Study on elastic deformation of substitution alloy AB with interstitial atom C and BCC structure under pressure

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Abstract. The analytic expressions of the free energy, the mean nearest neighbor distance between two atoms, the elastic moduli such as the Young modulus E, the bulk modulus K, the rigidity modulus G and the elastic constants C₁₁, C₁₂, C₄₄ for substitution alloy AB with interstitial atom C and BCC structure under pressure are derived from the statistical moment method. The elastic deformations of main metal A, substitution alloy AB and interstitial alloy AC are special cases of elastic deformation for alloy ABC. The theoretical results are applied to alloy FeCrSi. The numerical results for alloy FeCrSi are compared with the numerical results for main metal Fe, substitution alloy FeCr, interstitial alloy FeSi and experiments.

1. Introduction
Thermodynamic and elastic properties of interstitial alloys are specially interested by many theoretical and experimental researchers [1, 2, 5, 7-18].

The binary FeCr system is the basis for a large class of important engineering materials known as stainless steels. Stainless steels combine good corrosion resistance with attractive mechanical properties. Some other features of the FeCr alloys are also of interest, such as spin glass formation, sluggish formation of the σ phase and strong swelling resistance in an irradiative environment [11].

Iron silicides have attracted a lot of attention in recent decades, due to their unusual physical properties and functional applications [12]. The distribution of the Si-atoms in alloy FeCrSi is discussed in comparison with some common transition metal silicide structures [18].

In this paper, we build the theory of elastic deformation for substitution alloy AB with interstitial atom C and body-centered cubic (BCC) structure under pressure by the statistical moment method (SMM) [3-5].

2. Content of research
2.1. Analytic results
2.1.1. Mean nearest neighbor distance between two atoms in alloy In interstitial alloy AC with BCC structure, 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) in the approximation of three coordination spheres with the center C and the radii r₁, r₁√2, r₁√5 is determined by [3-5]
\[ u_{0C} = \frac{1}{2} \sum_{i=1}^{n_i} \varphi_{AC} (r_i) = \frac{1}{2} \left[ 2 \varphi_{AC} (r_1) + 4 \varphi_{AC} (r_1 \sqrt{2}) + 8 \varphi_{AC} (r_1 \sqrt{5}) \right] = \varphi_{AC} (r_1) + 2 \varphi_{AC} (r_1 \sqrt{2}) + 4 \varphi_{AC} (r_1 \sqrt{5}). \]

(1)

where \( \varphi_{AC} \) is the interaction potential between the atom A and the atom C, \( n_i \) is the number of atoms on the \( i \)th coordination sphere with the radius \( r_i \), \( i = 1, 2, 3 \), \( r_1 = r_{01C} + y_{0A1} (T) \) is the nearest neighbor distance between the interstitial atom C and the metallic atom A at temperature \( T \), \( r_{01C} \) 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 \( u_{0C} \), \( y_{0A1} (T) \) is the displacement of the atom \( A_1 \) (the atom A stays in the body center of cubic unit cell) from equilibrium position at temperature \( T \). The alloy’s parameters for the atom C in the approximation of three coordination spheres have the form [3-5]

\[
\begin{align*}
\kappa_C &= \frac{1}{2} \sum_i \left( \frac{\partial^2 \varphi_{AC}}{\partial u_{i\beta}^2} \right)_{eq} = \varphi^{(2)}_{AC} (r_1) + \frac{\sqrt{2}}{r_1} \varphi^{(1)}_{AC} (r_1 \sqrt{2}) + \frac{16}{5 \sqrt{5} r_1^5} \varphi^{(1)}_{AC} (r_1 \sqrt{5}), \\
\gamma_C &= 4 (\gamma_{1C} + \gamma_{2C}), \\
\gamma_{1C} &= \frac{1}{48} \sum_i \left( \frac{\partial^4 \varphi_{AC}}{\partial u_{i\alpha}^2 \partial u_{i\beta}^2} \right)_{eq} = \frac{1}{24} \varphi^{(4)}_{AC} (r_1) + \frac{1}{8 r_1^4} \varphi^{(2)}_{AC} (r_1 \sqrt{2}) - \frac{\sqrt{2}}{16 r_1^3} \varphi^{(1)}_{AC} (r_1), \\
&+ \frac{1}{150} \varphi^{(4)}_{AC} (r_1 \sqrt{2}) + \frac{4 \sqrt{3}}{125 r_1^5} \varphi^{(3)}_{AC} (r_1 \sqrt{5}), \\
\gamma_{2C} &= \frac{6}{48} \sum_i \left( \frac{\partial^4 \varphi_{AC}}{\partial u_{i\alpha}^2 \partial u_{i\beta}^2} \right)_{eq} = \frac{1}{4 r_1^4} \varphi^{(3)}_{AC} (r_1) - \frac{1}{4 r_1^4} \varphi^{(2)}_{AC} (r_1) + \frac{5}{8 r_1^3} \varphi^{(1)}_{AC} (r_1), \\
&+ \frac{\sqrt{2}}{8 r_1^4} \varphi^{(3)}_{AC} (r_1 \sqrt{2}) - \frac{1}{8 r_1^4} \varphi^{(2)}_{AC} (r_{01C} \sqrt{2}) + \frac{2}{25} \varphi^{(4)}_{AC} (r_1 \sqrt{5}) \\
&+ \frac{3}{25 r_1 \sqrt{5}} \varphi^{(3)}_{AC} (r_1 \sqrt{5}) + \frac{2}{25 r_1^2} \varphi^{(2)}_{AC} (r_1 \sqrt{5}) - \frac{3}{25 r_1 \sqrt{3}} \varphi^{(1)}_{AC} (r_1 \sqrt{5}). \\
\end{align*}
\]

