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BUILD THEORY OF NONLINEAR DEFORMATION FOR BCC AND FCC SUBSTITUTIONAL ALLOYS AB WITH INTERSTITIAL ATOM C UNDER PRESSURE

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Abstract. Analytic expressions of characteristic nonlinear deformation quantities such as the density of deformation energy, the maximum real stress and the limit of elastic deformation for bcc and fcc substitutional alloys AB with interstitial atom C under pressure are derived by the statistical moment method. The nonlinear deformations of the main metal A, the substitutional alloy AB and the interstitial alloy AC are special cases for nonlinear deformation of substitutional alloy AB with interstitial atom C and the same structure.

Keywords: Interstitial and substitutional alloy, binary and ternary alloys, nonlinear deformation, density of deformation energy, maximum real stress, limit of elastic deformation, statistical moment method.

1. Introduction

Thermodynamic and elastic properties of metals and interstitial alloys are specially interested by many theoretical and experimental researchers [1-14]. For example in [1], strengthening effects interstitial carbon solute atoms in (i.e., ferritic of bcc) Fe-C alloys are understood, owning chiefly to the interaction of C with crystalline defects (e.g. dislocations and grain boundaries) to resist plastic deformation via dislocation glide. High-strength steels developed in current energy and infrastructure applications include alloys where in the bcc Fe matrix is thermodynamically supersaturated in carbon. In [2], structural, elastic and thermal properties of cementite (Fe_3C) were studied using a Modified Embedded Atom Method (MEAM) potential for iron-carbon (Fe-C) alloys. The predictions of this potential are in good agreement with first-principle calculations and experiments. In [3], the thermodynamic properties of binary interstitial alloys with bcc structure are considered by the statistical moment method (SMM).

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The analytic expressions of the elastic moduli for anharmonic fcc and bcc crystals are also obtained by the SMM and the numerical calculation results are carried out for metals Al, Ag, Fe, W and Nb in [4].

In this paper, we build the theory of nonlinear deformation for bcc and fcc substitutional alloys AB with interstitial atom C by the SMM [3, 4, 15, 16].

2. Content

In the case of interstitial alloy AC with bcc structure (where the main atoms A stay in body center and peaks, the interstitial atom C stays in face centers of cubic unit cell), the cohesive energy of the atom C(in face centers of cubic unit cell) with the atoms A (in body center and peaks of cubic unit cell) and the alloy's parameters in the approximation of three coordination spheres with the center C and the radii $r_1^{bcc}, r_1^{bcc}\sqrt{2}, r_1^{bcc}\sqrt{5}$ are determined by [3, 15]

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

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

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

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

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

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

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

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 *i*th atom in the direction β.

The cohesive energy of the atom A_1 (which contains the interstitial atom C on the first coordination sphere) with the atoms in crystalline lattice and the corresponding alloy's parameters in the approximation of three coordination spheres with the center A_1 is determined by [3, 15].

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

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

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

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

where $r_{1A_1}^{bcc} \approx r_{1C}^{bcc}$ is the nearest neighbor distance between atom A_1 and atoms in crystalline lattice.

The cohesive energy of the atom A_2 (which contains the interstitial atom C on the first coordination sphere) with the atoms in crystalline lattice and the corresponding alloy's parameters in the approximation of three coordination spheres with the center A_2 is determined by [3, 15]

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

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

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

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

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

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

where $r_{1A_2}^{bcc} = r_{01A_2}^{bcc} + y_{0C}^{bcc}(T), r_{01A_2}^{bcc}$ is the nearest neighbor distance between the 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 [3, 15, 16].

