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Original Article

Study on Elastic Deformation of Interstitial Alloy FeC with 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 C_{11}, C_{12}, C_{44} for interstitial alloy AB with BCC structure under pressure are derived from the statistical moment method. The elastic deformations of main metal A is special case of elastic deformation for interstitial alloy AB. The theoretical results are applied to alloy FeC under pressure. The numerical results for this alloy are compared with the numerical results for main metal Fe and experiments.

Keywords: interstitial alloy, elastic deformation, Young modulus, bulk modulus, rigidity modulus, elastic constant, Poisson ratio.

1. Introduction

Elastic properties of interstitial alloys are especially interested in many theoretical and experimental researchers [1-4, 7-12]. For example, in [3] the strengthening effects interstitial carbon solute atoms in (i.e., ferritic or 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 wherein the bcc Fe matrix is thermodynamically supersaturated in carbon. In [4], 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-principles calculations and experiments. In [7], the thermodynamic properties of binary interstitial alloy with bcc structure are considered by the statistical moment method (SMM). 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 [12]

In this paper, we build the theory of elastic deformation for interstitial AB with body-centered cubic (BCC) structure under pressure by the SMM [5-7]. The theoretical results are applied to alloy FeCunder pressure.

2. Content of research

2.1. Analytic results

In interstitial alloy AB with BCC structure, the cohesive energy of the atom B (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 B and the radii $r_1, r_1\sqrt{2}, r_1\sqrt{5}$ are determined by [5-7]

$$u_{0B} = \sum_{i=1}^{n_i} \varphi_{AB}(r_i) = 2\varphi_{AB}(r_1) + 4\varphi_{AB}(r_1\sqrt{2}) + 8\varphi_{AB}(r_1\sqrt{5}), \qquad (2.1)$$

where φ_{AB} is the interaction potential between the atom A and the atom B, n_i is the number of atoms on the ith coordination sphere with the radius $r_i(i = 1, 2, 3)$, $r_1 \equiv r_{1B} = r_{01B} + y_{0A_1}(T)$ is the nearest neighbor distance between the interstitial atom B and the metallic atom A at temperature T, r_{01B} 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_{0B}, $y_{0A_1}(T)$ 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 B in the approximation of three coordination spheres have the form [5-7]

$$k_B = \frac{1}{2}\sum_i \left(\frac{\partial^2 \varphi_{AB}}{\partial u_{i\beta}^2}\right)_{eq} = \varphi_{AB}^{(2)}(r_1) + \frac{\sqrt{2}}{r_1}\varphi_{AB}^{(1)}(r_1\sqrt{2}) + \frac{16}{5r_1\sqrt{5}}\varphi_{AB}^{(1)}(r_1\sqrt{5}),$$

$$\gamma_B = 4(\gamma_{1B} + \gamma_{2B}),$$

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

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

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

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

$$+\frac{2}{25r_1^2}\varphi_{AB}^{(2)}(r_1\sqrt{5})-\frac{3}{25r_1^3\sqrt{5}}\varphi_{AB}^{(1)}(r_1\sqrt{5}),\tag{2.2}$$

where $\phi_{AB}^{(m)}\equiv\partial^m\phi_{AB}(r_i)/\partial r_i^m$ $(m=1,2,3,4,\alpha,\beta=x,y.z,\alpha\neq\beta$ and $u_{i\beta}$ is the displacement of the ith atom in the direction β.

