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Original Article

Combining the Mie-Lennard-Jones and the Morse Potentials in Studying the Elastic Deformation of Interstitial Alloy AGC with FCC Structure under Pressure

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Abstract: In this study, the mean nearest neighbor distance between two atoms, the Helmholtz free energy and characteristic quantities for elastic deformation such as elastic moduli E, G, K and elastic constants C_{11}, C_{12}, C_{44} for binary interstitial alloys with FCC structure under pressure are derived with the statistical moment method. The numerical calculations for interstitial alloy AGC were performed by combining the Mie-Lennard-Jones potential and the Morse potential. Our calculated results were compared with other calculations and the experimental data.

Keywords: Elastic deformation, interstitial alloy, Morse potential, Mie-Lennard-Jones potential, elastic moduli, elastic constants, statistical moment method.

1. Introduction

The elastic deformation for body centered cubic (BCC) and face centered cubic (FCC) ternary and binary interstitial alloys under pressure in [1-10] has been studied with the statistical moment method (SMM). In this paper, we separately apply the Mie-Lennard-Jones pair potential [11], the Morse pair potential [12] and the Finnis-Sinclair many-body potential [13].

In this paper, we will present the theory of elastic deformation for binary interstitial alloys with FCC structure at zero pressure and various pressures built by the SMM. Then, we apply this theory to

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study the elastic deformation of interstitial alloy AgC by combining the Mie-Lennard-Jones pair potential [14] and the Morse pair potential [15].

2. Content of Research

2.1. Theory of Elastic Deformation for FCC Interstitial Alloy AB under Pressure

In our model for interstitial alloy AB with FCC structure and concentration condition $c_B << c_A$, the cohesive energy u_0 and the alloy parameters $k, \gamma_1, \gamma_2, \gamma$ (k is the harmonic parameter and $\gamma_1, \gamma_2, \gamma$ are anharmonic parameters) for the interstitial atom B in body center, the main metal atom A_1 in face centers and the main metal atom A_2 in corners of the cubic unit cell in the approximation of two coordination spheres have the form [1-10,16]

$$u_{0B} = \frac{1}{2}\sum_{i=1}^{n_i}\varphi_{AB}(r_i) = 3\varphi_{AB}(r_{1B}) + 4\varphi_{AB}(r_{2B}), r_{2B} = \sqrt{3}r_{1B}, \tag{1}$$

$$k_B = \frac{1}{2}\sum_i\left(\frac{\partial^2\varphi_{AB}}{\partial u_{i\beta}^2}\right)_{eq} = \frac{d^2\varphi_{AB}(r_{1B})}{dr_{1B}^2} + \frac{2}{r_{1B}}\frac{d\varphi_{AB}(r_{1B})}{dr_{1B}} + \frac{4}{3}\frac{d^2\varphi_{AB}(r_{2B})}{dr_{2B}^2} + \frac{8}{3r_{2B}}\frac{d\varphi_{AB}(r_{2B})}{dr_{2B}}, \tag{2}$$

$$\gamma_B = 4(\gamma_{1B} + \gamma_{2B}), \tag{3}$$

$$\gamma_{1B} = \frac{1}{48}\sum_i\left(\frac{\partial^4\varphi_{AB}}{\partial u_{i\beta}^4}\right)_{eq} = \frac{1}{24}\frac{d^4\varphi_{AB}(r_{1B})}{dr_{1B}^4} + \frac{1}{4r_{1B}^2}\frac{d^2\varphi_{AB}(r_{1B})}{dr_{1B}^2} - \frac{1}{4r_{1B}^3}\frac{d\varphi_{AB}(r_{1B})}{dr_{1B}} +$$
$$+ \frac{1}{54}\frac{d^4\varphi_{AB}(r_{2B})}{dr_{2B}^4} + \frac{2}{9r_{2B}}\frac{d^3\varphi_{AB}(r_{2B})}{dr_{2B}^3} - \frac{2}{9r_{2B}^2}\frac{d^2\varphi_{AB}(r_{2B})}{dr_{2B}^2} + \frac{2}{9r_{2B}^3}\frac{d\varphi_{AB}(r_{2B})}{dr_{2B}}, \tag{4}$$