In the action of rather large external force F, the alloy transfers to the process of nonlinear deformation. When the bcc interstititial alloy AC is deformed, the nearest neighbour distance $r_{1X}^{bccF}(\mathrm{X} = \mathrm{A}, \mathrm{A}_1, \mathrm{A}_2, \mathrm{C})$ at temperature T has the form

$$r_{1X}^{bccF} \approx r_{1X}^{bcc} + r_{01X}^{bcc}\varepsilon + r_{01X}^{bcc}\varepsilon(1+\varepsilon) = r_{1X}^{bcc} + r_{01X}^{bcc}\varepsilon(2+\varepsilon), \tag{5}$$

where $\varepsilon = \dfrac{E}{\sigma}$ (σ is the stress and *E* is the Young modulus), $r_{1X}^{bcc} = r_{1X}^{bcc}(P,T)$ is the nearest neighbour distance in bcc alloy before deformation. When the alloy is deformed, the mean nearest neighbour distance r_{01X}^{bccF} at 0K has the form

$$r_{01X}^{bccF} = r_{01X}^{bcc}(1+\varepsilon). \tag{6}$$

The equation of state for bcc interstitial alloy AC at temperature *T* and pressure *P* is written in the form [3]

$$Pv^{bcc} = -r_1^{bcc}\left(\frac{1}{6}\frac{\partial u_0^{bcc}}{\partial r_1^{bcc}} + \theta x^{bcc} cthx^{bcc}\frac{1}{2k^{bcc}}\frac{\partial k^{bcc}}{\partial r_1^{bcc}}\right), v^{bcc} = \frac{4\left(r_1^{bcc}\right)^3}{3\sqrt{3}}. \tag{7}$$

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

$$Pv^{bcc} = -r_1^{bcc}\left(\frac{1}{6}\frac{\partial u_0^{bcc}}{\partial r_1^{bcc}} + \frac{\hbar\omega_0^{bcc}}{4k^{bcc}}\frac{\partial k^{bcc}}{\partial r_1^{bcc}}\right). \tag{8}$$

If we know the interaction potential φ_{i0}, the equation (8) 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.After finding $r_{1X}^{bcc}(P,0)$, we can determine

$$r_{1X}^{bccF}(P,0) = r_{1X}^{bcc}(P,0)\left(1 + 2\varepsilon + \varepsilon^2\right) \tag{9}$$

and then determine the parameters $k_X^{bccF}(P,0), \gamma_{1X}^{bccF}(P,0), \gamma_{2X}^{bccF}(P,0), \gamma_X^{bccF}(P,0)$ at pressure *P*and 0K for each case of X when alloy is deformed. Then, the displacement $y_{0X}^{bccF}(P,T)$ of atom X from the equilibrium position at temperature *T* and pressure *P* is calculated a in [3, 15].

When alloy is deformed, the nearest neighbour distance $r_{1X}^{bccF}(P,T)$ is determined by [3]

$$r_{1C}^{bccF}(P,T) = r_{1C}^{bccF}(P,0) + y_{A_1}^{bccF}(P,T), r_{1A}^{bccF}(P,T) = r_{1A}^{bccF}(P,0) + y_A^{bccF}(P,T),$$
$$r_{1A_1}^{bccF}(P,T) \approx r_{1C}^{bccF}(P,T), r_{1A_2}^{bccF}(P,T) = r_{1A_2}^{bccF}(P,0) + y_C^{bccF}(P,T). \tag{10}$$

When alloy is deformed, the mean nearest neighbour distance $\overline{r_{1A}^{bccACF}(P,T)}$ has the form [3]

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

$$\overline{r_{1A}^{bccACF}(P,0)} = \left[(1-c_C)r_{1A}^{bccF}(P,0) + c_C r_{1A}'^{bccACF}(P,0)\right]\left(1+2\varepsilon+\varepsilon^2\right), r_{1A}'^{bccF}(P,0) = \sqrt{3}r_{1C}^{bccF}(P,0),$$

$$\overline{y^{bccACF}(P,T)} = (1-7c_C)y_A^{bccF}(P,T) + c_C y_C^{bccF}(P,T) + 2c_C y_{A_1}^{bccF}(P,T) + 4c_C y_{A_2}^{bccF}(P,T), \quad (11)$$