The cohesive energy of the atom A_1 (which contains the interstitial atom B 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 [5-7]

$$u_{0A_1}=u_{0A}+\varphi_{AB}\left(r_{1A_1}\right),$$

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

$$\gamma_{A_1}=4\left(\gamma_{1A_1}+\gamma_{2A_1}\right),$$

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

$$\gamma_{2A_1}=\gamma_{2A}+\frac{6}{48}\sum_i\left[\left(\frac{\partial^4\varphi_{AB}}{\partial u_{i\alpha}^2\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_1}}=\gamma_{2A}+\frac{1}{2r_{1A_1}}\varphi_{AB}^{(3)}(r_{1A_1})-\frac{3}{4r_{1A_1}^2}\varphi_{AB}^{(2)}(r_{1A_1})+\frac{3}{4r_{1A_1}^3}\varphi_{AB}^{(1)}(r_{1A_1}).\tag{2.3}$$

where .. 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 B on the first coordination sphere) with the atoms in a crystalline lattice and the corresponding alloy's parameters in the approximation of three coordination spheres with the center A_2 is determined by [5-7]

$$u_{0A_2}=u_{0A}+\varphi_{AB}\left(r_{1A_2}\right),$$

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

$$\gamma_{A_2}=4\left(\gamma_{1A_2}+\gamma_{2A_2}\right),$$

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

$$-\frac{1}{8r_{1A_2}^2}\varphi_{AB}^{(2)}(r_{1A_2})+\frac{1}{8r_{1A_2}^3}\varphi_{AB}^{(1)}(r_{1A_2}),$$

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

$$+\frac{1}{4r_{1A_2}}\varphi_{AB}^{(3)}(r_{1A_2})+\frac{3}{8r_{1A_2}^2}\varphi_{AB}^{(2)}(r_{1A_2})-\frac{3}{8r_{1A_2}^3}\varphi_{AB}^{(1)}(r_{1A_2}),\tag{2.4}$$

where..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}, $y_{0B}(T)$ is the displacement of the atom C at temperature T.

In Eqs. (2.3) and (2.4), $u_{0A}, k_A, \gamma_{1A}, \gamma_{2A}$ are the corresponding quantities in clean metal A in the approximation of two coordination sphere [5-7]

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

$$Pv=-r_1\left(\frac{1}{6}\frac{\partial u_0}{\partial r_1}+\theta x\coth x\frac{1}{2k}\frac{\partial k}{\partial r_1}\right).\tag{2.5}$$

where $v=\dfrac{4r_1^3}{3\sqrt{3}}$ is the unit cell volume per atom, r_1 is the nearest neighbor distance, $\theta=k_{Bo}T$, k_{Bo} is the Boltzmann constant, $x=\dfrac{\hbar}{2\theta}\sqrt{\dfrac{k}{m}}=\dfrac{\hbar\omega}{2\theta}$, m is the atomic mass and ω is the vibrational frequencies of atoms. At temperature $T=0$ K, Eq. (2.5) will be simply reduced to

$$Pv=-r_1\left(\frac{1}{6}\frac{\partial u_0}{\partial r_1}+\frac{\hbar\omega}{4k}\frac{\partial k}{\partial r_1}\right).\tag{2.6}$$

Note that Eq.(2.5) permits us to find r_1 at temperature T under the condition that the quantities k, x, u_0 at temperature T_0 (for example $T_0 = 0$K) are known. If the temperature T_0 is not far from T, then one can see that the vibration of an atom around a new equilibrium position (corresponding to T_0) is harmonic. Eq.(2.5) only is a good equation of state in that condition. Eq. (2.6) also is the equation of state in the case of $T_0 = 0$K. In Eq. (2.6), the first term is the change of energy potential of atoms in euilibrium position and the second term is the change of energy of zeroth vibration. If knowing the form of interaction potential φ_{i0}, eq. (2.6) permits us to determine the nearest neighbor distance $r_{1X}(P,0)(X=B,A,A_1,A_2)$ at 0 K and pressure P. After knowing , we can determine alloy parametrs $k_X(P,0), \gamma_{1X}(P,0), \gamma_{2X}(P,0), \gamma_X(P,0), \omega_X(P,0)$ at 0K and pressure P. After that, we can calculate the displacements [5-7]