$$\gamma_{2B} = \frac{6}{48}\sum_i\left(\frac{\partial^4\varphi_{AB}}{\partial u_{i\alpha}^2\partial u_{i\beta}^2}\right)_{eq} = \frac{1}{2r_{1B}}\frac{d^3\varphi_{AB}(r_{1B})}{dr_{1B}^3} - \frac{3}{4r_{1B}^2}\frac{d^2\varphi_{AB}(r_{1B})}{dr_{1B}^2} + \frac{3}{4r_{1B}^3}\frac{d\varphi_{AB}(r_{1B})}{dr_{1B}} +$$
$$+ \frac{1}{9}\frac{d^4\varphi_{AB}(r_{2B})}{dr_{2B}^4} + \frac{2}{3r_{2B}^2}\frac{d^2\varphi_{AB}(r_{2B})}{dr_{2B}^2} - \frac{2}{3r_{2B}^3}\frac{d\varphi_{AB}(r_{2B})}{dr_{2B}}, \tag{5}$$

$$u_{0A_1} = u_{0A} + \phi_{AB}(r_{1A_1}), \tag{6}$$

$$k_{A_1} = k_A + \frac{1}{2}\sum_i\left[\left(\frac{\partial^2\varphi_{AB}}{\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_1}} = k_A + \frac{d^2\varphi_{AB}(r_{1A_1})}{dr_{1A_1}^2}, \tag{7}$$

$$\gamma_{A_1} = 4(\gamma_{1A_1} + \gamma_{2A_1}), \tag{8}$$

$$\gamma_{1A_1} = \gamma_{1A} + \frac{1}{48}\sum_i\left[\left(\frac{\partial^4\varphi_{AB}}{\partial u_{i\beta}^4}\right)_{eq}\right]_{r=r_{1A_1}} = \gamma_{1A} + \frac{1}{24}\frac{d^4\varphi_{AB}(r_{1A_1})}{dr_{1A_1}^4}, \tag{9}$$

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

$$= \gamma_{2A} + \frac{1}{4r_{1A_1}}\frac{d^3\varphi_{AB}(r_{1A_1})}{dr_{1A_1}^3} - \frac{1}{2r_{1A_1}^2}\frac{d^2\varphi_{AB}(r_{1A_1})}{dr_{1A_1}^2} + \frac{1}{2r_{1A_1}^3}\frac{d\varphi_{AB}(r_{1A_1})}{dr_{1A_1}}, \quad (10)$$

$$u_{0A_2} = u_{0A} + \phi_{AB}\left(r_{1A_2}\right), \quad (11)$$

$$k_{A_2} = k_A + \frac{1}{2}\sum_i \left[\left(\frac{\partial^2 \varphi_{AB}}{\partial u_{i\beta}^2}\right)_{eq}\right]_{r=r_{1A_2}} = k_A + \frac{1}{6}\frac{d^2\varphi_{AB}\left(r_{1A_2}\right)}{dr_{1A_2}^2} + \frac{23}{6r_{1A_2}}\frac{d\varphi_{AB}\left(r_{1A_2}\right)}{dr_{1A_2}}, \quad (12)$$

$$\gamma_{A_2} = 4\left(\gamma_{1A_2} + \gamma_{2A_2}\right), \quad (13)$$

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

$$- \frac{2}{9r_{1A_2}^2}\frac{d^2\varphi_{AB}(r_{1A_2})}{dr_{1A_2}^2} + \frac{2}{9r_{1A_2}^3}\frac{d\varphi_{AB}(r_{1A_2})}{dr_{1A_2}}, \quad (14)$$

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

$$+ \frac{4}{27r_{1A_2}}\frac{d^3\varphi_{AB}(r_{1A_2})}{dr_{1A_2}^3} + \frac{14}{27r_{1A_2}^2}\frac{d^2\varphi_{AB}(r_{1A_2})}{dr_{1A_2}^2} - \frac{14}{27r_{1A_2}^3}\frac{d\varphi_{AB}(r_{1A_2})}{dr_{1A_2}}, \quad (15)$$

where φ_{AB} is the interaction potential between atoms A and B, $r_{1X} = r_{01X} + y_{0X}(T)$ is the nearest neighbor distance between the atom X (X = A, A_1, A_2, B)(A in clean metal, A_1, A_2 and B in interstitial alloy AB) and other atoms at temperature T, r_{01X} is the nearest neighbor distance between the atom X and other atoms at T = 0K and is determined from the minimum condition of the cohesive energy, $u_{0X}, y_{0X}(T)$ is the displacement of atom X from equilibrium position at temperature T. $u_{0A}, k_A, \gamma_{1A}, \gamma_{2A}$ is the corresponding quantities in the clean metal A with FCC structure in the approximation of two coordination spheres [16]