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

In the case of fcc interstitial alloy AC (where the main atom A_1 stay in face centers, themain 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 [3, 15]

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

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

$$+ 4\varphi_{AC}^{(2)}\left(r_1^{fcc}\sqrt{5}\right) + \frac{8\sqrt{5}}{5r_1^{fcc}}\varphi_{AC}^{(1)}\left(r_1^{fcc}\sqrt{5}\right), \gamma_C^{fcc} = 4\left(\gamma_{1C}^{fcc} + \gamma_{2C}^{fcc}\right),$$

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

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

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

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

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

$$+\frac{4}{25}\varphi_{AC}^{(4)}\left(r_1^{fcc}\sqrt{5}\right)+\frac{26\sqrt{5}}{125r_1^{fcc}}\varphi_{AC}^{(3)}\left(r_1^{fcc}\sqrt{5}\right)-\frac{3}{25\left(r_1^{bcc}\right)^2}\varphi_{AC}^{(2)}\left(r_1^{bcc}\sqrt{5}\right)+\frac{3\sqrt{5}}{125\left(r_1^{bcc}\right)^3}\varphi_{AC}^{(1)}\left(r_1^{bcc}\sqrt{5}\right), \quad (13)$$

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

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

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

$$\gamma_{2A_1}^{fcc}=\gamma_{2A}^{fcc}+\frac{6}{48}\sum_i\left[\left(\frac{\partial^4\varphi_{AC}}{\partial u_{i\alpha}^2\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_1}^{fcc}}=\gamma_{2A}^{fcc}+\frac{1}{4r_{1A_1}^{fcc}}\varphi_{AC}^{(3)}\left(r_{1A_1}^{fcc}\right)-\frac{1}{2\left(r_{1A_1}^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_1}^{fcc}\right)+\frac{1}{2\left(r_{1A_1}^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_1}^{fcc}\right), \quad (14)$$

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

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

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

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

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

$$+\frac{14}{27\left(r_{1A_2}^{fcc}\right)^2}\varphi_{AC}^{(2)}\left(r_{1A_2}^{fcc}\right)-\frac{14}{27\left(r_{1A_2}^{fcc}\right)^3}\varphi_{AC}^{(1)}\left(r_{1A_2}^{fcc}\right), \quad (15)$$

$$r_{1X}^{fccF}\approx r_{1X}^{fcc}+r_{01X}^{fcc}\varepsilon+r_{01X}^{fcc}\varepsilon(1+\varepsilon)=r_{1X}^{fcc}+r_{01X}^{fcc}\varepsilon(2+\varepsilon), \quad (16)$$

$$r_{01X}^{fccF}=r_{01X}^{fcc}(1+\varepsilon), \quad (17)$$

$$Pv^{fcc}=-r_1^{fcc}\left(\frac{1}{6}\frac{\partial u_0^{fcc}}{\partial r_1^{bcc}}+\theta x^{fcc}cthx^{fcc}\frac{1}{2k^{fcc}}\frac{\partial k^{fcc}}{\partial r_1^{fcc}}\right),v^{fcc}=\frac{\sqrt{2}\left(r_1^{fcc}\right)^3}{2}, \quad (18)$$

$$Pv^{fcc}=-r_1^{fcc}\left(\frac{1}{6}\frac{\partial u_0^{fcc}}{\partial r_1^{fcc}}+\frac{\hbar\omega_0^{fcc}}{4k^{fcc}}\frac{\partial k^{fcc}}{\partial r_1^{fcc}}\right), \quad (19)$$

$$r_{1X}^{fccF}(P,0)=r_{1X}^{fcc}(P,0)\left(1+2\varepsilon+\varepsilon^2\right), \tag{20}$$

$$r_{1C}^{fccF}(P,T)=r_{1C}^{fccF}(P,0)+y_{A_1}^{bccF}(P,T), r_{1A}^{fccF}(P,T)=r_{1A}^{fccF}(P,0)+y_{A}^{fccF}(P,T),$$

$$r_{1A_1}^{fccF}(P,T)\approx\sqrt{2}r_{1C}^{fccF}(P,T), r_{1A_2}^{fccF}(P,T)=r_{1A_2}^{fccF}(P,0)+y_{C}^{fccF}(P,T), \tag{21}$$