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

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

$$a_{2X}=\frac{13}{3}+\frac{47}{6}Y_X+\frac{23}{6}Y_X^2+\frac{1}{2}Y_X^3,\quad a_{3X}=-\left(\frac{25}{3}+\frac{121}{6}Y_X+\frac{50}{3}Y_X^2+\frac{16}{3}Y_X^3+\frac{1}{2}Y_X^4\right),$$

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

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

$$a_{6X} = 65 + \frac{561}{2}Y_X + \frac{1489}{3}Y_X^2 + \frac{927}{2}Y_X^3 + \frac{733}{3}Y_X^4 + \frac{145}{2}Y_X^5 + \frac{31}{3}Y_X^6 + \frac{1}{2}Y_X^7, Y_X \equiv x_X \coth x_X. \qquad (2.7)$$

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

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

$$r_{1A_1}(P,T) \approx r_{1B}(P,T), r_{1A_2}(P,T) = r_{1A_2}(P,0) + y_B(P,T). \qquad (2.8)$$

Then, we calculate the mean nearest neighbor distance in interstitial alloy AB by the expressions as follows [5-7]

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

$$\overline{r_{1A}(P,0)} = (1 - c_B)r_{1A}(P,0) + c_B r'_{1A}(P,0), r'_{1A}(P,0) = \sqrt{3}r_{1B}(P,0), \qquad (2.9)$$

where $\overline{r_{1A}(P,T)}$ is the mean nearest neighbor distance between atoms A in interstitial alloy AB at pressure P and temperature T, $\overline{r_{1A}(P,0)}$ is the mean nearest neighbor distance between atoms A in interstitial alloy AB 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 B at pressure P and 0K and c_B is the concentration of interstitial atoms B.

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

$$\psi_{AB} = (1 - 7c_B)\psi_A + c_B\psi_B + 2c_B\psi_{A_1} + 4c_B\psi_{A_2} - TS_c,$$

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

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

$$\psi_{0X} = 3N\theta\left[x_X + \ln(1 - e^{-2x_X})\right], X_X \equiv x_X \coth x_X, \qquad (2.10)$$

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

The Young modulus of alloy AB with BCC structure at temperature T and pressure P is determined by

$$E_{AB}(c_B,P,T) = E_A\left(1 - 7c_B + c_B\frac{\dfrac{\partial^2\psi_B}{\partial\varepsilon^2} + 2\dfrac{\partial^2\psi_{A_1}}{\partial\varepsilon^2} + 4\dfrac{\partial^2\psi_{A_2}}{\partial\varepsilon^2}}{\dfrac{\partial^2\psi_A}{\partial\varepsilon^2}}\right), E_A = \frac{1}{\pi.r_{1A}A_{1A}},$$

$$A_{1A} = \frac{1}{k_A}\left[1+\frac{2\gamma_A^2\theta^2}{k_A^4}\left(1+\frac{X_A}{2}\right)(1+X_A)\right],$$

$$\frac{\partial^2\psi_X}{\partial\varepsilon^2} = \left\{\frac{1}{2}\frac{\partial^2 u_{0X}}{\partial r_{1X}^2}+\frac{3}{4}\frac{\hbar\omega_X}{k_X}\left[\frac{\partial^2 k_X}{\partial r_{1X}^2}-\frac{1}{2k_X}\left(\frac{\partial k_X}{\partial r_{1X}}\right)^2\right]\right\}4r_{01X}^2 +$$

$$+\left(\frac{1}{2}\frac{\partial u_{0X}}{\partial r_{1X}}+\frac{3}{2}\hbar\omega_X cthx_X\frac{1}{2k_X}\frac{\partial k_X}{\partial r_{1X}}\right)2r_{01X}, \tag{2.11}$$

where ε is the relative deformation.