$$u_{0A} = 6\varphi_{AA}\left(r_{1A}\right) + 3\varphi_{AA}\left(r_{2A}\right), r_{2A} = \sqrt{2}r_{1A}, \quad (16)$$

$$k_A = 2\frac{d^2\varphi_{AA}\left(r_{1A}\right)}{dr_{1A}^2} + \frac{4}{r_{1A}}\frac{d\varphi_{AA}\left(r_{1A}\right)}{dr_{1A}} + \frac{d^2\varphi_{AA}\left(r_{2A}\right)}{dr_{2A}^2} + \frac{2}{r_{2A}}\frac{d\varphi_{AA}\left(r_{2A}\right)}{dr_{2A}}, \quad (17)$$

$$\gamma_{1A} = \frac{1}{24}\frac{d^4\varphi_{AA}\left(r_{1A}\right)}{dr_{1A}^4} + \frac{1}{4r_{1A}}\frac{d^3\varphi_{AA}\left(r_{1A}\right)}{dr_{1A}^3} - \frac{1}{8r_{1A}^2}\frac{d^2\varphi_{AA}\left(r_{1A}\right)}{dr_{1A}^2} + \frac{1}{8r_{1A}^3}\frac{d\varphi_{AA}\left(r_{1A}\right)}{dr_{1A}} +$$

$$+\frac{1}{24}\frac{d^4\varphi_{AA}(r_{2A})}{dr_{2A}^4}+\frac{1}{4r_{2A}^2}\frac{d^2\varphi_{AA}(r_{2A})}{dr_{2A}^2}-\frac{1}{4r_{2A}^3}\frac{d\varphi_{AA}(r_{2A})}{dr_{2A}}, \tag{18}$$

$$\gamma_{2A}=\frac{1}{48}\frac{d^4\varphi_{AA}(r_{1A})}{dr_{1A}^4}+\frac{7}{8r_{1A}}\frac{d^3\varphi_{AA}(r_{1A})}{dr_{1A}^3}-\frac{31}{16r_{1A}^2}\frac{d^2\varphi_{AA}(r_{1A})}{dr_{1A}^2}+\frac{31}{16r_{1A}^3}\frac{d\varphi_{AA}(r_{1A})}{dr_{1A}}+$$
$$+\frac{1}{2r_{2A}}\frac{d^3\varphi_{AA}(r_{2A})}{dr_{2A}^3}-\frac{9}{8r_{2A}^2}\frac{d^2\varphi_{AA}(r_{2A})}{dr_{2A}^2}+\frac{9}{8r_{2A}^3}\frac{d\varphi_{AA}(r_{2A})}{dr_{2A}}. \tag{19}$$

The equations of state for FCC interstitial alloy at temperature T and pressure P and at 0K and pressure P are written in the form [16]

$$Pv=-r_1\left(\frac{1}{6}\frac{\partial u_0}{\partial r_1}+\theta x\,\mathrm{cth}x\,\frac{1}{2k}\frac{\partial k}{\partial r_1}\right),v=\frac{r_1^3}{\sqrt{2}}, \tag{20}$$

$$Pv=-r_1\left(\frac{1}{6}\frac{\partial u_0}{\partial r_1}+\frac{\hbar\omega_0}{4k}\frac{\partial k}{\partial r_1}\right). \tag{21}$$

From (21), we can calculate the nearest neighbor distance $r_{1X}(P,0)$ ($X = A, A_1, A_2, B$), the parameters $k_X(P,0), \gamma_{1X}(P,0), \gamma_{2X}(P,0), \gamma_X(P,0)$, the displacement $y_X(P,T)$ of atom X from equilibrium position as in [16], the nearest neighbor distance $r_{1X}(P,T)$ and the mean nearest neighbor distance between two atoms in alloy $\overline{r_{1A}(P,T)}$ as follows: [1-10]