(2)

where \( \varphi^{(i)}_{AC} (r_i) = \frac{\partial^i \varphi_{AC} (r_i)}{\partial u_{i\alpha}^i} (i = 1, 2, 3, 4), \alpha, \beta = x, y, z, \alpha \neq \beta \) and \( u_{i\beta} \) is the displacement of the \( i \)th atom in the direction \( \beta \).

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 [3-5]

\[
\begin{align*}
\epsilon_{0A} &= u_{0A} + \varphi_{AC} (r_{1A_1}), \\
\kappa_{A_1} &= \kappa_A + \frac{1}{2} \sum_i \left[ \left( \frac{\partial^2 \varphi_{AC}}{\partial u_{i\beta}^2} \right)_{eq} \right]_{r=r_{1A_1}} = \kappa_A + \varphi^{(2)}_{AC} (r_{1A_1}) + \frac{5}{2 r_{1A_1}^4} \varphi^{(1)}_{AC} (r_{1A_1}), \\
\gamma_{A_1} &= 4 (\gamma_{1A_1} + \gamma_{2A_1}), \\
\gamma_{1A_1} &= \gamma_{1A} + \frac{1}{48} \sum_i \left[ \left( \frac{\partial^4 \varphi_{AC}}{\partial u_{i\alpha}^2 \partial u_{i\beta}^2} \right)_{eq} \right]_{r=r_{1A_1}},
\end{align*}
\]
energy $u$ atoms in crystalline lattice at 0K and is determined from the minimum condition of the cohesive
neighbor distance $P$

If knowing the form of interaction potential by $[3-5]$ $A$
parameters in the approximation of three coordination spheres with the center $P$

The equation of state for interstitial alloy AC with BCC structure at temperature $T$

$$\gamma_{2A} = \gamma_{2A} + \frac{6}{48} \sum_i \left[ \left( \frac{\partial^4 \varphi_{AC}}{\partial u_{\alpha} \partial u_{\beta}^2} \right)_{eq} \right]_{r=r_{1A1}}$$
$$= \gamma_{2A} + \frac{1}{2 r_{1A1}} \varphi_{AC}^{(3)}(r_{1A1}) - \frac{3}{4 r^2_{1A1}} \varphi_{AC}^{(2)}(r_{1A1}) + \frac{3}{8 r^3_{1A1}} \varphi_{AC}^{(1)}(r_{1A1})$$ (3)

where $r_{1A1} \approx r_{1C}$ is the nearest neighbor distance between the 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 alloys parameters in the approximation of three coordination spheres with the center $A_2$ is determined by $[3-5]$

$$u_{0A_2} = u_{0A} + \varphi_{AC}(r_{1A_2})$$,
$$k_{A_2} = k_A + \frac{1}{2} \sum_i \left[ \left( \frac{\partial^2 \varphi_{AC}}{\partial u_{\alpha}^2} \right)_{eq} \right]_{r=r_{1A_2}}$$
$$= k_A + \frac{1}{2} \gamma_{2A} + 2 \varphi_{AC}^{(2)}(r_{1A_2}) + \frac{4}{r_{1A_2}} \varphi_{AC}^{(1)}(r_{1A_2})$$,
$$\gamma_{A_2} = 4 \gamma_{1A_2} + \gamma_{2A_2} \gamma_{1A_2} + \frac{1}{48} \sum_i \left[ \left( \frac{\partial^4 \varphi_{AC}}{\partial u_{\alpha} \partial u_{\beta}^2} \right)_{eq} \right]_{r=r_{1A_2}}$$
$$= \gamma_{1A} + \frac{1}{24} \varphi_{AC}^{(4)}(r_{1A_2}) + \frac{1}{4 r_{1A_2}} \varphi_{AC}^{(3)}(r_{1A_2}) - \frac{1}{8 r^2_{1A_2}} \varphi_{AC}^{(2)}(r_{1A_2}) + \frac{1}{8 r^3_{1A_2}} \varphi_{AC}^{(1)}(r_{1A_2})$$,
$$\gamma_{2A_1} = \gamma_{2A} + \frac{6}{48} \sum_i \left[ \left( \frac{\partial^4 \varphi_{AC}}{\partial u_{\alpha} \partial u_{\beta}^2} \right)_{eq} \right]_{r=r_{1A_1}}$$
$$= \gamma_{2A} + \frac{1}{8} \varphi_{AC}^{(4)}(r_{1A_2}) + \frac{1}{4 r_{1A_2}} \varphi_{AC}^{(3)}(r_{1A_2}) + \frac{3}{8 r^2_{1A_2}} \varphi_{AC}^{(2)}(r_{1A_2}) - \frac{3}{8 r^3_{1A_2}} \varphi_{AC}^{(1)}(r_{1A_2})$$ (4)

where $r_{1A1} = r_{01A1} + y_0 C(T)$, $r_{01A1}$ 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 $u_{0A_2}$, $y_0 C(T)$ is the displacement of the atom $C$ at temperature $T$.