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

$$\overline{r_{1A}^{fccACF}(P,0)}=\left[(1-c_C)r_{1A}^{fccF}(P,0)+c_C r_{1A}'^{fccACF}(P,0)\right]\left(1+2\varepsilon+\varepsilon^2\right), r_{1A}'^{fccF}(P,0)=\sqrt{2}r_{1C}^{fccF}(P,0),$$

$$\overline{y^{fccACF}(P,T)}=(1-15c_C)y_{A}^{fccF}(P,T)+c_C y_{C}^{fccF}(P,T)+6c_C y_{A_1}^{fccF}(P,T)+8c_C y_{A_2}^{fccF}(P,T). \tag{22}$$

The mean nearest neighbor distance between two atoms A in the deformed bcc substitutional alloy AB with interstitial atom C at pressure P and temperature T is determined by [3, 15].

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

$$a_{ABC}^{bccF}\equiv\overline{r_{1A}^{bccABCF}(P,T)}, a_{AC}^{bccF}\equiv\overline{r_{1A}^{bccACF}(P,T)}, a_B^{bccF}\equiv r_{1B}^{bccF}(P,T),$$

$$B_{TAC}^{bccF}=\frac{1}{\chi_{TAC}^{bccF}}=\frac{2P+\frac{3\sqrt{3}}{4a_{AC}^{bccF}}\frac{1}{3N}\left(\frac{\partial^2\psi_{AC}^{bccF}}{\partial a_{AC}^{bccF2}}\right)_T}{3\left(\frac{a_{AC}^{bccF}}{a_{0AC}^{bccF}}\right)^3}, B_{TB}^{bccF}=\frac{1}{\chi_{TB}^{bccF}}=\frac{2P+\frac{3\sqrt{3}}{4a_{B}^{bccF}}\frac{1}{3N}\left(\frac{\partial^2\psi_{B}^{bccF}}{\partial a_{B}^{bccF2}}\right)_T}{3\left(\frac{a_{B}^{bccF}}{a_{0B}^{bccF}}\right)^3},$$

$$\left(\frac{\partial^2\psi_{AC}^{bccF}}{\partial a_{AC}^{bccF2}}\right)_T\approx(1-7c_C)\left(\frac{\partial^2\psi_{A}^{bccF}}{\partial a_{A}^{bccF2}}\right)_T+c_C\left(\frac{\partial^2\psi_{C}^{bccF}}{\partial a_{C}^{bccF2}}\right)_T+2c_C\left(\frac{\partial^2\psi_{A_1}^{bccF}}{\partial a_{A_1}^{bccF2}}\right)_T+4c_C\left(\frac{\partial^2\psi_{A_2}^{bccF}}{\partial a_{A_2}^{bccF2}}\right)_T,$$

$$\frac{1}{3N}\left(\frac{\partial^2\psi_{X}^{bccF}}{\partial a_{X}^{bccF2}}\right)_T=\frac{1}{6}\frac{\partial^2 u_{0X}^{bccF}}{\partial a_{X}^{bccF2}}+\frac{\hbar\omega_X^{bccF}}{4k_X^{bccF}}\left[\frac{\partial^2 k_X^{bccF}}{\partial a_X^{bccF2}}-\frac{1}{2k_X^{bccF}}\left(\frac{\partial k_X^{bccF}}{\partial a_X^{bccF}}\right)^2\right], X=A,A_1,A_2,B,C. \tag{23}$$

