right. \\ &\quad \left. - \frac{1}{6} \frac{\partial \gamma_{1X}}{\partial r_{1X}} (4 + X_X + Y_X^2) - \left(\frac{2\gamma_{2X}}{k_X} \frac{\partial k_X}{\partial r_{1X}} - \frac{\partial \gamma_{2X}}{\partial r_{1X}} \right) \right], Y_X \equiv \frac{x_X}{\sinh x_X}.\end{aligned}\quad (8)$$

The heat capacity at constant volume of interstitial alloy AB is determined by

$$\begin{aligned}C_{VAB} &= (1 - 7c_B)C_{VA} + c_B C_{VB} + 2c_B C_{VA_1} + 4c_B C_{VA_2}, \\ C_{VX} &= 3Nk_B \left\{ Y_X^2 + \frac{2\theta}{k_X^2} \left[\left(2\gamma_2 + \frac{\gamma_{1X}}{3} \right) X_X Y_X^2 \right. \right. \\ &\quad \left. \left. + \frac{2\gamma_{1X}}{3} (1 + Y_X^2) - \gamma_{2X} (Y_X^4 + 2X_X^2 Y_X^2) \right] \right\}.\end{aligned}\quad (9)$$

The heat capacity at constant pressure of interstitial alloy AB is determined by

$$C_{PAB} = C_{VAB} + \frac{9TV_{AB}\alpha_{TAB}^2}{\chi_{TAB}}. \quad (10)$$

2.2. Elastic Quantities. The Young modulus of alloy AB with BCC structure at temperature T and zero pressure is determined as the one of alloy AC at $P = 0$ in [9].

The bulk modulus of alloy AB has the following form:

$$K_{AB} = \frac{E_{AB}}{3(1 - 2\nu_A)}. \quad (11)$$

The rigidity modulus of alloy AB at temperature T and zero pressure is as follows:

$$G_{AB} = \frac{E_{AB}}{2(1 + \nu_A)}. \quad (12)$$

The elastic constants of alloy AB at temperature T and zero pressure are as follows:

$$\begin{aligned}C_{11AB} &= \frac{E_{AB}(1 - \nu_A)}{(1 + \nu_A)(1 - 2\nu_A)}, \\ C_{12AB} &= \frac{E_{AB}\nu_A}{(1 + \nu_A)(1 - 2\nu_A)}, \\ C_{44AB} &= \frac{E_{AB}}{2(1 + \nu_A)}.\end{aligned}\quad (13)$$

The Poisson ratio of alloy AB is as follows:

$$\nu_{AB} = c_A \nu_A + c_B \nu_B \approx \nu_A, \quad (14)$$

where ν_A and ν_B , respectively, are the Poisson ratio of materials A and B and are determined from the experimental data.

2.3. Numerical Results for Interstitial Alloy FeC. For pure metal Fe, we use the m-n potential that the m-n potential parameters between atoms Fe-Fe were given in [12]. For alloy FeC, we use the Finnis-Sinclair potential as follows:

$$\begin{aligned}U &= -A \sqrt{\sum_{i \neq j} \rho(r_{ij})} + \frac{1}{2} \sum_{i \neq j} \phi(r_{ij}), \\ \rho(r) &= t_1 (r - R_1)^2 + t_2 (r - R_1)^3 \quad (r < R_1), \\ \phi(r) &= (r - R_2)^2 (k_1 + k_2 r + k_3 r^2) \quad (r < R_2).\end{aligned}\quad (15)$$

where the Finnis-Sinclair potential parameters between atoms Fe-C are as shown in Table 1.

Our numerical results for the thermal expansion coefficient and the heat capacity at constant pressure, the Young modulus, the bulk modulus, the rigidity modulus and the elastic constants of alloy FeC are summarized in tables from Tables 2–5 and are described by figures from

TABLE 1: The Finnis–Sinclair potential parameters between atoms Fe-C [15].

A (eV)	R_1 (Å)	t_1 (Å) ⁻²	t_2 (Å) ⁻³	R_2 (Å)	k_1 (eV(Å) ⁻²)	k_2 (eV(Å) ⁻³)	k_3 (eV(Å) ⁻⁴)
2.958787	2.545937	10.024001	1.638980	2.468801	8.972488	-4.086410	1.483233

TABLE 2: Dependence of thermal expansion coefficient on temperature for Fe.