In Eqs. (3) and (4), $u_{0A}$, $k_A$, $\gamma_{1A}$, $\gamma_{2A}$ are the corresponding quantities in clean metal $A$ in the approximation of two coordination sphere $[3-5]$.

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

$$Pv = -r_1 \left( \frac{1}{6} \frac{\partial u_0}{\partial r_1} + \theta_0 c h x \frac{1}{2 k} \frac{\partial k}{\partial r_1} \right)$$ (5)

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

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

If knowing the form of interaction potential $\phi_0$, eq. (6) permits us to determine the nearest neighbor distance $r_{1X}(P, 0)$ ($X = C, A, A_1, A_2$) at 0K and pressure $P$. After knowing $r_{1X}(P, 0)$,
we can determine alloy parameters $k_X(P,0)$, $\gamma_{1X}(P,0)$, $\gamma_{2X}(P,0)$, $\gamma_X(P,0)$ at 0K and pressure $P$. After that, we can calculate the displacements [3-5]

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

$$A_X = a_{1X} + \sum_{i=2}^{5} \left( \frac{\gamma_X(\theta)}{k_X} \right)^i a_{iX},$$

$$k_X = m\omega_X^2,$$

$$x_X = \frac{h\omega_X}{\gamma_X},$$

$$a_{1X} = 1 + \frac{Y_X}{2},$$

$$a_{2X} = \frac{13}{3} + \frac{47}{6} Y_X + \frac{23}{5} Y_X^2 + \frac{1}{2} Y_X^3,$$

$$a_{3X} = -\left( \frac{25}{3} + \frac{121}{6} Y_X + \frac{50}{3} Y_X^2 + \frac{16}{3} Y_X^3 + \frac{1}{2} Y_X^4 \right),$$

$$a_{4X} = \frac{43}{3} + \frac{93}{2} Y_X + \frac{169}{3} Y_X^2 + \frac{83}{3} Y_X^3 + \frac{22}{4} Y_X^4 + \frac{1}{2} Y_X^5,$$

$$a_{5X} = -\left( \frac{103}{3} + \frac{749}{6} Y_X + \frac{363}{3} Y_X^2 + \frac{733}{3} Y_X^3 + \frac{148}{3} Y_X^4 + \frac{53}{6} Y_X^5 + \frac{1}{2} Y_X^6 \right),$$

$$a_{6X} = 65 + \frac{561}{2} Y_X + \frac{1489}{3} Y_X^2 + \frac{927}{2} Y_X^3 + \frac{733}{3} Y_X^4 + \frac{145}{2} Y_X^5 + \frac{31}{3} Y_X^6 + \frac{1}{2} Y_X^7,$$

$$Y_X = x_X \coth x_X$$  \hspace{1cm} (7)

From that, we derive the nearest neighbor distance $r_{1X}(P,T)$ at temperature $T$ and pressure $P$

$$r_{1C}(P,T) = r_{1C}(P,0) + y_{A_1}(P,T), r_{1A}(P,T) = r_{1A}(P,0), r_{1A_1}(P,T) = r_{1A_2}(P,0) + y_C(P,T).$$  \hspace{1cm} (8)

Then, we calculate the mean nearest neighbor distance in interstitial alloy $AC$ by the expressions as follows [3-5]

$$r_{1A}(P,T) = r_{1A}(P,0) + y(P,T), r_{1A}(P,0) = (1 - c_C) r_{1A}(P,0) + c_C r_{1A}^*(P,0),$$

$$r_{1A}^*(P,0) \approx \sqrt{3} r_{1C}(P,0), y(P,T) = (1 - 7c_C) y_A(P,T) + c_C y_C(P,T) + 2c_C y_{A_1}(P,0) + 4 c_C y_{A_2}(P,T),$$  \hspace{1cm} (9)

where $r_{1A}(P,T)$ is the mean nearest neighbor distance between atoms $A$ in interstitial alloy $AC$ at pressure $P$ and temperature $T$, $r_{1A}(P,0)$ is the mean nearest neighbor distance between atoms $A$ in interstitial alloy $AC$ at pressure $P$ and 0K, $r_{1A}(P,0)$ is the nearest neighbor distance between atoms $A$ in clean metal $A$ at pressure $P$ and 0K, $r_{1A}^*(P,0)$ is the nearest neighbor distance between atoms $A$ in the zone containing the interstitial atom $C$ at pressure $P$ and 0K and $c_C$ is the concentration of interstitial atoms $C$.