The mean nearest neighbor distance between atoms A in the deformed bcc substitutional alloy AB with interstitial atom C at pressure P and temperature T = 0K is determined by

$$a_{0ABC}^{bccF}=c_{AC}a_{0AC}^{bccF}\frac{B_{0TAC}^{bccF}}{B_{0T}^{bccF}}+c_B a_{0B}^{bccF}\frac{B_{0TB}^{bccF}}{B_{0T}^{bccF}}, \overline{B_{0T}^{bccF}}=c_{AC}B_{0TAC}^{bccF}+c_B B_{0TB}^{bccF},$$

$$a_{0ABC}^{bccF}\equiv\overline{r_{1A}^{bccABCF}(P,0)}, a_{0AC}^{bccF}\equiv\overline{r_{1A}^{bccACF}(P,0)}, a_{0B}^{bccF}\equiv r_{1B}^{bcc}(P,0). \tag{24}$$

The Helmholtz free energy of bcc substitutional alloy AB with interstitial atom C before deformation with the condition $c_C << c_B << c_A$ has the form [3]

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

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

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

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

$$\psi_{0X}^{bcc} = 3N\theta\left[x_X^{bcc} + \ln\left(1-e^{-2x_X^{bcc}}\right)\right], Y_X^{bcc} \equiv x_X^{bcc}\coth x_X^{bcc}, \quad (25)$$

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

In the case of fcc interstitial alloy AC, the corresponding formulas are as follows [3, 15]:

$$a_{ABC}^{fccF} = c_{AC}a_{AC}^{fccF}\frac{B_{TAC}^{fccF}}{\overline{B_T^{fccF}}} + c_Ba_B^{fccF}\frac{B_{TB}^{fccF}}{\overline{B_T^{fccF}}}, \overline{B_T^{bccF}} = c_{AC}B_{TAC}^{fccF} + c_BB_{TB}^{fccF}, c_{AC} = c_A + c_C,$$

$$a_{ABC}^{fccF} \equiv \overline{r_{1A}^{fccABCF}(P,T)}, a_{AC}^{fccF} \equiv \overline{r_{1A}^{fccACF}(P,T)}, a_B^{fccF} \equiv r_{1B}^{fccF}(P,T),$$

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

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

$$\frac{1}{3N}\left(\frac{\partial^2\psi_X^{fccF}}{\partial a_X^{fccF\,2}}\right)_T = \frac{1}{6}\frac{\partial^2 u_{0X}^{fccF}}{\partial a_X^{fccF\,2}} + \frac{\hbar\omega_X^{fccF}}{4k_X^{fccF}}\left[\frac{\partial^2 k_X^{fccF}}{\partial a_X^{fccF\,2}} - \frac{1}{2k_X^{fccF}}\left(\frac{\partial k_X^{fccF}}{\partial a_X^{fccF}}\right)^2\right], X = A, A_1, A_2, B, C. \quad (26)$$

$$a_{0ABC}^{fccF} = c_{AC}a_{0AC}^{fccF}\frac{B_{0TAC}^{fccF}}{\overline{B_{0T}^{fccF}}} + c_Ba_{0B}^{fccF}\frac{B_{0TB}^{fccF}}{\overline{B_{0T}^{fccF}}}, \overline{B_{0T}^{fccF}} = c_{AC}B_{0TAC}^{fccF} + c_BB_{0TB}^{fccF},$$

$$a_{0ABC}^{fccF} \equiv \overline{r_{1A}^{fccABCF}(P,0)}, a_{0AC}^{fccF} \equiv \overline{r_{1A}^{fccACF}(P,0)}, a_{0B}^{fccF} \equiv r_{1B}^{fccF}(P,0). \quad (27)$$

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

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

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

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

$$\psi_{0X}^{fcc} = 3N\theta\left[x_X^{fcc} + \ln\left(1-e^{-2x_X^{fcc}}\right)\right], Y_X^{fcc} \equiv x_X^{fcc}\coth x_X^{fcc}. \quad (28)$$

When the process of nonlinear deformation in both fcc and bcc alloy happens, the relationship between the stress and the strain is decribed by

$$\sigma_{1ABC} = \sigma_{oABC}\frac{\varepsilon_F^{\alpha_{ABC}}}{1+\varepsilon_F}. \quad (29)$$

Here, σ_{oABC} and α_{ABC} are constant depending on every interstitial alloy. We can find the strain ε_F corresponding to the maximum value of the real stress through the density of deformation energy.

