HNUE JOURNAL OF SCIENCE DOI: 10.18173/2354-1059.2019-0031
Natural Sciences, 2019, Volume 64, Issue 6, pp. 57-67
This paper is available online at http://stdb.hnue.edu.vn

STUDY ON STRUCTURAL PHASE TRANSITIONS IN DEFECTIVE AND PERFECT SUBSTITUTIONAL ALLOYS AB WITH INTERSTITIAL ATOMS C UNDER PRESSURE

Nguyen Quang Hoc[1], Dinh Quang Vinh[1], Le Hong Viet[2],
Ta Dinh Van[1] and Pham Thanh Phong[1]
[1]*Faculty of Physics, Hanoi National University of Education*
[2]*Tran Quoc Tuan University, Co Dong, Son Tay, Hanoi*

Abstract. The analytic expressions of the Helmholtz free energy, the Gibbs thermodynamic potential the mean nearest neighbor distance between two atoms, the crystal parameters for bcc, fcc and hcp phases of defective and perfect substitutional alloys AB with interstitial atoms C and structural phase transition temperatures of these alloys at zero pressure and under pressure are derived by the statistical moment method. The structural phase transition temperatures of the main metal A, the substitutional alloy AB and the interstitial alloy AC are special cases of ones of the substitutional alloy AB with interstitial atoms C.

Keywords: Statistical moment method, Helmholtz free energy, Gibbs thermodynamic potential, structural phase transition temperature.

1. Introduction

Structural phase transitions of crystals in general and metals and interstitial alloys in particular are specially interested by many theoretical and experimental researchers [1-7]. In [8], the body centered cubic (bcc) - face centered cubic (fcc) phase transition temperature determined in solid nitrogen and carbon monoxide on the basis of the self-consistent field approximation. In [9], this phase transition temperature in solid nitrogen is calculated by the statistical moment method (SMM). The $\alpha-\beta$ ($\alpha,\beta=$bcc, fcc, hexagonal close packed (hcp)) phase transition temperature for rare-earth metals and substitutional alloys is also derived from the SMM [10].

In this paper, we build the theory of $\alpha-\beta$ $\alpha,\beta=$bcc, fcc, hcp) structural phase transition for defective and perfect substitutional alloys AB with interstitial atoms C at zero pressure and under pressure by the SMM [11-13].

Received April 30, 2019. Revised June 15, 2019. Accepted July 22, 2019.
Contact Nguyen Quang Hoc, e-mail address: hocnq@hnue.edu.vn

2. Content

In the case of perfect interstitial alloy AC with bcc structure (where the main atom A_1 stays in body center, the main atom A_2 stays in peaks and the interstitial atom C stays in face centers of cubic unit cell), the cohesive energy and the alloy's parameters for atoms C, A_1 and A_2 in the approximation of three coordination spheres are determined by [11-13].

$$u_{0C}^{bcc} = \frac{1}{2}\sum_{i=1}^{n_i} \varphi_{AC}(r_i) = \varphi_{AC}(r_1^{bcc}) + 2\varphi_{AC}\left(r_1^{bcc}\sqrt{2}\right) + 4\varphi_{AC}\left(r_1^{bcc}\sqrt{5}\right), \quad (1)$$

$$k_C^{bcc} = \frac{1}{2}\sum_i \left(\frac{\partial^2 \varphi_{AC}}{\partial u_{i\beta}^2}\right)_{eq} = \varphi_{AC}^{(2)}\left(r_1^{bcc}\right) + \frac{\sqrt{2}}{r_1^{bcc}}\varphi_{AC}^{(1)}\left(r_1^{bcc}\sqrt{2}\right) + \frac{16}{5\sqrt{5}r_1^{bcc}}\varphi_{AC}^{(1)}\left(r_1^{bcc}\sqrt{5}\right), \gamma_C^{bcc} = 4\left(\gamma_{1C}^{bcc} + \gamma_{2C}^{bcc}\right),$$

$$\gamma_{1C}^{bcc} = \frac{1}{48}\sum_i \left(\frac{\partial^4 \varphi_{ACF}}{\partial u_{i\beta}^4}\right)_{eq} = \frac{1}{24}\varphi_{AC}^{(4)}\left(r_1^{bcc}\right) + \frac{1}{8\left(r_1^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{bcc}\sqrt{2}\right) -$$

$$- \frac{\sqrt{2}}{16\left(r_1^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{bcc}\sqrt{2}\right) + \frac{1}{150}\varphi_{AC}^{(4)}\left(r_1^{bcc}\sqrt{2}\right) + \frac{4\sqrt{5}}{125 r_1^{bcc}}\varphi_{AC}^{(3)}\left(r_1^{bcc}\sqrt{5}\right),$$

$$\gamma_{2C}^{bcc} = \frac{6}{48}\sum_i \left(\frac{\partial^4 \varphi_{AC}}{\partial u_{i\alpha}^2 \partial u_{i\beta}^2}\right)_{eq} = \frac{1}{4r_1^{bcc}}\varphi_{AC}^{(3)}\left(r_1^{bcc}\right) - \frac{1}{4\left(r_1^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{bcc}\right) + \frac{5}{8\left(r_1^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{bcc}\right) +$$

$$+ \frac{\sqrt{2}}{8r_1^{bcc}}\varphi_{AC}^{(3)}\left(r_1^{bcc}\sqrt{2}\right) - \frac{1}{8\left(r_1^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{bcc}\sqrt{2}\right) + \frac{1}{8\left(r_1^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{bcc}\sqrt{2}\right) + \frac{2}{25}\varphi_{AC}^{(4)}\left(r_1^{bcc}\sqrt{5}\right) +$$

$$+ \frac{3}{25\sqrt{5}r_1^{bcc}}\varphi_{AC}^{(3)}\left(r_1^{bcc}\sqrt{5}\right) + \frac{2}{25\left(r_1^{bcc}\right)^2}\varphi_{ACF}^{(2)}\left(r_1^{bcc}\sqrt{5}\right) - \frac{3}{25\sqrt{5}\left(r_1^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{bcc}\sqrt{5}\right), \quad (2)$$

$$u_{0A_1}^{bcc} = u_{0A}^{bcc} + \varphi_{AC}\left(r_{1A_1}^{bcc}\right), \gamma_{A_1}^{bcc} = 4\left(\gamma_{1A_1}^{bcc} + \gamma_{2A_1}^{bcc}\right),$$

$$k_{A_1}^{bcc} = k_A^{bcc} + \frac{1}{2}\sum_i \left[\left(\frac{\partial^2 \varphi_{AC}}{\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_1}^{bcc}} = k_A^{bcc} + \varphi_{AB}^{(2)}\left(r_{1A_1}^{bcc}\right) + \frac{5}{2r_{1A_1}^{bcc}}\varphi_{AC}^{(1)}\left(r_{1A_1}^{bcc}\right),$$