In alloy $ABC$ with BCC structure (interstitial alloy $AC$ with atoms $A$ in peaks and body center, interstitial atom $C$ in facer centers and then, atom $B$ substitutes atom $A$ in body center), the mean nearest neighbor distance between atoms $A$ at pressure $P$ and temperature $T$ is determined by [3-5]

$$a_{ABC} = c_{AC} a_{AC} \frac{B_{T,AC}}{B_T} + c_B a_B \frac{B_{T,B}}{B_T},$$
\[ B_T = c_{AC}B_{TAC} + c_BB_{TB}, \]
\[ c_{AC} = c_A + c_C, \]
\[ a_{AC} = r_{AC}(P,T), \]
\[ B_{TAC} = \frac{1}{\chi_{TAC}}, \]
\[ B_{TB} = \frac{1}{\chi_{TB}}. \]

\[ \chi_{TAC} = \frac{\left( \frac{a_{AC}}{n_{AC}} \right)^3}{2P + \sqrt{3} \frac{1}{3n_{AC}} \left( \frac{\partial^2 \psi_{AC}}{\partial a_{AC}^2} \right)}_T, \]
\[ \left( \frac{\partial^2 \psi_{AC}}{\partial a_{AC}^2} \right)_T \approx (1 - 7c_C) \left( \frac{\partial^2 \psi_{A}}{\partial a_{A}^2} \right)_T + c_C \left( \frac{\partial^2 \psi_{C}}{\partial a_{C}^2} \right)_T + 2c_C \left( \frac{\partial^2 \psi_{A_1}}{\partial a_{A_1}^2} \right)_T + 4c_C \left( \frac{\partial^2 \psi_{A_2}}{\partial a_{A_2}^2} \right)_T, \]
\[ \frac{1}{3n_{AC}} \left( \frac{\partial^2 \Psi_X}{\partial a_{X}^2} \right)_T = \frac{1}{6} \frac{\partial^2 U_{0X}}{\partial a_{X}^2} + \frac{\hbar \omega_X}{4k_X} \left[ \frac{\partial^2 \psi_X}{\partial a_{X}^2} \right] - \frac{1}{2k_X} \left( \frac{\partial k_X}{\partial a_X} \right)^2, \]
\[ a_X \equiv r_{1X}(P,T). \]

The mean nearest neighbor distance between atoms A in alloy ABC at pressure \( P \) and 0K is determined by
\[ a_{0ABC} = c_{AC}a_{0AC} \frac{B_{0TAC}}{B_{0T}} + c_Ba_{0B} \frac{B_{0TB}}{B_{0T}}. \]

2.1.2. Free energy The free energy of alloy ABC with BCC structure and the condition \( c_C \ll c_B \ll c_A \) has the form[5]
\[ \psi_{ABC} = \psi_{AC} + c_B(\psi_B - \psi_A) + TS_C^{AC} - TS_C^{ABC}, \]
\[ \psi_{AC} = (1 - 7c_C)\psi_A + c_C\psi_C + 2c_C\psi_{A_1} + 4c_C\psi_{A_2} - TS_C^{AC}, \]
\[ \psi_X \approx U_{0X} + \psi_{0X} + 3N \left\{ \frac{\theta^2}{k_X^2} \left[ \gamma_2 X^2 - \frac{2\gamma_1}{3} X X \right] + \frac{2\theta^3}{k_X^3} \left[ \frac{4}{3} \gamma_2 X X \left( 1 + \frac{X X}{2} \right) - 2 \left( \gamma_1 X + 2\gamma_1 X \right) \left( 1 + \frac{X X}{2} \right) \right] \right\}, \]
\[ \psi_{0X} = 3N\theta \left[ X X + \ln(1 - e^{-2X}) \right], \]
\[ X X \equiv X X \coth X X. \]

where \( \psi_X \) is the free energy of atom \( X \), \( \psi_{AC} \) is the free energy of interstitial alloy AC, \( S_C^{AC} \) is the configuration entropy of interstitial alloy AC and \( S_C^{ABC} \) is the configuration entropy of alloy ABC.

2.1.3. Characteristic quantities of elastic deformation The Young modulus of alloy ABC with BCC structure at temperature \( T \) and pressure \( P \) is determined by
\[ E_{ABC} = c_B(E_B - E_A) + E_{AC} = c_B E_B + c_A E_A - (c_A + c_B) E_A + E_{AC} = E_{AB} - (c_A + c_B) E_A + E_{AC}, E_{AB} = c_A E_A + c_B E_B, \]
\[ E_{AC} = E_A \left( 1 - 7c_C + c_C \frac{\partial^2 \psi_c}{\partial \varepsilon^2} + 2 \frac{\partial^2 \psi_{A1}}{\partial \varepsilon^2} + 4 \frac{\partial^2 \psi_{A2}}{\partial \varepsilon^2} \right), \]

\[ E_A = \frac{1}{\pi r_1 A_1 A}, \]