In order to determine the stress - strain dependence according to the above formula, it is necesary to determine two constants σ_{oABC} and α_{ABC} for every intestitial alloy. Therefore, we can calculate the density of deformation energy of substitutional alloy AB with interstitial atom C in the form

$$f_{ABC}(\varepsilon) = \frac{\Psi_{ABC}^F}{V_{ABC}^F} - \frac{\Psi_{ABC}}{V_{ABC}} = \frac{1}{N}\left(\frac{\Psi_{ABC}^F}{v_{ABC}^F} - \frac{\Psi_{ABC}}{v_{ABC}}\right) = \frac{1}{N}\left[c_A\left(\frac{\Psi_A^F}{v_{ABC}^F} - \frac{\Psi_A}{v_{ABC}}\right) + c_C\left(\frac{\Psi_A^F}{v_{ABC}^F} - \frac{\Psi_A}{v_{ABC}}\right) + \right.$$

$$\left. + c_{A_1}\left(\frac{\Psi_{A_1}^F}{v_{ABC}^F} - \frac{\Psi_{A_1}}{v_{ABC}}\right) + c_{A_2}\left(\frac{\Psi_{A_2}^F}{v_{ABC}^F} - \frac{\Psi_{A_2}}{v_{ABC}}\right) + c_B\left(\frac{\Psi_B^F}{v_{ABC}^F} - \frac{\Psi_B}{v_{ABC}}\right) - c_B\left(\frac{\Psi_A^F}{v_{ABC}^F} - \frac{\Psi_A}{v_{ABC}}\right)\right].$$

$$c_A = 1 - c_B - 7c_C, c_{A_1} = 2c_C, c_{A_2} = 4c_C \text{ for bcc alloy,}$$

$$c_A = 1 - c_B - 15c_C, c_{A_1} = 6c_C, c_{A_2} = 8c_C \text{ for fcc alloy.} \quad (30)$$

Since ε is very small (ε << 1), we can expand the expression of the Helmholtz free energy $\Psi_X^F(\mathrm{X} = \mathrm{A}, \mathrm{A}_1, \mathrm{A}_2, \mathrm{B}, \mathrm{C})$ in terms of the strain ε in the form of series and approximately,

$$\Psi_X^F(\varepsilon) = \Psi_X + \left(\frac{\partial\Psi_X^F}{\partial\varepsilon}\right)_T \varepsilon + \frac{1}{2}\left(\frac{\partial^2\Psi_X^F}{\partial\varepsilon^2}\right)_T \varepsilon^2. \quad (31)$$

Applying the following formulas:

$$\frac{\partial\Psi_X^F}{\partial\varepsilon} = \frac{\partial\Psi_X^F}{\partial r_{1X}^F}\frac{\partial r_{1X}^F}{\partial\varepsilon}, \frac{\partial^2\Psi_X^F}{\partial\varepsilon^2} = \frac{\partial}{\partial\varepsilon}\left(\frac{\partial\Psi_X^F}{\partial r_{1X}^F}\frac{\partial r_{1X}^F}{\partial\varepsilon}\right) = \frac{\partial^2\Psi_X^F}{\partial r_{1X}^{F2}}\left(\frac{\partial r_{1X}^F}{\partial\varepsilon}\right)^2 + \frac{\partial\Psi_X^F}{\partial r_{1X}^F}\frac{\partial^2 r_{1X}^F}{\partial\varepsilon^2}, \quad (32)$$

$$\frac{\partial r_{1X}^F}{\partial\varepsilon} = 2r_{01X}(1+\varepsilon) = 2r_{01X}^F, \frac{\partial^2 r_{1X}^F}{\partial\varepsilon^2} = 2r_{01X}. \quad (33)$$