The bulk modulus of BCC alloy AB with BCC structure at temperature T and pressure P has the form

$$K_{AB}\left(c_B,P,T\right)=\frac{E_{AB}\left(c_B,P,T\right)}{3(1-2\nu_{AB})}. \tag{2.12}$$

The rigidity modulus of alloy AB with BCC structure at temperature T and pressure P has the form

$$G_{AB}\left(c_B,P,T\right)=\frac{E_{AB}\left(c_B,P,T\right)}{2\left(1+\nu_{AB}\right)}. \tag{2.13}$$

The elastic constants of alloy AB with BCC structure at temperature T and pressure P has the form

$$C_{11AB}\left(c_B,P,T\right)=\frac{E_{AB}\left(c_B,P,T\right)\left(1-\nu_{AB}\right)}{\left(1+\nu_{AB}\right)\left(1-2\nu_{AB}\right)}, \tag{2.14}$$

$$C_{12AB}\left(c_B,P,T\right)=\frac{E_{AB}\left(c_B,P,T\right)\nu_{AB}}{\left(1+\nu_{AB}\right)\left(1-2\nu_{AB}\right)}, \tag{2.15}$$

$$C_{44AB}\left(c_B,P,T\right)=\frac{E_{AB}\left(c_B,P,T\right)}{2\left(1+\nu_{AB}\right)}. \tag{2.16}$$

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

$$\nu_{AB}=c_A\nu_A+c_B\nu_B\approx\nu_A, \tag{2.17}$$

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

When the concentration of interstitial atom B is equal to zero, the obtained results for alloy AB become the coresponding results for main metal A.

2.2. Numerical results for alloy FeC

For pure metal Fe, we use the m – n potential as follows

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

where the m – n potential parameters between atoms Fe-Fe are shown in Table 1.

For alloy FeC, we use the Finnis-Sinclair potential as follows

$$U = -A\sqrt{\sum_{i \neq j} \rho(r_{ij})} + \frac{1}{2}\sum_{i \neq j} \phi(r_{ij}),$$

$$\rho(r) = t_1(r - R_1)^2 + t_2(r - R_1)^3 \quad (r < R_1),$$

$$\phi(r) = (r - R_2)^2(k_1 + k_2 r + k_3 r^2) \quad (r < R_2). \tag{2.19}$$

where the Finnis-Sinclair potential parameters between atoms Fe-C are shown in Table 2.

Our numerical results are summarized in tables and illustrated in figures. Our calculated results for Young modulus E of alloy FeC in Table 3, Table 4, Fig.5 and Fig.6 are in good agreement with experiments [10].

Table 1. The m-n potential parameters between atoms Fe-Fe [8]

Interaction	m	n	$D(\text{eV})$	$r_0\left(\overset{o}{\text{A}}\right)$
Fe – Fe	7.0	11.5	0.4	2.4775

Table 2. The Finnis-Sinclair potential parameters between atoms Fe-C [9]

A (eV)	R_1 $\left(\overset{o}{\text{A}}\right)$	t_1 $\left(\overset{o}{\text{A}}\right)^{-2}$	t_2 $\left(\overset{o}{\text{A}}\right)^{-3}$	R_2 $\left(\overset{o}{\text{A}}\right)$	k_1 $\left(\text{eV}\left(\overset{o}{\text{A}}\right)^{-2}\right)$	k_2 $\left(\text{eV}\left(\overset{o}{\text{A}}\right)^{-3}\right)$	k_3 $\left(\text{eV}\left(\overset{o}{\text{A}}\right)^{-4}\right)$
2.958787	2.545937	10.024001	1.638980	2.468801	8.972488	-4.086410	1.483233

Table 3. The dependence of Young modulus $E(10^{10}\text{Pa})$ for alloy FeC with $c_C = 0.2\%$ from the SMM and alloy FeC with $c_C \leq 0.3\%$ from EXPT[10] at zero pressure

T(K)	73	144	200	294	422	533	589	644	700	811	866
SMM	22.59	22.03	21.58	20.75	19.49	18.28	17.65	16.96	16.26	14.81	14.06
EXPT	21.65	21.24	20,82	20.34	19.51	18.82	18.41	17.58	16.69	14.07	12.41