T (K)	100	200	300	500	700	1000
α_T (10 ⁻⁶ K ⁻¹)						
This paper	5.71	10.93	12.77	14.64	16.15	18.66
EXPT [11]	5.6	10.0	11.7	14.3	16.3	19.2

TABLE 3: Dependence of heat capacity at constant pressure on temperature for Fe.

T (K)	100	200	300	400	500
C_P (J/mol.K)					
This paper	10.68	20.13	22.92	24.13	24.77
EXPT [11]	12.07	21.50	25.13	27.43	29.64

TABLE 4: The dependence of Young modulus E (10¹⁰ Pa) for alloy FeC with $c_C = 0.2\%$ from the SMM and alloy FeC with $c_C \leq 0.3\%$ from EXPT [17].

T (K)	73	144	200	294	422	533	589	644	700	811	866
SMM	22.59	22.03	21.58	20.75	19.49	18.28	17.65	16.96	16.26	14.81	14.06
EXPT	21.65	21.24	20.82	20.34	19.51	18.82	18.41	17.58	16.69	14.07	12.41

TABLE 5: The dependence of Young modulus E (10¹⁰ Pa) for alloy FeC with $c_C = 0.4\%$ from the SMM and alloy FeC with $c_C \geq 0.3\%$ from EXPT [17].

T (K)	73	144	200	294	422	533	589	644	700	811	866	922
SMM	22.46	21.90	21.45	20.62	19.38	18.18	17.53	16.87	16.17	14.72	13.98	13.21
EXPT	21.51	21.10	20.68	20.20	19.37	18.62	18.27	17.44	16.55	13.93	12.34	10.62

FIGURE 1: α_T (T) for FeC at $P = 0$, $c_C = 0, 1, 2$, and 4% . FIGURE 2: α_T (c_C) for FeC at $P = 0$, $T = 100, 300, 500$, and 700 K.

FIGURE 3: C_p (T) for FeC at $P = 0$, $c_C = 0, 1, 3$, and 5% . FIGURE 4: C_p (c_C) for FeC at $P = 0$, $T = 100, 200, 300$, and 500 K.

Figures 1–12. When the concentration $c_C \rightarrow 0$, we obtain thermodynamic quantities of Fe. Our calculated results shown in Tables 2–4 and Figures 5, 6, 11, and 12 are in rather good agreement with experiments (the obtained deviations are smaller than 15%).

For alloy FeC at the same temperature when the concentration of interstitial atoms increases, the thermal expansion coefficient α_T and the heat capacity at constant pressure C_p decrease. For example, for FeC at $T = 1000$ K when c_C increases from 0 to 5%, α_T decreases from $18.66 \cdot 10^{-6}$ to $12.95 \cdot 10^{-6} \text{ K}^{-1}$, and C_p decreases from 26.67 to $25.59 \text{ J}/(\text{mol K})$.

For alloy FeC at the same concentration of interstitial atoms when temperature increases, the thermal expansion

FIGURE 5: α_T (T) for Fe at $P = 0$ from the SMM and the experimental data [11]. FIGURE 6: C_p (T) for Fe at $P = 0$ from the SMM and the experimental data [11].

coefficient α_T and the heat capacity at constant pressure C_p increase. For example, for FeC at $c_C = 5\%$ when T increases from 100 to 1000 K, α_T increases from $3.23 \cdot 10^{-6}$ to $12.95 \cdot 10^{-6} \text{ K}^{-1}$, and C_p increases from 9.26 to $25.59 \text{ J}/(\text{mol K})$.