$$\gamma_{1A_1}^{bcc} = \gamma_{1A}^{bcc} + \frac{1}{48}\sum_i \left[\left(\frac{\partial^4 \varphi_{AC}}{\partial u_{i\beta}^4}\right)_{eq}\right]_{r=r_{1A_1}^{bcc}} = \gamma_{1A}^{bcc} + \frac{1}{24}\varphi_{AC}^{(4)}\left(r_{1A_1}^{bcc}\right) + \frac{1}{8\left(r_{1A_1}^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_1}^{bcc}\right) - \frac{1}{8\left(r_{1A_1}^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_1}^{bcc}\right),$$

$$\gamma_{2A_1}^{bcc} = \gamma_{2A}^{bcc} + \frac{6}{48}\sum_i \left[\left(\frac{\partial^4 \varphi_{AC}}{\partial u_{i\alpha}^2 \partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_1}^{bcc}} = \gamma_{2A}^{bcc} + \frac{1}{2r_{1A_1}^{bcc}}\varphi_{AC}^{(3)}\left(r_{1A_1}^{bcc}\right) - \frac{3}{4\left(r_{1A_1}^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_1}^{bcc}\right) + \frac{3}{4\left(r_{1A_1}^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_1}^{bcc}\right), \quad (3)$$

$$u_{0A_2}^{bcc} = u_{0A}^{bcc} + \varphi_{AC}\left(r_{1A_2}^{bcc}\right), \gamma_{A_2}^{bcc} = 4\left(\gamma_{1A_2}^{bcc} + \gamma_{2A_2}^{bcc}\right),$$

$$k_{A_1}^{bcc} = k_A^{bcc} + \frac{1}{2}\sum_i \left[\left(\frac{\partial^2 \varphi_{AC}}{\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_2}^{bcc}} = k_A^{bcc} + 2\varphi_{AC}^{(2)}\left(r_{1A_2}^{bcc}\right) + \frac{4}{r_{1A_2}^{bcc}}\varphi_{AC}^{(1)}\left(r_{1A_2}^{bcc}\right),$$

$$\gamma_{1A_2}^{bcc} = \gamma_{1A}^{bcc} + \frac{1}{48}\sum_i \left[\left(\frac{\partial^4 \varphi_{AC}}{\partial u_{i\beta}^4}\right)_{eq}\right]_{r=r_{1A_2}^{bcc}} = \gamma_{1A}^{bcc} + \frac{1}{24}\varphi_{AC}^{(4)}\left(r_{1A_2}^{bcc}\right) + \frac{1}{4r_{1A_2}^{bcc}}\varphi_{AC}^{(3)}\left(r_{1A_2}^{bcc}\right) -$$

$$-\frac{1}{8\left(r_{1A_2}^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_2}^{bcc}\right) + \frac{1}{8\left(r_{1A_2}^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_2}^{bcc}\right) +,$$

$$\gamma_{2A_2}^{bcc} = \gamma_{2A}^{bcc} + \frac{6}{48}\sum_i \left[\left(\frac{\partial^4 \varphi_{AC}}{\partial u_{i\alpha}^2 \partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_2}^{bcc}} = \gamma_{2A}^{bcc} + \frac{1}{8}\varphi_{AC}^{(4)}\left(r_{1A_2}^{bcc}\right) + \frac{1}{4r_{1A_2}^{bcc}}\varphi_{AC}^{(3)}\left(r_{1A_2}^{bcc}\right) +$$

$$+\frac{3}{8\left(r_{1A_2}^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_2}^{bcc}\right) - \frac{3}{8\left(r_{1A_2}^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_2}^{bcc}\right), \tag{4}$$

where φ_{AC} is the interaction potential between the atom A and the atom C, n_i is the number of atoms on the ith coordination sphere with the radius $r_i (i = 1, 2, 3)$, $r_1^{bcc} \equiv r_{1C}^{bcc} = r_{01C}^{bcc} + y_{0A_1}^{bcc}(T)$ is the nearest neighbor distance between the interstitial atom C and the metallic atom A at temperature *T*, r_{01C}^{bcc} is the nearest neighbor distance between the interstitial atom C and the metallic atom A at 0K and is determined from the minimum condition of the cohesive energy u_{0C}^{bcc}, $y_{0A_1}^{bcc}(T)$ is the displacement of the atom A_1 (the atom A stays in the bcc unit cell) from equilibrium position at temperature *T*.

$\varphi_{AB}^{(m)} \equiv \partial^m \varphi_{AC}(r_i)/\partial r_i^m (m = 1,2,3,4, \alpha, \beta = x, y.z, \alpha \neq \beta$ and $u_{i\beta}$ is the displacement of the ith atom in the direction β. $r_{1A_1}^{bcc} \approx r_{1C}^{bcc}$ is the nearest neighbor distance between the atom A_1 and atoms in crystalline lattice. $r_{1A_2}^{bcc} = r_{01A_2}^{bcc} + y_{0C}^{bcc}(T), r_{01A_2}^{bcc}$ is the nearest neighbor distance between atom A_2 and atoms in crystalline lattice at 0K and is determined from the minimum condition of the cohesive energy $u_{0A_2}^{bcc}, y_{0C}^{bcc}(T)$ is the displacement of the atom C at temperature *T*. In Eqs. (3) and (4), $u_{0A}^{bcc}, k_A^{bcc}, \gamma_{1A}^{bcc}, \gamma_{2A}^{bcc}$ are the coressponding quantities in clean bcc metal A in the approximation of two coordination sphere [11-13].

The equation of state for bcc interstitial alloy AC at temperature *T* and pressure *P* is written in the form

$$Pv^{bcc} = -r_1^{bcc}\left(\frac{1}{6}\frac{\partial u_0^{bcc}}{\partial r_1^{bcc}} + \theta x^{bcc} cthx^{bcc} \frac{1}{2k^{bcc}}\frac{\partial k^{bcc}}{\partial r_1^{bcc}}\right), v^{bcc} = \frac{4\left(r_1^{bcc}\right)^3}{3\sqrt{3}}. \tag{5}$$

At 0K and pressure *P*, this equation has the form

$$Pv^{bcc} = -r_1^{bcc}\left(\frac{1}{6}\frac{\partial u_0^{bcc}}{\partial r_1^{bcc}} + \frac{\hbar\omega_0^{bcc}}{4k^{bcc}}\frac{\partial k^{bcc}}{\partial r_1^{bcc}}\right). \tag{6}$$