Table 4. The dependence of Young modulus $E(10^{10}\text{Pa})$ for alloy FeC with $c_C = 0.4\%$ from the SMM and alloy FeC with $c_C \geq 0.3\%$ from EXPT[10] at zero pressure

T(K)	73	144	200	294	422	533	589	644	700	811	866	922
SMM	22.46	21.90	21.45	20.62	19.38	18.18	17.53	16.87	16.17	14.72	13.98	13.21
EXPT	21.51	21.10	20.68	20.20	19.37	18.62	18.27	17.44	16.55	13.93	12.34	10.62
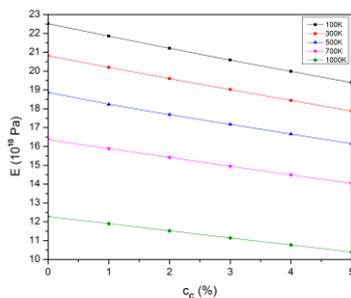
Fig 1. E(c_C) for FeC at P = 0.
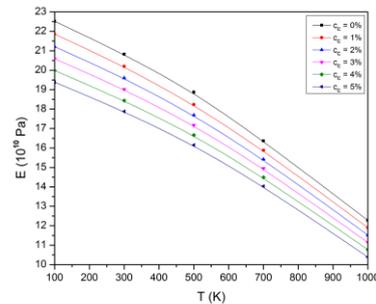
Fig 2. E(T) for FeC at P = 0.
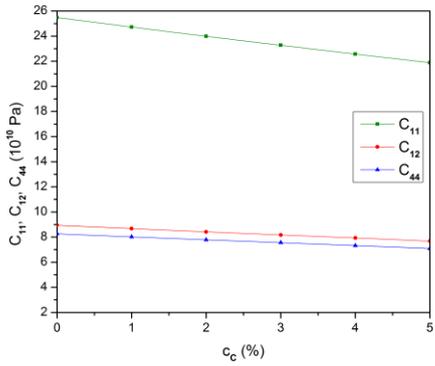
Fig 3. C_{11}, C_{12}, C_{44} (c_C) for FeC at P = 0.
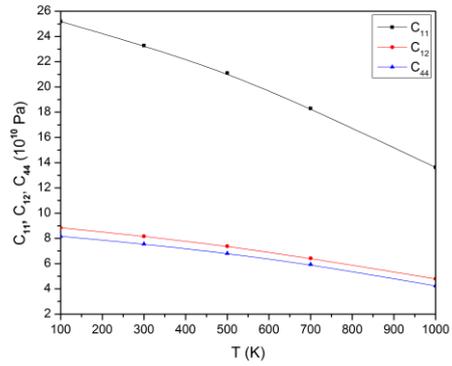
Fig 4. C_{11}, C_{12}, C_{44} (T) for FeC at P = 0.
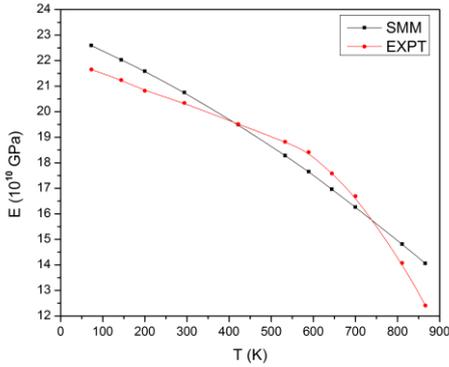