For alloy FeC at the same temperature when the concentration of interstitial atoms increases, the elastic moduli E , G , K , and the elastic constants C_{11} , C_{12} , C_{44} decrease. For example, for FeC at $T = 1000$ K when c_C increases from 0 to 5%, E decreases from 12.28×10^{10} to $10.39 \times 10^{10} \text{ Pa}$, G decreases from 4.87×10^{10} to $4.12 \times 10^{10} \text{ Pa}$, K decreases from 8.53×10^{10} to $7.21 \times 10^{10} \text{ Pa}$, C_{11} decreases from 15.02×10^{10} to $12.71 \times 10^{10} \text{ Pa}$, C_{12} decreases from 5.28×10^{10} to

FIGURE 7: $E(c_C)$ for FeC at different temperatures T . FIGURE 9: C_{11} , C_{12} , and $C_{44}(c_C)$ for FeC at $T = 300$ K. FIGURE 8: $E(T)$ for FeC at different concentrations c_C . FIGURE 10: C_{11} , C_{12} , and $C_{44}(T)$ for FeC at $c_C = 3\%$.

4.46×10^{10} Pa, and C_{44} decreases from 4.87×10^{10} to 4.12×10^{10} Pa.

For alloy FeC at the same concentration of interstitial atoms when temperature increases, the elastic moduli E , G , and K , and the elastic constants C_{11} , C_{12} , and C_{44} also decrease. For example, for FeC at $c_C = 5\%$ when T increases from 100 to 1000 K, E decreases from $19.39 \cdot 10^{10}$ to $10.39 \cdot 10^{10}$ Pa, G decreases from $7.69 \cdot 10^{10}$ to $4.12 \cdot 10^{10}$ Pa, K decreases from $13.47 \cdot 10^{10}$ to $7.21 \cdot 10^{10}$ Pa, C_{11} decreases from $23.72 \cdot 10^{10}$ to $12.71 \cdot 10^{10}$ Pa, C_{12} decreases from $8.33 \cdot 10^{10}$ to $4.46 \cdot 10^{10}$ Pa, and C_{44} decreases from $7.69 \cdot 10^{10}$ to $4.12 \cdot 10^{10}$ Pa.

The calculated values from the SMM for the Young modulus E in Tables 4 and 5 and Figures 11 and 12 and therefore other elastic quantities, such as the elastic moduli G and K , the elastic constants C_{11} , C_{12} , and C_{44} of alloy FeC, are in good agreement with experiments. The nearest neighbor distance, the elastic moduli E , G , and K , the elastic constants C_{11} , C_{12} , and C_{44} , and the isothermal elastic modulus B_T of main metal Fe at $P = 0$, $T = 300$ K according to the SMM, the other calculation [21] and experiments [18–20] are given in [9]. Our obtained deviations are smaller than 15%.

FIGURE 11: $E(T)$ for alloy FeC with $c_C = 0.2\%$ from the SMM and alloy FeC with $c_C \leq 0.3\%$ from EXPT [17].

FIGURE 12: $E(T)$ for alloy FeC with $c_C = 0.4\%$ from the SMM and alloy FeC with $c_C \geq 0.3\%$ from EXPT [17].

3. Conclusion

From the SMM, using the minimum condition of cohesive energies and the method of three coordination spheres, we find the mean nearest neighbor distance, the free energy, the isothermal compressibility, the thermal expansion coefficient, the heat capacities at constant volume and at constant pressure, the Young modulus, the bulk modulus, the rigidity modulus, and the elastic constants of binary interstitial alloy with BCC structure with very small concentration of interstitial atoms. The obtained expressions of these quantities depend on temperature and concentration

of interstitial atoms. At zero concentration of interstitial atoms, thermodynamic and elastic quantities of interstitial alloy become ones of main metal in alloy. The theoretical results are applied to interstitial alloy FeC. Our calculated results for the nearest neighbor distance, the elastic moduli, the elastic constants, and the isothermal elastic modulus at 300 K, the thermal expansion coefficient in the range from 100 to 1000 K and the heat capacity at constant pressure in the range from 100 to about 450 K of main metal Fe, the Young modulus, the bulk modulus, the rigidity modulus, and the elastic constants of alloy FeC with $c_C = 0.2\%$ and $c_C = 0.4\%$ are in rather good agreement with experiments.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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References