If we know the interaction potential φ_{i0}, Equation (6) permits us to determine the nearest neighbour distance $r_{1X}^{bcc}(P,0)(\mathrm{X}=\mathrm{A},\mathrm{A}_1,\mathrm{A}_2,\mathrm{C})$ at pressure P and temperature 0K. When we know $r_{1X}^{bcc}(P,0)$ we can determine the parameters $k_X^{bcc}(P,0),\gamma_{1X}^{bcc}(P,0),\gamma_{2X}^{bcc}(P,0),\gamma_X^{bcc}(P,0)$ at pressure P and 0K for each case of X. Then, the displacement $y_{0X}^{bcc}(P,T)$ of atom X from the equilibrium position at temperature T and pressure P is calculated as in [11]. From that, we can calculate the nearest neighbour distance $r_{1X}^{bcc}(P,T)$ at temperature T and pressure P as follows:

$$r_{1B}^{bcc}(P,T)=r_{1B}^{bcc}(P,0)+y_{A_1}^{bcc}(P,T),r_{1A}^{bcc}(P,T)=r_{1A}^{bcc}(P,0)+y_{A}^{bcc}(P,T),$$
$$r_{1A_1}^{bcc}(P,T)\approx r_{1B}^{bcc}(P,T),r_{1A_2}^{bcc}(P,T)=r_{1A_2}^{bcc}(P,0)+y_{B}^{bcc}(P,T). \tag{7}$$

The mean nearest neighbour distance between two atoms in bcc interstitial alloy AC has the form

$$\overline{r_{1A}^{bcc}(P,T)}=\overline{r_{1A}^{bcc}(P,0)}+\overline{y^{bcc}(P,T)},$$
$$\overline{r_{1A}^{bcc}(P,0)}=(1-c_C)r_{1A}^{bcc}(P,0)+c_C r_{1A}'^{bcc}(P,0),r_{1A}'^{bcc}(P,0)=\sqrt{3}r_{1C}^{bcc}(P,0),$$
$$\overline{y^{bcc}(P,T)}=(1-7c_C)y_A^{bcc}(P,T)+c_C y_B^{bcc}(P,T)+2c_C y_{A_1}^{bcc}(P,T)+4c_C y_{A_2}^{bcc}(P,T), \tag{8}$$

where $\overline{r_{1A}^{bcc}(P,T)}$ is the mean nearest neighbor distance between atoms A in the interstitial alloy AC at pressure P and temperature T, $\overline{r_{1A}^{bcc}(P,0)}$ is the mean nearest neighbor distance between atoms A in the interstitial alloy AC at pressure P and temperature 0K, $r_{1A}^{bcc}(P,0)$ is the nearest neighbor distance between atoms A in the deformed clean metal A at pressure P and temperature 0K, $r_{1A}'^{bcc}(P,0)$ is the nearest neighbor distance between atoms A in the zone containing the interstitial atom C at pressure P and temperature 0K and c_C is the concentration of interstitial atoms C.

In the case of fcc interstitial alloy AC (where the main atom A_1 stay in face centers, the main atom A_2 stay in peaks and the interstitial atom C stays in body center of cubic unit cell), the corresponding formulas are as follows [11-13]:

$$u_{0C}^{fcc}=\frac{1}{2}\sum_{i=1}^{n_i}\varphi_{AC}(r_i)=3\varphi_{AC}(r_1^{fcc})+4\varphi_{AC}\left(r_1^{fcc}\sqrt{3}\right)+12\varphi_{AC}\left(r_1^{fcc}\sqrt{5}\right), \tag{9}$$

$$k_C^{fcc}=\frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{AC}}{\partial u_{i\beta}^2}\right)_{eq}=\varphi_{AC}^{(2)}\left(r_1^{fcc}\right)+\frac{2}{r_1^{fcc}}\varphi_{AC}^{(1)}\left(r_1^{fcc}\right)+\frac{4}{3}\varphi_{AC}^{(2)}\left(r_1^{fcc}\sqrt{3}\right)+\frac{8\sqrt{3}}{9r_1^{fcc}}\varphi_{AC}^{(2)}\left(r_1^{fcc}\sqrt{3}\right)+$$
$$+4\varphi_{AC}^{(2)}\left(r_1^{fcc}\sqrt{5}\right)+\frac{8\sqrt{5}}{5r_1^{fcc}}\varphi_{AC}^{(1)}\left(r_1^{fcc}\sqrt{5}\right),\gamma_C^{fcc}=4\left(\gamma_{1C}^{fcc}+\gamma_{2C}^{fcc}\right),$$

$$\gamma_{1C}^{fcc}=\frac{1}{48}\sum_i\left(\frac{\partial^4\varphi_{AB}}{\partial u_{i\beta}^4}\right)_{eq}=\frac{1}{24}\varphi_{AC}^{(4)}\left(r_1^{fcc}\right)+\frac{1}{4\left(r_1^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{fcc}\right)-\frac{1}{4\left(r_1^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{fcc}\right)+\frac{1}{54}\varphi_{AC}^{(4)}\left(r_1^{fcc}\sqrt{3}\right)+$$

$$+\frac{2\sqrt{3}}{27r_1^{fcc}}\varphi_{AC}^{(3)}\left(r_1^{fcc}\sqrt{3}\right)-\frac{2}{27\left(r_1^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{fcc}\sqrt{3}\right)+\frac{2\sqrt{3}}{81\left(r_1^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{fcc}\sqrt{3}\right)+\frac{17}{150}\varphi_{AC}^{(4)}\left(r_1^{fcc}\sqrt{5}\right)+$$

$$+\frac{8\sqrt{5}}{125r_1^{fcc}}\varphi_{AC}^{(3)}\left(r_1^{fcc}\sqrt{5}\right)+\frac{1}{25\left(r_1^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{fcc}\sqrt{5}\right)-\frac{\sqrt{5}}{125\left(r_1^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{fcc}\sqrt{5}\right),$$

$$\gamma_{2C}^{fcc}=\frac{6}{48}\sum_i\left(\frac{\partial^4\varphi_{AC}}{\partial u_{i\alpha}^2\partial u_{i\beta}^2}\right)_{eq}=\frac{1}{2r_1^{fcc}}\varphi_{AC}^{(3)}\left(r_1^{fcc}\right)-\frac{3}{4\left(r_1^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{fcc}\right)+\frac{3}{4\left(r_1^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{fcc}\right)+$$

$$+\frac{1}{4}\varphi_{AC}^{(4)}\left(r_1^{fcc}\sqrt{2}\right)+\frac{\sqrt{2}}{8r_1^{fcc}}\varphi_{AC}^{(3)}\left(r_1^{fcc}\sqrt{2}\right)+\frac{7}{8\left(r_1^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{fcc}\sqrt{2}\right)-\frac{7\sqrt{2}}{16\left(r_1^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{fcc}\sqrt{2}\right)+$$