Fig 5. E(T) for alloy FeC with $c_C = 0.2\%$
from the SMM and alloy FeC with $c_C \leq 0.3\%$
from EXPT [17].
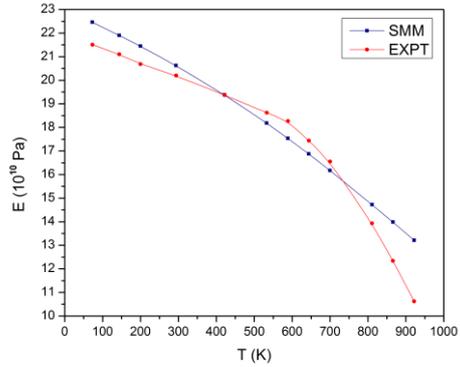
Fig 6. E(T) for alloy FeC with $c_C = 0.4\%$
from the SMM and alloy FeC with $c_C \geq 0.3\%$
from EXPT [17].
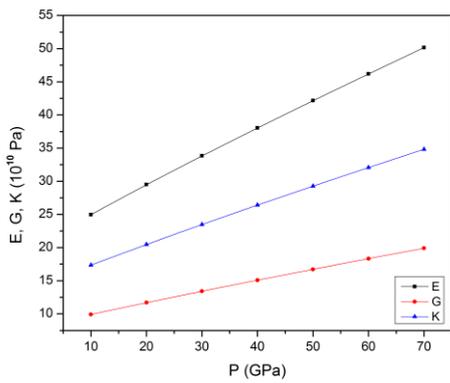
Fig 7. E(P), G(P), K(P) for alloy FeC
with $c_C = 1\%$ at T = 300K.
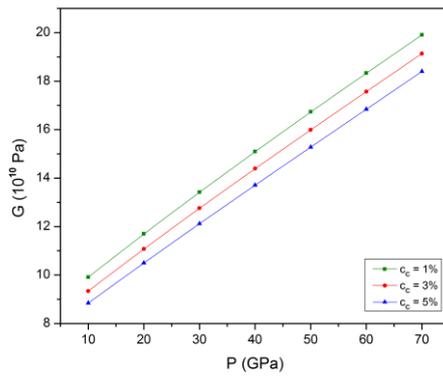
Fig 8. G(P) for alloy FeC with $c_C = 1, 3$ and 5%
at T = 300K.
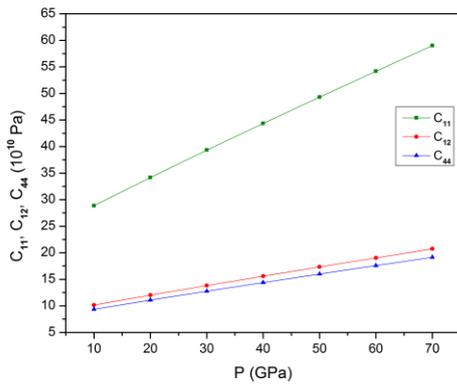
Fig 9. $C_{11}(P)$, $C_{12}(P)$, $C_{44}(P)$ for alloy FeC
with c_C = 3% at T = 300K.
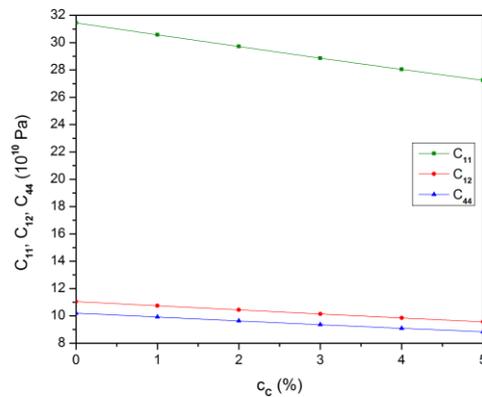
Fig 10. $C_{11}(c_C)$, $C_{12}(c_C)$, $C_{44}(c_C)$ for alloy FeC
at P = 10 GPa at T = 300K.