$$r_{1B}(P,T)=r_{1B}(P,0)+y_B(P,T),r_{1A}(P,T)=r_{1A}(P,0)+y_A(P,T),$$
$$r_{1A_1}(P,T)\approx r_{1B}(P,T),r_{1A_2}(P,T)=r_{1A_2}(P,0)+y_{A_2}(P,T), \tag{22}$$
$$\overline{r_{1A}(P,T)}=\overline{r_{1A}(P,0)}+\overline{y(P,T)},$$
$$\overline{r_{1A}(P,0)}=(1-c_B)r_{1A}(P,0)+c_Br'_{1A}(P,0),r'_{1A}(P,0)=\sqrt{2}r_{1B}(P,0),$$
$$\overline{y(P,T)}=(1-15c_B)y_A(P,T)+c_By_B(P,T)+6c_By_{A_1}(P,T)+8c_By_{A_2}(P,T). \tag{23}$$

The Helmholtz free energy ψ of FCC interstitial alloy AB with the condition $c_B << c_A$ is determined by [1-10,16]

$$\psi=(1-15c_B)\psi_A+c_B\psi_B+6c_B\psi_{A_1}+8c_B\psi_{A_2}-TS_c,$$
$$\psi_X\approx U_{0X}+\psi_{0X}+3N\left\{\frac{\theta^2}{(k_X)^2}\left[\gamma_{2X}(Y_X)^2-\frac{2\gamma_{1X}}{3}\left(1+\frac{Y_X}{2}\right)\right]+\right.$$
$$\left.+\frac{2\theta^3}{(k_X)^4}\left[\frac{4}{3}\gamma_{2X}Y_X\left(1+\frac{Y_X}{2}\right)-2\left[(\gamma_{1X})^2+2\gamma_{1X}\gamma_{2X}\right]\left(1+\frac{Y_X}{2}\right)(1+Y_X)\right]\right\},$$
$$\psi_{0X}=3N\theta\left[x_X+\ln\left(1-e^{-2x_X}\right)\right],Y_X\equiv x_X\mathrm{cth}x_X, \tag{24}$$

where ψ_X is the Helmholtz free energy of one atom X, U_{0X} is the cohesive energy and S_c is the configurational entropy of FCC interstitial alloy AB.

The Young modulus E, the bulk modulus K, the shearing modulus G, the elastic constants C_{11}, C_{12}, C_{44} and the Poisson ratio of FCC interstitial alloy AB have the form [3,6.8-10,16]

$$E = \frac{1}{\pi r_{1A} A_{1A}}\left(1-15c_B + c_B\frac{\frac{\partial^2\psi_B}{\partial\varepsilon^2}+6\frac{\partial^2\psi_{A_1}}{\partial\varepsilon^2}+8\frac{\partial^2\psi_{A_2}}{\partial\varepsilon^2}}{\frac{\partial^2\psi_A}{\partial\varepsilon^2}}\right),$$

$$A_{1A} = \frac{1}{k_A}\left[1+\frac{2\gamma_A^2\theta^2}{k_A^4}\left(1+\frac{Y_A}{2}\right)\left(1+Y_A\right)\right],\ x_X = \frac{\hbar\omega_X}{2\theta},\ \omega_X = \sqrt{\frac{k_X}{m}},$$

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

$$K_{AB} = \frac{E_{AB}}{3\left(1-2\nu_A\right)},\ G_{AB} = \frac{E_{AB}}{2\left(1+\nu_A\right)}, \tag{25}$$

$$C_{11AB} = \frac{E_{AB}\left(1-\nu_A\right)}{\left(1+\nu_A\right)\left(1-2\nu_A\right)},\ C_{12AB} = \frac{E_{AB}\nu_A}{\left(1+\nu_A\right)\left(1-2\nu_A\right)},\ C_{44AB} = \frac{E_{AB}}{2\left(1+\nu_A\right)}, \tag{26}$$

$$\nu_{AB} = c_A\nu_A + c_B\nu_B \approx \nu_A, \tag{27}$$

where ν_A, ν_B are the Poisson ratios of materials A and B determined from experiments.

2.2. Numerical results for alloy AgC

To describe the interaction Ag-Ag, we apply the Mie-Lennard-Jones pair interaction potential in the form [14]

$$\varphi(r) = \frac{D}{n-m}\left[m\left(\frac{r_0}{r}\right)^n - n\left(\frac{r_0}{r}\right)^m\right], \tag{28}$$

where D is the depth of potential well corresponding to the equilibrium distance r_0, m and n are determined empirically. The Mie-Lennard-Jones potential parameters for the interaction Ag-Ag are given in Table 1. The Poisson ratio of Ag is 0.38 [18].