$$+\frac{4}{25}\varphi_{AC}^{(4)}\left(r_1^{fcc}\sqrt{5}\right)+\frac{26\sqrt{5}}{125r_1^{fcc}}\varphi_{AC}^{(3)}\left(r_1^{fcc}\sqrt{5}\right)-\frac{3}{25\left(r_1^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{bcc}\sqrt{5}\right)+\frac{3\sqrt{5}}{125\left(r_1^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{bcc}\sqrt{5}\right), \quad (10)$$

$$u_{0A_1}^{fcc}=u_{0A}^{fcc}+\varphi_{AC}\left(r_{1A_1}^{fcc}\right), \gamma_{A_1}^{fcc}=4\left(\gamma_{1A_1}^{fcc}+\gamma_{2A_1}^{fcc}\right),$$

$$k_{A_1}^{fcc}=k_A^{fcc}+\frac{1}{2}\sum_i\left[\left(\frac{\partial^2\varphi_{AC}}{\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_1}^{fcc}}=k_A^{fcc}+\varphi_{AC}^{(2)}\left(r_{1A_1}^{fcc}\right),$$

$$\gamma_{1A_1}^{fcc}=\gamma_{1A}^{fcc}+\frac{1}{48}\sum_i\left[\left(\frac{\partial^4\varphi_{AC}}{\partial u_{i\beta}^4}\right)_{eq}\right]_{r=r_{1A_1}^{fcc}}=\gamma_{1A}^{fcc}+\frac{1}{24}\varphi_{AC}^{(4)}\left(r_{1A_1}^{fcc}\right),$$

$$\gamma_{2A_1}^{fcc}=\gamma_{2A}^{fcc}+\frac{6}{48}\sum_i\left[\left(\frac{\partial^4\varphi_{AC}}{\partial u_{i\alpha}^2\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_1}^{fcc}}=\gamma_{2A}^{fcc}+\frac{1}{4r_{1A_1}^{fcc}}\varphi_{AC}^{(3)}\left(r_{1A_1}^{fcc}\right)-\frac{1}{2\left(r_{1A_1}^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_1}^{fcc}\right)+\frac{1}{2\left(r_{1A_1}^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_1}^{fcc}\right), \quad (11)$$

$$u_{0A_2}^{fcc}=u_{0A}^{fcc}+\varphi_{AC}\left(r_{1A_2}^{fcc}\right), \gamma_{A_2}^{fcc}=4\left(\gamma_{1A_2}^{fcc}+\gamma_{2A_2}^{fcc}\right),$$

$$k_{A_1}^{fcc}=k_A^{fcc}+\frac{1}{2}\sum_i\left[\left(\frac{\partial^2\varphi_{AC}}{\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_2}^{fcc}}=k_A^{fcc}+\frac{1}{6}\varphi_{AC}^{(2)}\left(r_{1A_2}^{fcc}\right)+\frac{23}{6r_{1A_2}^{fcc}}\varphi_{AC}^{(1)}\left(r_{1A_2}^{fcc}\right),$$

$$\gamma_{1A_2}^{fcc}=\gamma_{1A}^{fcc}+\frac{1}{48}\sum_i\left[\left(\frac{\partial^4\varphi_{AC}}{\partial u_{i\beta}^4}\right)_{eq}\right]_{r=r_{1A_2}^{fcc}}=\gamma_{1A}^{fcc}+\frac{1}{54}\varphi_{AC}^{(4)}\left(r_{1A_2}^{fcc}\right)+\frac{2}{9r_{1A_2}^{fcc}}\varphi_{AC}^{(3)}\left(r_{1A_2}^{fcc}\right)-$$

$$-\frac{2}{9\left(r_{1A_2}^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_2}^{fcc}\right)+\frac{2}{9\left(r_{1A_2}^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_2}^{fcc}\right)+,$$

$$\gamma_{2A_2}^{fcc}=\gamma_{2A}^{fcc}+\frac{6}{48}\sum_i\left[\left(\frac{\partial^4\varphi_{AC}}{\partial u_{i\alpha}^2\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_2}^{fcc}}=\gamma_{2A}^{fcc}+\frac{1}{81}\varphi_{AC}^{(4)}\left(r_{1A_2}^{fcc}\right)+\frac{4}{27r_{1A_2}^{fcc}}\varphi_{AC}^{(3)}\left(r_{1A_2}^{fcc}\right)+$$

$$+\frac{14}{27\left(r_{1A_2}^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_2}^{fcc}\right)-\frac{14}{27\left(r_{1A_2}^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_2}^{fcc}\right), \quad (12)$$

$$Pv^{fcc}=-r_1^{fcc}\left(\frac{1}{6}\frac{\partial u_0^{fcc}}{\partial r_1^{bcc}}+\theta x^{fcc}cthx^{fcc}\frac{1}{2k^{fcc}}\frac{\partial k^{fcc}}{\partial r_1^{fcc}}\right), v^{fcc}=\frac{\sqrt{2}\left(r_1^{fcc}\right)^3}{2}, \quad (13)$$

$$Pv^{fcc}=-r_1^{fcc}\left(\frac{1}{6}\frac{\partial u_0^{fcc}}{\partial r_1^{fcc}}+\frac{\hbar\omega_0^{fcc}}{4k^{fcc}}\frac{\partial k^{fcc}}{\partial r_1^{fcc}}\right), \quad (14)$$

$$r_{1B}^{fcc}(P,T)=r_{1B}^{fcc}(P,0)+y_{A_1}^{fcc}(P,T), r_{1A}^{fcc}(P,T)=r_{1A}^{fcc}(P,0)+y_A^{fcc}(P,T),$$

$$r_{1A_1}^{fcc}(P,T)\approx r_{1B}^{fcc}(P,T), r_{1A_2}^{fcc}(P,T)=r_{1A_2}^{fcc}(P,0)+y_B^{fcc}(P,T). \quad (15)$$

$$\overline{r_{1A}^{fcc}(P,T)}=\overline{r_{1A}^{fcc}(P,0)}+\overline{y^{fcc}(P,T)},$$

$$\overline{r_{1A}^{cc}(P,0)}=(1-c_C)r_{1A}^{fcc}(P,0)+c_C r_{1A}'^{fcc}(P,0), r_{1A}'^{fcc}(P,0)=\sqrt{2}r_{1C}^{fcc}(P,0),$$

$$\overline{y^{fcc}(P,T)}=(1-15c_C)y_A^{fcc}(P,T)+c_C y_B^{fcc}(P,T)+6c_C y_{A_1}^{fcc}(P,T)+8c_C y_{A_2}^{fcc}(P,T), \quad (16)$$