For alloy FeC at the same temperature and pressure when the concentration of interstitial atoms increases, the elastic moduli E, G, K and the elastic constants C_{11}, C_{12}, C_{44} decrease. For example, for FeC at T = 1000K , P = 0 when c_C increases from 0 to 5%, E decreases from $12.28.10^{10}$ to $10.39.10^{10}$ Pa, G decreases from $4.87.10^{10}$ to $4.12.10^{10}$ Pa, K decreases from $8.53.10^{10}$ to $7.21.10^{10}$Pa, C_{11} decreases from $15.02.10^{10}$ to $12.71.10^{10}$ Pa, C_{12} decreases from $5.28.10^{10}$ to $4.46.10^{10}$ Pa and C_{44} decreases from $4.87.10^{10}$ to $4.12.10^{10}$ Pa.

For alloy FeC at the same pressrure and concentration of interstitial atoms when temperature increases, the elastic moduli E, G, K and the elastic constants C_{11}, C_{12}, C_{44} also decrease. For example, for FeC at c_C = 5%, P = 0 when T increases from 100 to 1000K, E decreases from $19.39.10^{10}$ to $10.39.10^{10}$ Pa, G decreases from $7.69.10^{10}$ to $4.12.10^{10}$ Pa, K decreases from $13.47.10^{10}$ to $7.21.10^{10}$Pa, C_{11} decreases from $23.72.10^{10}$ to $12.71.10^{10}$ Pa, C_{12} decreases from $8.33.10^{10}$ to $4.46.10^{10}$ Pa and C_{44} decreases from $7.69.10^{10}$ to $4.12.10^{10}$ Pa.

For alloy FeC at the same temperature and concentration of interstitial atoms when pressure increases, the elastic moduli E, G, K and the elastic constants C_{11}, C_{12}, C_{44} increase. For example, for FeC at c_C = 5%, T = 300K when P increases from 10 to 70 GPa, E increases $22.27.10^{10}$ to $46.36.10^{10}$ Pa, G increases $8.84.10^{10}$ to $18.40.10^{10}$ Pa, K increases $15.46.10^{10}$ to $32.20.10^{10}$ Pa, C_{11} increases $27.24.10^{10}$ to $56.73.10^{10}$ Pa, C_{12} increases $9.57.10^{10}$ to $19.93.10^{10}$ Pa and C_{44} increases $8.84.10^{10}$ to $18.40.10^{10}$ Pa.

For main metal Fe in alloy FeC at T = 300 K, our calculated results of elastic moduli and elastic constantsare in good agreement with experiments in Tables 5-7.

Table 5. The elastic moduli E, G, K (10^{-10}Pa) and elastic constants C_{11}, C_{12}, C_{44}(10^{11}Pa) according to the SMM and EXPT [11] for Fe at P = 0 and T = 300 K

	E	G	K	C_{11}	C_{12}	C_{44}
SMM	20.82	8.26	14.46	2.55	0.90	0.83
EXPT [11]	20.98	8.12	---	2.33	1.35	1.18

Table 6. The shear modulus G (GPa) according to the SMM, EXPT [13] and CAL [14]
for Fe at T = 300 K and P = 0, 9.8 GPa

P (GPa)	SMM	EXPT [13]	CAL [14]
0	82.6	84	100
9.8	101.6	101	120

Table 7. Isothermal elastic modulus for Fe at P = 0 and T = 300K
according to the SMM, CAL [16] and EXPT [15]

Method	SMM	EXPT[150]	CAL[16]
B_T[GPa]	170.09	168	281

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 interstitial atoms for interstitial alloy AB with BCC structure under pressure are derived by the SMM. The numerical results for alloy FeC are in good agreement with the numerical results for main metal Fe. The numerical results for alloy FeC with $c_C = 0.2\%$ and $c_C = 0.4\%$ at zero pressure are in good agreement with experiments. The temperature changes from 73K to 1000K and the concentration of interstitial atoms C changes from 0 to 5%.

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APPENDIX

The Hamiltonian of atom X can be written in the form

$$\hat{H}_X = \hat{H}_{0X} - \alpha_X \hat{V}_X \tag{A1}$$

where α_X is the parameter and proceeding from the condition of normalization for the statistical operator, it is easy to find the expression

$$< \hat{V}_X >_{\alpha_X} = -\frac{\partial \psi_X(\alpha_X)}{\partial \alpha_X} \tag{A2}$$

where $< ... >_{\alpha_X}$ expresses the averaging over the equilibrium ensemble with the Hamiltonian $\hat{H}_X$ and $\psi_X(\alpha_X)$ is the free energy.