\[ A_{1A} = \frac{1}{k_A} \left[ 1 + 2 \gamma_A^2 \theta^2 \left( 1 + \frac{1}{2} x_{A \text{c} \text{h}x_A} \right) \left( 1 + x_{A \text{c} \text{h}x_A} \right) \right], \]

\[ x_A = \frac{\hbar \omega_A}{2 \theta}, \]

\[ \frac{\partial^2 \psi \varepsilon}{\partial \varepsilon^2} = \left\{ \frac{1}{2} \frac{\partial^2 U_0}{\partial r_{1X}^2} + \frac{3}{4} \frac{h \omega_X}{k_X} \left[ \frac{\partial^2 k_X}{\partial r_{1X}^2} - \frac{1}{2k_X} \left( \frac{\partial k_X}{\partial r_{1X}} \right)^2 \right] \right\} 4r_{01X}^2 \]

\[ + \left( \frac{1}{2} \frac{\partial U_0}{\partial r_{1X}} + \frac{3}{2} \frac{h \omega_X}{k_X} \text{c} \text{h}x_X \frac{1}{2k_X} \frac{\partial k_X}{\partial r_{1X}} \right) 2r_{01X}, \]

\[ x_X = \frac{\hbar \omega_X}{2 \theta}, \]

\[ \omega_X = \sqrt{\frac{k_X}{m}}, \quad (13) \]

where \( \varepsilon \) is the relative deformation, \( E_{AB} \) is the Young modulus of substitution alloy AB and \( E_{AC} \) is the Young modulus of interstitial alloy AC.

The bulk modulus of alloy ABC with BCC structure at temperature \( T \) and pressure \( P \) has the form

\[ K_{ABC} = \frac{E_{ABC}}{3(1 - 2\nu_{AB})}. \quad (14) \]

The rigidity modulus of alloy ABC with BCC structure at temperature \( T \) and pressure \( P \) has the form

\[ G_{ABC} = \frac{E_{ABC}}{2(1 + \nu_{AB})}. \quad (15) \]

The elastic constants of alloy ABC with BCC structure at temperature \( T \) and pressure \( P \) has the form

\[ C_{11ABC} = \frac{E_{ABC}(1 - \nu_{AB})}{(1 + \nu_{AB})(1 - 2\nu_{AB})}, \quad (16) \]

\[ C_{12ABC} = \frac{E_{ABC} \nu_{AB}}{(1 + \nu_{AB})(1 - 2\nu_{AB})}, \quad (17) \]

\[ C_{44ABC} = \frac{E_{ABC}}{2(1 + \nu_{AB})}. \quad (18) \]

The Poisson ratio of alloy ABC with BCC structure has the form

\[ \nu_{ABC} = c_A \nu_A + c_B \nu_B + c_C \nu_C \approx c_A \nu_A + c_B \nu_B = \nu_{AB}. \quad (19) \]

where \( \nu_A, \nu_B \) and \( \nu_A \) respectively are the Poisson ratios of materials A, B and C and are determined from the experimental data.

When the concentration of interstitial atom C is equal to zero, the obtained results for alloy ABC become the corresponding results for substitution alloy AB. When the concentration of substitution atom B is equal to zero, the obtained results for alloy ABC become the corresponding results for interstitial alloy AC. When the concentrations of substitution atoms B and interstitial atoms C are equal to zero, the obtained results for alloy ABC become the corresponding results for main metal A.
2.2. Numerical results for alloy FeCrSi

For alloy FeCrSi, we use the n-m pair potential

\[ \varphi(r) = \frac{D}{n-m} \left[ m \left( \frac{r_0}{r} \right)^n - n \left( \frac{r_0}{r} \right)^m \right]. \]  

(20)

where the potential parameters are given in Table 1[6]

| Material | \(m\) | \(n\) | \(D \ (10^{-16} \text{erg})\) | \(r_0 \ (10^{-10} \text{m})\) |
|---------|------|------|---------------------|---------------------|
| Fe      | 7.0  | 11.5 | 6416.448            | 2.4775             |
| Cr      | 6.0  | 15.5 | 6612.96             | 2.4950             |
| Si      | 6.0  | 12.0 | 45128.24            | 2.2950             |

Table 1. Potential parameters \(m, n, D, r_0\) of materials.

Considering the interaction between Fe and Si and between Fe and Cr, we use the following approximation

\[ \varphi_{Fe-Cr} \approx \frac{1}{2} \left( \varphi_{Fe-Fe} + \varphi_{Cr-Cr} \right), \varphi_{Fe-Si} \approx \frac{1}{2} \left( \varphi_{Fe-Fe} + \varphi_{Si-Si} \right). \]  

(21)

and ignore the interaction between Cr and Si.

According to our numerical results for alloy FeCrSi at the same pressure, temperature and concentration of substitution atoms when the concentration of interstitial atoms increases, the mean nearest neighbor distance also increases. For example for alloy FeCrSi at \(T = 300\text{K}, P = 70 \text{ GPa} \) and \(c_{Cr} = 10\%\) when \(c_{Si}\) increases from 0 to 5\%, \(r_1\) increases from 2.3228 Å to 2.3989 Å.