The mean nearest neighbor distance between two atoms A in the perfect bcc substitutional alloy AB with interstitial atom C at pressure P and temperature T is

$$a_{ABC}^{bcc}=c_{AC}a_{AC}^{bcc}\frac{B_{TAC}^{bcc}}{\overline{B_T^{bccF}}}+c_B a_B^{bcc}\frac{B_{TB}^{bcc}}{\overline{B_T^{bcc}}}, \overline{B_T^{bcc}}=c_{AC}B_{TAC}^{bcc}+c_B B_{TB}^{bcc}, c_{AC}=c_A+c_C,$$

$$a_{ABC}^{bcc}\equiv\overline{r_{1A}^{bccABC}(P,T)}, a_{AC}^{bcc}\equiv\overline{r_{1A}^{bccAC}(P,T)}, a_B^{bcc}\equiv r_{1B}^{bcc}(P,T),$$

$$B_{TAC}^{bcc}=\frac{1}{\chi_{TAC}^{bcc}}=\frac{2P+\frac{3\sqrt{3}}{4a_{AC}^{bccF}}\frac{1}{3N}\left(\frac{\partial^2\psi_{AC}^{bcc}}{\partial a_{AC}^{bcc2}}\right)_T}{3\left(\frac{a_{AC}^{bcc}}{a_{0AC}^{bccF}}\right)^3}, B_{TB}^{bcc}=\frac{1}{\chi_{TB}^{bcc}}=\frac{2P+\frac{3\sqrt{3}}{4a_B^{bcc}}\frac{1}{3N}\left(\frac{\partial^2\psi_B^{bcc}}{\partial a_B^{bcc2}}\right)_T}{3\left(\frac{a_B^{bcc}}{a_{0B}^{bcc}}\right)^3},$$

$$\left(\frac{\partial^2\psi_{AC}^{bcc}}{\partial a_{AC}^{bcc2}}\right)_T\approx(1-7c_C)\left(\frac{\partial^2\psi_A^{bcc}}{\partial a_A^{bcc2}}\right)_T+c_C\left(\frac{\partial^2\psi_C^{bcc}}{\partial a_C^{bcc2}}\right)_T+2c_C\left(\frac{\partial^2\psi_{A_1}^{bcc}}{\partial a_{A_1}^{bcc2}}\right)_T+4c_C\left(\frac{\partial^2\psi_{A_2}^{bcc}}{\partial a_{A_2}^{bcc2}}\right)_T,$$

$$\frac{1}{3N}\left(\frac{\partial^2\psi_X^{bcc}}{\partial a_X^{bcc2}}\right)_T=\frac{1}{6}\frac{\partial^2u_{0X}^{bcc}}{\partial a_X^{bcc2}}+\frac{\hbar\omega_X^{bcc}}{4k_X^{bcc}}\left[\frac{\partial^2k_X^{bcc}}{\partial a_X^{bcc2}}-\frac{1}{2k_X^{bcc}}\left(\frac{\partial k_X^{bcc}}{\partial a_X^{bcc}}\right)^2\right], \mathrm{X}=\mathrm{A},\mathrm{A}_1,\mathrm{A}_2,\mathrm{B},\mathrm{C}. \quad (17)$$

The Helmholtz free energy of perfect bcc substitutional alloy AB with interstitial atom C before deformation with the condition $c_C << c_B << c_A$ has the form

$$\psi_{ABC}^{bcc}=\psi_{AC}^{bcc}+c_B\left(\psi_B^{bcc}-\psi_A^{bcc}\right)+TS_c^{bccAC}-TS_c^{bccABC},$$

$$\psi_{AC}^{bcc}=(1-7c_C)\psi_A^{bcc}+c_C\psi_C^{bcc}+2c_C\psi_{A_1}^{bcc}+4c_C\psi_{A_2}^{bcc}-TS_c^{bccAC},$$

$$\psi_X^{bcc} \approx U_{0X}^{bcc} + \psi_{0X}^{bcc} + 3N\left\{ \frac{\theta^2}{\left(k_X^{bcc}\right)^2}\left[\gamma_{2X}^{bcc}\left(Y_X^{bcc}\right)^2 - \frac{2\gamma_{1X}^{bcc}}{3}\left(1+\frac{Y_X^{bcc}}{2}\right)\right] + \right.$$

$$\left. + \frac{2\theta^3}{\left(k_X^{bcc}\right)^4}\left[\frac{4}{3}\gamma_{2X}^{bcc}Y_X^{bcc}\left(1+\frac{Y_X^{bcc}}{2}\right) - 2\left[\left(\gamma_{1X}^{bcc}\right)^2 + 2\gamma_{1X}^{bcc}\gamma_{2X}^{bcc}\right]\left(1+\frac{Y_X^{bcc}}{2}\right)\left(1+Y_X^{bcc}\right)\right]\right\},$$

$$\psi_{0X}^{bcc} = 3N\theta\left[x_X^{bcc} + \ln\left(1-e^{-2x_X^{bcc}}\right)\right], Y_X^{bcc} \equiv x_X^{bcc}\coth x_X^{bcc}, \tag{18}$$

where ψ_X^{bcc} is the Helmholtz free energy, Y_X^{bcc} is an atom X in clean metals A, B or interstitial alloy AC, S_c^{bccAC} is the configuration entropy of bcc interstitial alloy AC and S_c^{bccABC} is the configuration entropy of bcc alloy ABC.

In the case of fcc interstitial alloy AC, the corresponding formulas are as follows:

$$a_{ABC}^{fcc} = c_{AC}a_{AC}^{fcc}\frac{B_{TAC}^{fcc}}{\overline{B_T^{fcc}}} + c_B a_B^{fcc}\frac{B_{TB}^{fcc}}{\overline{B_T^{fcc}}}, \overline{B_T^{bcc}} = c_{AC}B_{TAC}^{fcc} + c_B B_{TB}^{fcc}, c_{AC} = c_A + c_C,$$

$$a_{ABC}^{fcc} \equiv \overline{r_{1A}^{fccABC}(P,T)}, a_{AC}^{fcc} \equiv \overline{r_{1A}^{fccAC}(P,T)}, a_B^{fcc} \equiv r_{1B}^{fcc}(P,T),$$

$$B_{TAC}^{fcc} = \frac{1}{\chi_{TAC}^{fccF}}\frac{2P + \frac{\sqrt{2}}{a_{AC}^{fccF}}\frac{1}{3N}\left(\frac{\partial^2\psi_{AC}^{fcc}}{\partial a_{AC}^{fcc2}}\right)_T}{3\left(\frac{a_{AC}^{fcc}}{a_{0AC}^{fcc}}\right)^3}, B_{TB}^{fcc} = \frac{1}{\chi_{TB}^{fcc}} = \frac{2P + \frac{\sqrt{2}}{a_B^{fccF}}\frac{1}{3N}\left(\frac{\partial^2\psi_B^{fcc}}{\partial a_B^{fcc2}}\right)_T}{3\left(\frac{a_B^{fcc}}{a_{0B}^{fcc}}\right)^3},$$