Therefore,

$$f_{ABC}(\varepsilon)=\frac{1}{N}c_A\left\{\Psi_A\left(\frac{1}{v_{AB}^F}-\frac{1}{v_{AB}}\right)+\frac{2\varepsilon r_{01A}^F}{v_{AB}^F}\left(\frac{\partial\Psi_A^F}{\partial r_{1A}^F}\right)_T+\frac{\varepsilon^2}{2v_{AB}^F}\left[\left(\frac{\partial^2\Psi_A^F}{\partial r_{1A}^{F2}}\right)_T\left(2r_{01A}^F\right)^2+\left(\frac{\partial\Psi_A^F}{\partial r_{1A}^F}\right)_T 2r_{01A}^F\right]\right\}+$$

$$+\frac{c_C}{N}\left\{\Psi_B\left(\frac{1}{v_{AB}^F}-\frac{1}{v_{AB}}\right)+\frac{2\varepsilon r_{01B}^F}{v_{AB}^F}\left(\frac{\partial\Psi_B^F}{\partial r_{1B}^F}\right)_T+\frac{\varepsilon^2}{2v_{AB}^F}\left[\left(\frac{\partial^2\Psi_B^F}{\partial r_{1B}^{F2}}\right)_T\left(2r_{01B}^F\right)^2+\left(\frac{\partial\Psi_B^F}{\partial r_{1B}^F}\right)_T 2r_{01B}^F\right]\right\}+$$

$$+\frac{c_{A_1}}{N}\left\{\Psi_{A_1}\left(\frac{1}{v_{AB}^F}-\frac{1}{v_{AB}}\right)+\frac{2\varepsilon r_{01A_1}^F}{v_{AB}^F}\left(\frac{\partial\Psi_{A_1}^F}{\partial r_{1A_1}^F}\right)_T+\frac{\varepsilon^2}{2v_{AB}^F}\left[\left(\frac{\partial^2\Psi_{A_1}^F}{\partial r_{1A_1}^{F2}}\right)_T\left(2r_{01A_1}^F\right)^2+\left(\frac{\partial\Psi_{A_1}^F}{\partial r_{1A_1}^F}\right)_T 2r_{01A_1}^F\right]\right\}+$$

$$+\frac{c_{A_2}}{N}\left\{\Psi_{A_2}\left(\frac{1}{v_{AB}^F}-\frac{1}{v_{AB}}\right)+\frac{2\varepsilon r_{01A_2}^F}{v_{AB}^F}\left(\frac{\partial\Psi_{A_2}^F}{\partial r_{1A_2}^F}\right)_T+\frac{\varepsilon^2}{2v_{AB}^F}\left[\left(\frac{\partial^2\Psi_{A_2}^F}{\partial r_{1A_2}^{F2}}\right)_T\left(2r_{01A_2}^F\right)^2+\left(\frac{\partial\Psi_{A_2}^F}{\partial r_{1A_2}^F}\right)_T 2r_{01A_2}^F\right]\right\}+$$

$$+\frac{c_B}{N}\left\{\Psi_B\left(\frac{1}{v_{AB}^F}-\frac{1}{v_{AB}}\right)+\frac{2\varepsilon r_{01B}^F}{v_{AB}^F}\left(\frac{\partial\Psi_B^F}{\partial r_{1B}^F}\right)_T+\frac{\varepsilon^2}{2v_{AB}^F}\left[\left(\frac{\partial^2\Psi_B^F}{\partial r_{1B}^{F2}}\right)_T\left(2r_{01B}^F\right)^2+\left(\frac{\partial\Psi_B^F}{\partial r_{1B}^F}\right)_T 2r_{01B}^F\right]\right\}-$$