For alloy FeCrSi at the same temperature, concentration of substitution atoms and concentration of interstitial atoms when pressure increases, the mean nearest neighbor distance decreases. For example for alloy FeCrSi at \(T = 300\text{K}, c_{Cr} = 10\%, c_{Si} = 3\%\) when \(P\) increases from 0 to 70 GPa, \(r_1\) decreases from 2.4715 Å to 2.3683 Å.

For alloy FeCrSi at the same pressure, temperature and concentration of interstitial atoms when the concentration of substitution atoms increases, the mean nearest neighbor distance decreases. For example for alloy FeCrSi at \(T = 300\text{K}, P = 50 \text{ GPa}, c_{Si} = 5\%\) when \(c_{Cr}\) increases from 0 to 15\% \(r_1\) decreases from 2.4216 Å to 2.4178 Å.

For alloy FeCrSi at the same pressure, temperature and concentration of substitution atoms when pressure increases, the elastic moduli \(E, G, K\) increases. For example for alloy FeCrSi at \(T = 300\text{K}, P = 10\text{GPa}\) and \(c_{Cr} = 10\% \) when \(c_{Si}\) increases from 0 to 5\%, \(E\) increases from 18.4723.10\(^{10}\) Pa to 30.0379.10\(^{10}\) Pa.

For alloy FeCrSi at the same temperature, concentration of substitution atoms and concentration of interstitial atoms when pressure increases, the elastic moduli \(E, G, K\) increases. For example for alloy FeCrSi at \(T = 300\text{K}, c_{Cr} = 10\%, c_{Si} = 1\%\) when \(P\) increases from 0 to 70 GPa, \(E\) increases from 15,2862.10\(^{10}\) Pa to 48,0400.10\(^{10}\) Pa.

For alloy FeCrSi at the same pressure, temperature and concentration of interstitial atoms when the concentration of substitution atoms increases, the elastic moduli \(E, G, K\) decreases.
For example for alloy FeCrSi at $T = 300\text{K}$, $P = 30\text{GPa}$, $c_{\text{Si}} = 5\%$ when $c_{\text{Cr}}$ descases from 0 to 15%. $E$ descases from $39.389310^{10}\text{Pa}$ to $39.2128.10^{10}\text{Pa}$.

For alloy FeCrSi at the same pressure, concentration of substitution atoms and concentration of interstitial atoms when temperature increases, the elastic moduli $E, G, K$ descases. For example for alloy FeCrSi at $P = 70\text{GPa}$, $c_{\text{Cr}} = 10\%$, $c_{\text{Si}} = 5\%$ when $T$ increases from 50K to 1000K $E$ descases from $53.6239.10^{10}\text{Pa}$ to $52.9651.10^{10}\text{Pa}$.

For alloy FeCrSi at the same pressure, temperature and concentration of substitution atoms when the concentration of interstitial atoms increases, the elastic constants, $C_{11}, C_{12}, C_{44}$ increases. For example for alloy FeCrSi at $T = 300\text{K}$, $P = 10\text{GPa}$, $c_{\text{Cr}} = 10\%$ when $c_{\text{Si}}$ increases from 0 to 5%, $C_{11}$ increases from $23.7286.10^{10}\text{Pa}$ to $38.5851.10^{10}\text{Pa}$.

For alloy FeCrSi at the same temperature, concentration of substitution atoms and concentration of interstitial atoms when pressure increases, the elastic constants $C_{11}, C_{12}, C_{44}$ increases. For example for alloy FeCrSi at $T = 300\text{K}$, $c_{\text{Cr}} = 10\%$, $c_{\text{Si}} = 1\%$ when $P$ increases from 0 to 70GPa, $C_{11}$ increases from $14.6358.10^{10}\text{Pa}$ to $61.7096.10^{10}\text{Pa}$.

For alloy FeCrSi at the same pressure, temperature and concentration of interstitial atoms when the concentration of substitution atoms increases, the elastic constants $C_{11}, C_{12}, C_{44}$ descases. For example for alloy FeCrSi at $T = 300\text{K}$, $P = 30\text{GPa}$, $c_{\text{Si}} = 5\%$ when $c_{\text{Cr}}$ increases from 0 to 15% $C_{11}$ descases from $51.6175.10^{10}\text{Pa}$ to $49.8943.10^{10}\text{Pa}$.

For alloy FeCrSi at the same pressure, concentration of substitution atoms and concentration of interstitial atoms when temperature increases, the elastic constants $C_{11}, C_{12}, C_{44}$ descases. For example for alloy FeCrSi at $P = 70\text{GPa}$, $c_{\text{Cr}} = 10\%$, $c_{\text{Si}} = 5\%$ when $T$ increases from 50K to 1000K, $C_{11}$ descases from $68.8824.10^{10}\text{Pa}$ to $68.0362.10^{10}\text{Pa}$.