Expression (A2) gives the general formula

$$\psi_X(\alpha_X) = \psi_{0X} - \int_0^{\alpha_X} \left\langle \hat{V}_X \right\rangle_{\alpha_X} d\alpha_X \tag{A3}$$

in which ψ_{0X} is the free energy of atom X corresponding to the Hamiltonian H_{0X}. For many cases $\left\langle V_X \right\rangle_{\alpha_X}$ can be written through the moments and thus we can determine it with the aid of the momentum formula. Therefore, using (A3) the free energy $\psi_X(\alpha_X)$ can be found.

In the approximation up to fourth order the average potential energy is equal to

$$\left\langle U_X \right\rangle = U_{0X} + 3N \left[\frac{k_X}{2} \left\langle u_X^2 \right\rangle + \gamma_{1X} \left\langle u_X^4 \right\rangle + \gamma_{2X} \left\langle u_X^2 \right\rangle^2 \right] \tag{A4}$$

where $U_{0X} = \frac{N}{2} u_{0X}$, $k_X, \gamma_{1X}, \gamma_{2X}$ are the crystal parameters, $\left\langle u_X^2 \right\rangle$ and $\left\langle u_X^4 \right\rangle$ have been derived by using statistical moment method in [6].

To find free energy ψ_X, we must calculate the integrals

$$
\int_0^{\gamma_{2X}} \left\langle u_X^2 \right\rangle^2 d\gamma_{2X}, \ \int_0^{\gamma_{1X}} \left\langle u_X \right\rangle^4 d\gamma_{1X} \tag{A5}
$$

By combining the equations (A3), (A4) and (A5) we have

$$
\psi_X \approx \frac{N}{2} u_{0X} + 3N\theta \left[x_X + \ln(1 - e^{-2x_X}) \right] + 3N \left\{ \frac{\theta^2}{k_X^2} \left[\gamma_{2X} X_X^2 - \frac{2\gamma_{1X}}{3} \left(1 + \frac{X_X}{2} \right) \right] + \right.
$$

$$
\left. + \frac{2\theta^3}{k_X^4} \left[\frac{4}{3} \gamma_{2X}^2 X_X \left(1 + \frac{X_X}{2} \right) - 2 \left(\gamma_{1X}^2 + 2\gamma_{1X}\gamma_{2X} \right) \left(1 + \frac{X_X}{2} \right) (1 + X_X) \right] \right\} \tag{A6}
$$

Thus free energy of interstitial alloy AB per atom with BCC structure can be simply given by

$$
\frac{\psi_{AB}}{N} = (N - 7N_B) \frac{\psi_A}{N} + N_B \frac{\psi_B}{N} + 2N_B \frac{\psi_{A_1}}{N} + 4N_B \frac{\psi_{A_2}}{N} - TS_c =
$$

$$
= \left(1 - 7\frac{N_B}{N} \right) \psi_A + \frac{N_B}{N} \psi_B + 2\frac{N_B}{N} \psi_{A_1} + 4\frac{N_B}{N} \psi_{A_2} - TS_c =
$$

$$
= \left(1 - 7c_B \right) \psi_A + c_B \psi_B + 2c_B \psi_{A_1} + 4c_B \psi_{A_2} - TS_c, c_B = \frac{N_B}{N}, \tag{7}
$$

where c_B is the concentration of interstitial atom B, N is the number of atoms in crystal, N_B is is the number of atoms in crystal and S_c is the configuration entropy. In crystal, there are N_B atoms B, $2N_B$ atoms A_1, $4N_B$ atoms A_2 and then the number of atoms A is $N - (N_B + 2N_B + 4N_B) = N - 7N_B$.