$$\left(\frac{\partial^2\psi_{AC}^{fcc}}{\partial a_{AC}^{fcc2}}\right)_T \approx \left(1-15c_C\right)\left(\frac{\partial^2\psi_A^{fcc}}{\partial a_A^{fcc2}}\right)_T + c_C\left(\frac{\partial^2\psi_C^{fcc}}{\partial a_C^{fcc2}}\right)_T + 6c_C\left(\frac{\partial^2\psi_{A_1}^{fcc}}{\partial a_{A_1}^{fcc2}}\right)_T + 8c_C\left(\frac{\partial^2\psi_{A_2}^{fcc}}{\partial a_{A_2}^{fcc2}}\right)_T,$$

$$\frac{1}{3N}\left(\frac{\partial^2\psi_X^{fcc}}{\partial a_X^{fcc2}}\right)_T = \frac{1}{6}\frac{\partial^2 u_{0X}^{fcc}}{\partial a_X^{fcc2}} + \frac{\hbar\omega_X^{fcc}}{4k_X^{fcc}}\left[\frac{\partial^2 k_X^{fcc}}{\partial a_X^{fcc2}} - \frac{1}{2k_X^{fcc}}\left(\frac{\partial k_X^{fcc}}{\partial a_X^{fcc}}\right)^2\right], \mathrm{X} = \mathrm{A}, \mathrm{A}_1, \mathrm{A}_2, \mathrm{B}, \mathrm{C}, \tag{19}$$

$$\psi_{ABC}^{fcc} = \psi_{AC}^{fcc} + c_B\left(\psi_B^{fcc} - \psi_A^{fcc}\right) + TS_c^{fccAC} - TS_c^{fccABC},$$

$$\psi_{AB}^{fcc} = \left(1-15c_B\right)\psi_A^{fcc} + c_B\psi_B^{fcc} + 6c_B\psi_{A_1}^{fcc} + 8c_B\psi_{A_2}^{fcc} - TS_c^{fccAC},$$

$$\psi_X^{fcc} \approx U_{0X}^{fcc} + \psi_{0X}^{fcc} + 3N\left\{ \frac{\theta^2}{\left(k_X^{fcc}\right)^2}\left[\gamma_{2X}^{fcc}\left(Y_X^{fcc}\right)^2 - \frac{2\gamma_{1X}^{fcc}}{3}\left(1+\frac{Y_X^{fcc}}{2}\right)\right] + \right.$$

$$\left. + \frac{2\theta^3}{\left(k_X^{fcc}\right)^4}\left[\frac{4}{3}\gamma_{2X}^{fcc}Y_X^{fcc}\left(1+\frac{Y_X^{fcc}}{2}\right) - 2\left[\left(\gamma_{1X}^{fcc}\right)^2 + 2\gamma_{1X}^{fcc}\gamma_{2X}^{fcc}\right]\left(1+\frac{Y_X^{fcc}}{2}\right)\left(1+Y_X^{fcc}\right)\right]\right\},$$

$$\psi_{0X}^{fcc} = 3N\theta\left[x_X^{fcc} + \ln\left(1-e^{-2x_X^{fcc}}\right)\right], Y_X^{fcc} \equiv x_X^{fcc}\coth x_X^{fcc}. \tag{20}$$

For perfect hcp interstitial alloy AC and perfect hcp substitutional alloy AB with interstitial atoms C, we have the same formulas as for perfect fcc interstitial alloy AC and perfect fcc substitutional alloy AB with interstitial atoms C. The numerical calculations of the cohesive energy u_0 and the alloy parameters $k,\gamma_1,\gamma_2,\gamma$ of fcc alloy and ones of the hcp alloys are different.

When the phase equilibrium happens between the α phase and the β phase of perfect substitutional alloy AB with interstitial atoms C at zero pressure,

$$\psi_{ABC}^{\alpha}=\psi_{ABC}^{\beta},T_{ABC}^{\alpha}=T_{ABC}^{\beta}\equiv T_{ABC}^{\alpha-\beta}, \tag{21}$$

where we call $T_{ABC}^{bcc-fcc}$ as the α-β phase transition temperature of substitutional alloy AB with interstitial atoms C. According to the thermodynamic relation, $\psi=E-TS$. Therefore, the α-β phase transition temperature of substitutional alloy AB with interstitial atoms Cat zero pressure can be determined by the following formular

$$T_{ABC}^{\alpha-\beta}(P=0)=\left|\frac{\Delta E_{ABC}}{\Delta S_{ABC}}\right|=\left|\frac{E_{ABC}^{\alpha}-E_{ABC}^{\beta}}{S_{ABC}^{\alpha}-S_{ABC}^{\beta}}\right|. \tag{22}$$

For example, when α ≡ bcc, β ≡ fcc,

$$E_{ABC}^{bcc}=(1-7c_C)E_A^{bcc}+c_CE_C^{bcc}+2c_CE_{A_1}^{bcc}+4c_CE_{A_2}^{bcc}+c_B\left(E_B^{bcc}-E_A^{bcc}\right),$$

$$E_X^{bcc}=U_{0X}^{bcc}+E_{0X}^{bcc}+\frac{3N\theta^2}{\left(k_X^{bcc}\right)^2}\left\{\gamma_{2X}^{bcc}\left(Y_X^{bcc}\right)^2+\frac{\gamma_{1X}^{bcc}}{3}\left[2+\left(Z_X^{bcc}\right)^2\right]-2\gamma_{2X}^{bcc}Y_X^{bcc}\left(Z_X^{bcc}\right)^2\right\},$$

$$E_{0X}^{bcc}=3N\theta Y_X^{bcc},Z_X^{bcc}\equiv\frac{x_X^{bcc}}{\sinh x_X^{bcc}},$$

$$S_{ABC}^{bcc}=(1-7c_C)S_A^{bcc}+c_CS_B^{bcc}+2c_CS_{A_1}^{bcc}+4c_CS_{A_2}^{bcc}+c_B\left(S_B^{bcc}-S_A^{bcc}\right),$$

$$S_X^{bcc}=S_{0X}^{bcc}+\frac{3Nk_{Bo}\theta}{\left(k_X^{bcc}\right)^2}\left\{\frac{\gamma_{1X}^{bcc}}{3}\left[4+Y_X^{bcc}+\left(Z_X^{bcc}\right)^2\right]-2\gamma_{2X}^{bcc}Y_X^{bcc}\left(Z_X^{bcc}\right)^2\right\},$$

$$S_{0X}^{bcc}=3Nk_{Bo}\left[Y_X^{bcc}-\ln\left(2\sinh x_X^{bcc}\right)\right],$$

$$E_{ABC}^{fcc}=(1-15c_C)E_A^{fcc}+c_CE_B^{fcc}+6c_CE_{A_1}^{fcc}+8c_CE_{A_2}^{fcc}+c_B\left(E_B^{fcc}-E_A^{fcc}\right),$$