When the concentration of substitution atoms and the concentration of interstitial atoms are equal to zero, the mean nearest neighbor distance, the elastic moduli and the elastic constants of alloy FeCrSi becomes the mean nearest neighbor distance, the elastic moduli and the elastic constants of metal Fe. The dependence of mean nearest neighbor distance, the elastic moduli and the elastic constants on pressure and concentration of interstitial atoms for alloy FeCrSi is the same as the dependence of mean nearest neighbor distance, the elastic moduli and the elastic constants on pressure and concentration of substitution atoms for alloy FeCrSi.

The dependences of elastic moduli $E, K, G$ on temperature for Fe at $P = 0$ are given in Table 2. The dependences of nearest neighbor distance $a$, relative change of volume $\Delta V / V$, elastic moduli $E, K, G$ and elastic constants $C_{11}, C_{12}, C_{44}$ on pressure for Fe at $T = 300\text{K}$ are given in Table 3. The nearest neighbor distance and temperature and the elastic moduli $E, G$ of Fe at $P = 0$, $T = 300\text{K}$ according to SMM and EXPT [7, 8] are given in Table 4. The dependences of elastic moduli $E, K, G$ and elastic constants $C_{11}, C_{12}, C_{44}$ on pressure for Fe-5%Si at $T = 300\text{K}$ are given in Table 5. The dependences of elastic moduli $E, K, G$ and elastic constants $C_{11}, C_{12}, C_{44}$ on concentration of substitution atoms Cr for Fe-Cr at $T = 300\text{K}$ and $P = 0$ are given in Table 6.

The isothermal modulus of FeSi at $T = 300\text{K}$ and $P = 0$ according to the SMM, the experiments (EXPT) and the tight-binding (TB) method are given in Table 7. The lattice constant, the volume of unit cell and the bulk modulus of FeSi at $T = 300\text{K}$ and $P = 0$ according to the SMM, the DFT and the EXPT are given in Tables 8, 9 and 10. Note that in these tables, FPPW is the first-principles plane-wave method combined with the quasi-harmonic Debye model, DFT$^a$ is the DFT with ultrasoft non-norm-conserving Vanderbilt pseudopotentials in GGA, DFT$^b$ is the DFT with Hartwigsen-Gedecker-Hutter pseudopotentials in GGA, DFT$^c$ is the DFT with Hartwigsen-Gedecker-Hutter pseudopotentials in LDA, DFT$^d$ is the DFT with ultrasoft pseudopotentials in LSD, DFT$^e$ is the DFT with ultrasoft pseudopotentials in GGA.
Table 2. Dependence of elastic moduli $E, K, G$ on temperature for Fe at $P = 0$.

| $T(K)$ | 100  | 200  | 300  | 500  | 700  | 1000 |
|--------|------|------|------|------|------|------|
| $E(10^{10} Pa)$ | 22.48 | 21.71 | 20.83 | 18.79 | 16.37 | 12.25 |
| $K(10^{10} Pa)$ | 15.61 | 15.07 | 14.47 | 13.05 | 11.37 | 6.50  |
| $G(10^{10} Pa)$ | 8.92  | 8.61  | 8.27  | 7.46  | 6.50  | 4.86  |

Table 3. Dependence of nearest neighbor distance $a$, relative change of volume $\frac{\Delta V}{V}$, elastic moduli $E, K, G$ and elastic constants $C_{11}, C_{12}, C_{44}$ on pressure for Fe at $T = 300K$.

| Method | $a$ (Å) | $E(10^{10} Pa)$ | $G(10^{10} Pa)$ | $C_{11}(10^{11} Pa)$ | $C_{12}(10^{11} Pa)$ | $C_{44}(10^{11} Pa)$ |
|--------|---------|-----------------|-----------------|----------------------|----------------------|----------------------|
| SMM    | 2.4298  | 20.83           | 8.27            | 2.48                 | 1.01                 | 0.73                 |
| EXPT   | 2.3729[7]| 20.98[8]        | 8.12[8]         | 2.33                 | 1.35[8]              | 1.18[8]              |

Table 4. Nearest neighbor distance, elastic moduli $E, G$ and elastic constants $C_{11}, C_{12}, C_{44}$ of Fe at $P = 0, T = 300K$ according to SMM and EXPT [7, 8].
Table 5. Dependences of elastic moduli $E$, $K$, $G$ and elastic constants $C_{11}$, $C_{12}$, $C_{44}$ on pressure for Fe-5\%Si at $T = 300K$.

| $P$ (GPa) | 10  | 30  | 50  | 70  |
|-----------|-----|-----|-----|-----|
| $E$ (10^{10} Pa) | 26.19 | 35.16 | 43.56 | 51.58 |
| $K$ (10^{10} Pa) | 18.19 | 24.42 | 30.25 | 35.82 |
| $G$ (10^{10} Pa) | 10.39 | 13.93 | 17.29 | 20.47 |
| $C_{11}$ (10^{10} Pa) | 32.04 | 43.02 | 53.30 | 63.11 |
| $C_{12}$ (10^{10} Pa) | 11.26 | 15.12 | 18.73 | 22.17 |
| $C_{44}$ (10^{10} Pa) | 10.39 | 13.93 | 17.29 | 20.47 |