$$-\frac{c_B}{N}\left\{\Psi_A\left(\frac{1}{v_{AB}^F}-\frac{1}{v_{AB}}\right)+\frac{2\varepsilon r_{01A}^F}{v_{AB}^F}\left(\frac{\partial\Psi_A^F}{\partial r_{1A}^F}\right)_T+\frac{\varepsilon^2}{2v_{AB}^F}\left[\left(\frac{\partial^2\Psi_A^F}{\partial r_{1A}^{F2}}\right)_T\left(2r_{01A}^F\right)^2+\left(\frac{\partial\Psi_A^F}{\partial r_{1A}^F}\right)_T 2r_{01A}^F\right]\right\}. \quad (34)$$

Similar to metal when the deformation rate is constant, the density of deformation energy of alloy has the form

$$f_{ABC}(\varepsilon) = C_{ABC}.\sigma_{ABC}.\varepsilon, \quad (35)$$

where C_{ABC} is a proportional factor.

The function $f_{ABC}(\varepsilon)$ gets its maximum at the strain ε_{ABC}^F. This means that

$$f_{ABC}\left(\varepsilon_{ABC}^F\right)= f_{ABC\max} = C_{ABC}\sigma_{ABC\max}\varepsilon_{ABC}^F. \quad (36)$$

then, we can find the maximum stress $\sigma_{ABC\max}$ and the maximum real stress $\sigma_{1ABC\max}$

$$\sigma_{ABC\max} = \frac{f_{ABC\max}}{C_{ABC}\varepsilon_{ABC}^F}, \sigma_{1ABC\max} = \frac{\sigma_{ABC\max}}{1+\varepsilon_{ABC}^F} = \frac{f_{ABC\max}}{C_{ABC}\varepsilon_{ABC}^F\left(1+\varepsilon_{ABC}^F\right)}. \quad (37)$$

From the maximum condition of stress $\left(\frac{\partial\sigma_{1ABC}}{\partial\varepsilon}\right)_{\varepsilon_{ABC}^F} = 0$, we determine the strain ε_{ABC}^F corresponding to the maximum value of the real stress as follows:

$$\varepsilon_{ABC}^F = \frac{\alpha_{ABC}}{1-\alpha_{ABC}} \Rightarrow \sigma_{1ABC\max} = \sigma_{0ABC}\frac{\left(\varepsilon_{ABC}^F\right)^{\alpha_{ABC}}}{1+\varepsilon_{ABC}^F}. \quad (38)$$

The proportional factor C_{ABC} is determined from the experimental condition of the stress $\sigma_{0,2ABC}$ in alloy in the form

$$C_{ABC} = \frac{f_{ABC}\left(\varepsilon_{0.2}\right)}{\sigma_{0.2ABC}\varepsilon_{0.2}}. \quad (39)$$

In substitutional alloy AB with interstitial atom C, if the concentration c_C of interstitial atoms is equal to zero, we obtain the expression of the density of deformation energy for substitutional alloy AB. In substitutional alloy AB with interstitial atom C,

if the concentration c_B of substitutional atoms is equal to zero, we obtain the expression of the density of deformation energy for interstitial alloy AC. In substitutional alloy AB with interstitial atom C, if both concentrations c_B and c_C are equal to zero, we obtain the expression of the density of deformation energy for main metal A.

After having the value of the strain ε_{ABC}^{F} corresponding to the maximum value of the density of deformation energy, we can find the expression to describe the relationship between the stress and the strain in the process of nonlinear deformation of bcc and fcc substitutional alloys AB with interstitial atom C

3. Conclusions

The analytic expressions of the Helmholtz free energy, the mean nearest neighbor distance and the characteristic nonlinear deformation quantities such as the density of deformation energy, the maximum real stress and the limit of elastic deformation for bcc and fcc substitutional alloys AB with interstitial atom C under pressure are derived from the statistical moment method. From that, we obtain the theory of nonlinear deformation for binary substitutional alloy, binary interstitial alloy and main metal. We will carry out the numerical calculations for real alloys in next paper.

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