$$E_X^{fcc}=U_{0X}^{bcc}+E_{0X}^{fcc}+\frac{3N\theta^2}{\left(k_X^{fcc}\right)^2}\left\{\gamma_{2X}^{fcc}\left(Y_X^{fcc}\right)^2+\frac{\gamma_{1X}^{fcc}}{3}\left[2+\left(Z_X^{fcc}\right)^2\right]-2\gamma_{2X}^{fcc}Y_X^{fcc}\left(Z_X^{fcc}\right)^2\right\},$$

$$E_{0X}^{fcc}=3N\theta Y_X^{fcc},Z_X^{fcc}\equiv\frac{x_X^{fcc}}{\sinh x_X^{fcc}},$$

$$S_{ABC}^{fcc}=(1-15c_C)S_A^{fcc}+c_CS_B^{fcc}+6c_CS_{A_1}^{fcc}+8c_CS_{A_2}^{fcc}+c_B\left(S_B^{fcc}-S_A^{fcc}\right),$$

$$S_X^{fcc}=S_{0X}^{fcc}+\frac{3Nk_{Bo}\theta}{\left(k_X^{fcc}\right)^2}\left\{\frac{\gamma_{1X}^{fcc}}{3}\left[4+Y_X^{fcc}+\left(Z_X^{fcc}\right)^2\right]-2\gamma_{2X}^{fcc}Y_X^{fcc}\left(Z_X^{fcc}\right)^2\right\},$$

$$S_{0X}^{fcc}=3Nk_{Bo}\left[Y_X^{fcc}-\ln\left(2\sinh x_X^{ccc}\right)\right], \tag{23}$$

where k_{Bo} is the Boltzmann constant.

When the phase equilibrium happens between the α phase and the β phase of perfect substitutional alloy AB with interstitial atoms C at preesure P,

$$G^{\alpha}_{ABC} = G^{\beta}_{ABC}, T^{\alpha}_{ABC} = T^{\beta}_{ABC} \equiv T^{\alpha-\beta}_{ABC}, P^{\alpha}_{ABC} = P^{\beta}_{ABC} \equiv P, \quad (24)$$

where G is the Gibbs thermodynamic potential. According to the thermodynamic relation, $G = \psi + PV = U - TS + PV$. Therefore, the α-β phase transition temperature of substitutional alloy AB with interstitial atoms C at pressure P can be determined by the following formular:

$$T^{\alpha-\beta}_{ABC} = \left| \frac{\Delta E_{ABC} + P\Delta V_{ABC}}{\Delta S_{ABC}} \right| = \left| \frac{E^{\alpha}_{AB} - E^{\beta}_{AB} + P\left(V^{\alpha}_{AB} - V^{\beta}_{AB}\right)}{S^{\alpha}_{AB} - S^{\beta}_{AB}} \right|. \quad (25)$$

For example, when α ≡ bcc, β ≡ fcc, we also have Eq. (23) and

$$V^{bcc}_{ABC} = Nv^{bcc}_{ABC} = N\frac{4\left(a^{bcc}_{ABC}\right)^3}{3\sqrt{3}}, V^{fcc}_{ABC} = Nv^{fcc}_{ABC} = N\frac{\sqrt{2}\left(a^{fcc}_{ABC}\right)^3}{2}. \quad (26)$$

The Helmholtz free energy of defective (or real) substitutional alloy AB with interstitial atoms C has the form

$$\psi^{R}_{ABC} = \psi_{ABC} + ng^{f}_{v}(ABC) - TS^{ABC*}_{c},$$

$$g^{f}_{v}(ABC) = c_A g^{f}_{v}(A) + c_C g^{f}_{v}(C) + c_{A_1} g^{f}_{v}\left(A_1\right) + c_{A_2} g^{f}_{v}\left(A_2\right) + c_B g^{f}_{v}(B),$$

$$g^{f}_{v}(X) = n_1\left(\psi^{(1)}_{XX} - \psi_{XX}\right) + \left(B_X - 1\right)\psi_{XX}, B_X \approx 1 + \frac{U_{0X}}{\psi_X}, N\psi^{(1)}_{XX} = \psi^{(1)}_{X}, N\psi_{XX} = \psi_X, \quad (27)$$

where ψ_{ABC} is the Helmholtz free energy of perfect substitutional alloy AB with interstitial atoms C, $g^{f}_{v}(ABC)$ is the Gibbs thermodynamic potential change of substitutional alloy AB with interstitial atoms C when one vacancy is formulated, $g^{f}_{v}(X)$ isthe Gibbs thermodynamic potential change of an atom X when one vacancy is formulated, S^{ABC*}_{c} is the configurational entropy of alloy atoms and vacancies, N is the total numeber of atoms in alloy, n_1 is the number of atoms on the first coordination sphere, $\psi^{(1)}_{XX}$ is the Helmholtz free energy of an atom X on the first coordination sphere with vacancy as centre, $c_A = 1 - c_B - 7c_C, c_{A_1} = 2c_C, c_{A_2} = 4c_C$ for bcc alloy and $c_A = 1 - c_B - 15c_C, c_{A_1} = 6c_C, c_{A_2} = 8c_C$ for fcc alloy.

The concentration of equilibrium atom is determined from the minimum condition of the Helmholtz free energy

$$n_v = n^{A}_{v} \exp\left[-\frac{c_B g^{f}_{v}(B)}{k_{Bo}T}\right] \exp\left[-\frac{c_B g^{f}_{v}(C)}{k_{Bo}T}\right],$$

$$n^{A}_{v} = \exp\left[-\frac{c_A g^{f}_{v}(A) + c_{A_1} g^{f}_{v}(A_1) + c_{A_2} g^{f}_{v}(A_2)}{k_{Bo}T}\right]. \quad (28)$$

Approximately, the mean nearest neighbor distance between two atoms in defective alloy is equal to one in perfect alloy.