Table 6. Dependences of elastic moduli $E$, $K$, $G$ and elastic constants $C_{11}$, $C_{12}$, $C_{44}$ on concentration of substitution atoms Cr for Fe-Cr at $T = 300K$ and $P = 0$.

| $c_{Cr}$ (%) | 3   | 6   | 9   | 12  | 15  |
|--------------|-----|-----|-----|-----|-----|
| $E$ (10^{10} Pa) | 20.91 | 20.98 | 21.06 | 21.14 | 21.14 |
| $K$ (10^{10} Pa) | 14.65 | 14.83 | 15.02 | 15.21 | 15.40 |
| $G$ (10^{10} Pa) | 8.28  | 8.30  | 8.32  | 8.33  | 8.35  |
| $C_{11}$ (10^{10} Pa) | 25.69 | 25.90 | 26.11 | 26.32 | 26.54 |
| $C_{12}$ (10^{10} Pa) | 9.12  | 9.30  | 9.48  | 9.66  | 9.84  |
| $C_{44}$ (10^{10} Pa) | 8.28  | 8.30  | 8.32  | 8.33  | 8.35  |

Table 7. Isothermal elastic modulus of Fe at $T = 300K$ and $P = 0$.

| Method      | SMM | EXPT[9] | EXPT[10] |
|-------------|-----|---------|----------|
| $B_T$ [GPa] | 170.09 | 168     | 281      |

Table 8. Lattice constant of FeSi at $T = 300K$ and $P = 0$.

| Method      | SMM   | FPPW + QHD [12] | $DFT^\text{a}$ [13] | $DFT^\text{b}$ [14] | $DFT^\text{c}$ [14] | $DFT^\text{d}$ [15] | $DFT^\text{e}$ [15] | EXPT [16] | EXPT [17] |
|-------------|-------|----------------|----------------------|---------------------|---------------------|---------------------|---------------------|-----------|-----------|
| $2a/\sqrt{3}$ (Å) | 2.890 | 2.785          | 2.768                 | 2.772                | 2.708                | 2.72                | 2.77                | 2.791     | 2.773     |

Table 9. Volume of unit cell of FeSi at $T = 300K$ and $P = 0$.

| Method      | SMM   | FPPW + QHD [12] | EXPT [16] | EXPT [17] |
|-------------|-------|----------------|-----------|-----------|
| $V = (2a/\sqrt{3})^3$, Å$^3$ | 24.14 | 21.6           | 21.74 ± 0.02 | 21.32     |
Method | SMM | FPPW +QHD | $DFT^a$ | $DFT^d$ | $DFT^e$ | EXPT | EXPT  
--- | --- | --- | --- | --- | --- | --- |  
K(GPa) | 194.395 | 199 | 226 | 263 | 221 | 184 ± 5 | 225  

**Table 10.** Bulk modulus of FeSi at $T = 300K$ and $P = 0$.  

Figure 1. Dependence of elastic moduli $E, G, K$ on pressure for alloy Fe-10%Cr-5%Si at $T = 300K$.  

Figure 2. Dependence of elastic constants $C_{11}, C_{12}, C_{44}$ on pressure for alloy Fe-10%Cr-5%Si at $T = 300K$.  

Figure 3. Dependence of elastic moduli $E, G, K$ on concentration of Si for alloy Fe-10%Cr-xSi at $P = 30$GPa and $T = 300K$.  

Figure 4. Dependence of elastic constants $C_{11}, C_{12}, C_{44}$ on concentration of Si for alloy Fe-10%Cr-xSi at $P = 30$GPa and $T = 300K$.  

Figure 5. Dependence of elastic moduli $E, G, K$ on concentration of Cr for alloy Fe-xCr-5%Si at $P = 30$GPa and $T = 300$K.

Figure 6. Dependence of elastic constants $C_{11}, C_{12}, C_{44}$ on concentration of Cr for alloy Fe-xCr-5%Si at $P = 30$GPa and $T = 300$K.

Figure 7. Dependence of elastic moduli $E, G, K$ on temperature for alloy Fe-15%Cr-5%Si at $P = 70$GPa.

Figure 8. Dependence of elastic constants $C_{11}, C_{12}, C_{44}$ on temperature for alloy Fe-15%xCr-5%Si at $P = 70$GPa.
3. Conclusion

The analytic expressions of the free energy, the mean nearest neighbor distance between two atoms, the elastic moduli such as the Young modulus, the bulk modulus, the rigidity modulus and the elastic constants depending on temperature, concentration of substitution atoms and concentration of interstitial atoms for substitution alloy AB with interstitial atom C and BCC structure under pressure are derived by the SMM. The numerical results for alloy FeCrSi are in good agreement with the numerical results for substitution alloy FeCr, interstitial alloy FeSi and main metal Fe. Temperature changes from 5 to 1000K, pressure changes from 0 to 70 GPa, the concentration of substitution atoms Cr changes from 0 to 15% and the concentration of interstitial atoms Si changes from 0 to 5%.

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