- [1] A. A. Smirnov, *Theory of Interstitial Alloys*, Nauka, Moscow, Russia, 1979.
- [2] V. A. Volkov and S. I. Masharov, "The effect of thermal redistribution of various interstitial impurities on equilibrium vacancy concentration in BCC substitutional-interstitial alloys," *Russian Physics Journal*, vol. 50, no. 4, pp. 400-404, 2007.
- [3] S. E. Andryushechkin and M. G. Karpman, "Calculation of the melting temperature of interstitial alloys of transition metals," *Metal Science and Heat Treatment*, vol. 41, no. 2, pp. 80-82, 1999.
- [4] M. Hirabayashi, S. Yamaguchi, H. Asano, and K. Hiraga, *Order-Disorder Transformations in Alloys*, Springer-Verlag, Berlin, Germany, 1974.
- [5] K. E. Mironov, *Interstitial alloy*, Plenum Press, New York, USA, 1967.
- [6] A. G. Morachevskii and I. V. Sladkov, *Thermodynamic Calculations in Metallurgy*, Metallurgiya, Moscow, Russia, 1993.
- [7] N. Eliaz, D. Fuks, and D. Eliezer, "Non-Arrhenius behavior of the diffusion coefficient of hydrogen in amorphous metals," *Materials Letters*, vol. 39, no. 5, pp. 255-259, 1999.
- [8] N. Tang and V. V. Hung, "Investigation of the thermodynamic properties of anharmonic crystals by the momentum method. I. General results for face-centred cubic crystals," *Physica Status Solidi (B)*, vol. 149, no. 2, pp. 511-519, 1988.
- [9] N. Q. Hoc and N. D. Hien, "Study on elastic deformation of substitution AB with interstitial alloy C and BCC structure under pressure," *IOP Conf. Series: Journal of Physics: Conference Series*, vol. 1034, article 012005, 2018.
- [10] N. Q. Hoc and D. Q. Vinh, "Thermodynamic properties of binary interstitial alloy with fcc structure: dependence on

- temperature and concentration of interstitial atoms," *Journal of Science of HNUE*, vol. 62, no. 8, pp. 72–81, 2017.
- [11] W. B. Pearson, *A Handbook of Lattice Spacings of Metals and Alloys*, Pergamon, New York, 1958.
 - [12] M. N. Magomedov, *Zhurnal Fizicheskoi Khimii*, vol. 61, no. 4, p. 1003, 1987 (in Russian).
 - [13] N. V. Hung, T. T. Hue, and N.B. Duc, "Calculation of morse potential parameters of bcc crystals and application to anharmonic interatomic effective potential, local force constant," *VNU Journal of Science:Mathematical-Physics*, vol. 31, no. 3, pp. 23–30, 2015.
 - [14] J. M. Philibert, *Atom Movements-Diffusion and Mass Transport in Solids*, EDP Sciences, F-91944 les UlisCedex A, France, 1991.
 - [15] T. L. Timothy, J. F. Clemens, L. Xi, D. G. Julian, Y. Sidney, and J. V. V. Krystyn, "Many-body potential for point defect clusters in Fe-C alloys," *Physical Review Letters*, vol. 98, no. 21, article 215501, 2007.
 - [16] L. S. I. Liyanage, S. G. Kim, J. Houze et al., "Structural, elastic, and thermal properties of cementite (Fe_3C) calculated using a modified embedded atom method," *Physical Review B*, vol. 89, article 094102, 2014.
 - [17] http://www.engineeringtoolbox.com/young-modulus-d_773.htm. Young's modulus of elasticity for metals and alloys.
 - [18] D. R. Lide, *CRC Handbook of Chemistry and Physics*, 86th Ed., Taylor & Francis, Boca Raton London, New York, Singapore, 2005.
 - [19] L. V. Tikhonov, V. A. Kononenko, G. I. Prokonenko et al., *Structure and properties of metals and alloys*, NaukovaDumka, Kiev, 1986 (in Russian).
 - [20] H. Cyunn and C.-S. Yoo, "Equation of state of tantalum to 174 GPa," *Physical Review B*, vol. 59, no. 13, p. 8526, 1999.
 - [21] M. J. Mehl and D. A. Papaconstantopoulos, "Applications of a tight-binding total-energy method for transition and noble metals: elastic constants, vacancies and surfaces of monatomic metals," *Physical Riview B*, vol. 54, no. 7, p. 4519, 1996.