The α-β phase transition temperature of defective substitutional alloy AB with interstitial atoms C at zero pressure and at pressure P is determined by

$$T_{ABC}^{R\alpha-\beta}(P=0)=\left|\frac{\Delta E_{ABC}^{R}}{\Delta S_{ABC}^{R}}\right|=\left|\frac{E_{ABC}^{R\alpha}-E_{ABC}^{R\beta}}{S_{ABC}^{R\alpha}-S_{ABC}^{R\beta}}\right|, \tag{29}$$

$$E_{ABC}^{Rbcc}=[1-n_v n_1+n_v(B_A-1)](1-c_B-7c_C)E_A+n_v n_1(1-c_B-7c_C)E_A^{(1)}+[1-n_v n_1+n_v(B_B-1)]c_B E_B+n_v n_1 c_B E_B^{(1)}+$$
$$+2[1-n_v n_1+n_v(B_{A_1}-1)]c_C E_{A_1}+2n_v n_1 c_C E_{A_1}^{(1)}+4[1-n_v n_1+n_v(B_{A_2}-1)]c_C E_{A_2}+4n_v n_1 c_C E_{A_2}^{(1)}+$$
$$+[1-n_v n_1+n_v(B_C-1)]c_C E_C+n_v n_1 c_C E_C^{(1)},$$

$$E_{ABC}^{Rfcc}=[1-n_v n_1+n_v(B_A-1)](1-c_B-15c_C)E_A+n_v n_1(1-c_B-15c_C)E_A^{(1)}+[1-n_v n_1+n_v(B_B-1)]c_B E_B+n_v n_1 c_B E_B^{(1)}+$$
$$+6[1-n_v n_1+n_v(B_{A_1}-1)]c_C E_{A_1}+6n_v n_1 c_C E_{A_1}^{(1)}+8[1-n_v n_1+n_v(B_{A_2}-1)]c_C E_{A_2}+8n_v n_1 c_C E_{A_2}^{(1)}+$$
$$+[1-n_v n_1+n_v(B_C-1)]c_C E_C+n_v n_1 c_C E_C^{(1)},$$

$$S_{ABC}^{Rbcc}=[1-n_v n_1+n_v(B_A-1)](1-c_B-7c_C)S_A+n_v n_1(1-c_B-7c_C)S_A^{(1)}+[1-n_v n_1+n_v(B_B-1)]c_B S_B+n_v n_1 c_B S_B^{(1)}+$$
$$+2[1-n_v n_1+n_v(B_{A_1}-1)]c_C S_{A_1}+2n_v n_1 c_C S_{A_1}^{(1)}+4[1-n_v n_1+n_v(B_{A_2}-1)]c_C S_{A_2}+4n_v n_1 c_C S_{A_2}^{(1)}+$$
$$+[1-n_v n_1+n_v(B_C-1)]c_C S_C+n_v n_1 c_C S_C^{(1)},$$

$$S_{ABC}^{Rfcc}=[1-n_v n_1+n_v(B_A-1)](1-c_B-15c_C)S_A+n_v n_1(1-c_B-15c_C)S_A^{(1)}+[1-n_v n_1+n_v(B_B-1)]c_B S_B+n_v n_1 c_B S_B^{(1)}+$$
$$+6[1-n_v n_1+n_v(B_{A_1}-1)]c_C S_{A_1}+6n_v n_1 c_C S_{A_1}^{(1)}+8[1-n_v n_1+n_v(B_{A_2}-1)]c_C S_{A_2}+8n_v n_1 c_C S_{A_2}^{(1)}+$$
$$+[1-n_v n_1+n_v(B_C-1)]c_C S_C+n_v n_1 c_C S_C^{(1)}, \tag{30}$$

$$T_{ABC}^{R\alpha-\beta}=\left|\frac{\Delta E_{ABC}^{R}+P\Delta V_{ABC}}{\Delta S_{ABC}^{R}}\right|=\left|\frac{E_{ABC}^{R\alpha}-E_{ABC}^{R\beta}+P\left(V_{ABC}^{\alpha}-V_{ABC}^{\beta}\right)}{S_{ABC}^{R\alpha}-S_{ABC}^{R\beta}}\right|. \tag{31}$$

When the concentration of interstitial atoms C is equal to zero, the theory of structural phase transition of substitutional alloy AB with interstitial atoms C becomes that of substitutional alloy AB. When the concentration of substitutional atoms B is equal to zero, the theory of structural phase transition of substitutional alloy AB with interstitial atoms C becomes that of interstitial alloy AC. When the concentrations of substitutional and interstitial atoms are equal to zero, the theory of structural phase transition of substitutional alloy AB with interstitial atoms C becomes that of main metal A.

3. Conclusions

The analytic expressions of the alloy parameters, the mean nearest neighbour distance between two atoms, the Helmholtz free energy, the Gibbs thermodynamic potential, the energy and entropy for bcc, fcc and hcp phases of substitutional alloy AB with interstitial atoms C and the structural phase transition temperatures of these alloys at zero pressure and under pressure are derived by the statistical moment method. The structural phase transition temperature of substitutional alloy AB, interstitial alloy AC and main metal A are special cases of that of substitutional alloy AB with interstitial atoms C. In next paper, we will carry out numertical calculations for some real ternary ABC.

REFERENCES

[1] B. R. Cuenya, M.Doi, S.Löbus, R.Courths and W.Keune, 2001. *Observation of the fcc-to-bcc Bain transformation in epitaxial Fe ultrathin films on Cu_3Au (001)*. Surface science **493**(1-3), 338-360.

[2] B.Wang and H.M.Urbassek, 2014. *Atomistic dynamics of the bcc↔fcc phase transition in iron: Competition of homo-and heterogeneous phase growth.* Computational Materials Science **81**C, 170-177.

[3] X.Ou, 2017. *Molecular dynamics simulations of fcc-to-bcc transformation in pure iron: a review*. Materials Science and Technology **33**(7), 822-835.

[4] V.V.Hung and D.T.Hai, 2013. *Melting curve of metals with defect: Pressure dependence.* Computational Materials Science **79**, 789-794.

[5] M.N.Magomedov, 2017. *Change in the lattice properties and melting temperature of a face-centered cubic iron under compression.* Technical Physics **62**(4), 569-576.

[6] H.M.Strong, R.E.Tuft and R.E.Hanneman, 1973. *The iron fusion curve and γ-δ-l triple point*. Metallurgical Transactions **4**(11), 2657-2661.

[7] F.P.Bundy, 1965. *Pressure-temperature phase diagram of iron to 200 kbar and 900^oC*. Journal of Applied Physics **36**(2), 616-620.

[8] N.V.Kotenok, 1972. *Vestnik MU*, Ser. Fiz. Astrono. No.1, p.40.

[9] N.Q.Hoc, D.D.Thand and N.Tang, 1996. *Communications in Physics* **6**, 4, pp.1-8

[10] D.T.Hai, 2015. PhD Thesis, HNUE.

[11] N. Tang, V. V. Hung, 1989, 1990, 1990, 1990. Phys. Stat. Sol. (b)**149,** 511; **161,** 165; **162,** 371; **162,** 379.

[12] V. V. Hung, 2009. *Statistical moment method in studying thwermodynamic and elastic property of crystal*. HNUE Publishing House.

[13] N. Q. Hoc, D. Q. Vinh, B. D. Tinh, T. T. C. Loan, N. L. Phuong, T. T. Hue, D. T. T. Thuy, 2015. Journal of Science of HNUE, Math. and Phys. Sci. Vol. 60, Number 7, p. 146.