Table 1. Mie-Lennard-Jones potential parameters for interaction Ag-Ag

Interaction	D/k_B(K)	r_0 (10^{-10} m)	M	n
Ag-Ag	5737.19[14]	2.876[17]	3.08[14]	10.35[14]

For the interaction Ag-C, Ag-C, we use the Morse potential as follows: [15]

$$\varphi(r) = \beta\left[e^{-N\delta(r-r_w)} - Ne^{-\delta(r-r_w)}\right]. \tag{29}$$

where the parameters β, δ, r_W, N are given in Table 2.

Table 2. Morse potential parameters for interaction Ag-C [15]

Interaction	$\beta(eV)$ β	$\delta\left(\overset{o}{A}\right)^{-1}$	$r_w(\overset{o}{A})$	N
Ag-C	0.297	2.662	2.349	$\sqrt{12}$

Our calculation results are summarized in Tables 3-10 and shown in Figures 1-6. For AgC at zero pressure and at the same temperature when the concentration of interstitial atoms increases, the mean nearest neighbor distance also increases. For AgC at zero pressure and with the constant concentration of interstitial atoms when temperature increases, the mean nearest neighbor distance also increases (see Table 3). That agrees with the experimental rules.

Table 3. The mean nearest neighbor distance a_{AgC} (Å) for FCC-AgC at P = 0 calculated by the SMM

T (K)	c_C(%)	0	1	2	3	4	5
100	a_{AgC}(Å)	2.8243	2.8363	2.8483	2.8603	2.8723	2.8843
300		2.8340	2.8451	2.8563	2.8674	2.8786	2.8898
500		2.8440	2.8543	2.8646	2.8748	2.8851	2.8954
700		2.8545	2.8639	2.8732	2.8825	2.8919	2.9012
900		2.8655	2.8738	2.8822	2.8905	2.8989	2.9072
1100		2.8770	2.8843	2.8916	2.8989	2.9062	2.9135
1300		2.8892	2.8954	2.9015	2.9077	2.9138	2.9200

Table 4. The dependence of elastic moduli E, G, K (10^{10} Pa) on temperature and concentration of interstitial atoms for FCC-AgC at P = 0 calculated by the SMM

T (K)	c_C(%)	0	1	2	3	4	5
100	E	8.7900	8.5100	8.4241	8.5169	8.7747	9.1850
	K	12.2083	11.8195	11.7002	11.8291	12.1871	12.7570
	G	3.1848	3.0833	3.0522	3.0858	3.1792	3.3279
300	E	8.2533	8.0644	8.0434	8.1771	8.4535	8.8615
	K	11.4629	11.2006	11.1713	11.3570	11.7409	12.3076
	G	2.9903	2.9219	2.9143	2.9627	3.0629	3.2107
500	E	7.6330	7.5235	7.5544	7.7141	7.9918	8.3769
	K	10.6014	10.4493	10.4922	10.7141	11.0997	11.6346
	G	2.7656	2.7259	2.7371	2.7950	2.8956	3.0351
700	E	6.9298	6.8892	6.9610	7.1351	7.4015	7.7507
	K	9.6247	9.5683	9.6681	9.9098	10.2799	10.7648
	G	2.5108	2.4961	2.5221	2.5852	2.6817	2.8082
900	E	6.1536	6.1731	6.2779	6.4594	6.7090	7.0183
	K	8.5467	8.5737	8.7193	8.9713	9.3180	9.7476
	G	2.2296	2.2366	2.2746	2.3403	2.4308	2.5429
1100	E	5.3260	5.3984	5.5313	5.7179	5.9513	6.2248
	K	7.3972	7.4978	7.6824	7.9415	8.2657	8.6455
	G	1.9297	1.9559	2.0041	2.0717	2.1563	2.2554
1300	E	4.4776	4.5969	4.7554	4.9480	5.1700	5.4166
	K	6.2188	6.3846	6.6047	6.8722	7.1805	7.5231
	G	1.6223	1.6656	1.7230	1.7927	1.8732	1.9626

Table 5. The dependence of elastic constants C_{11}, C_{12}, C_{44} (10^{10} Pa) on temperature and concentration of interstitial atoms for FCC-AgC at P = 0 calculated by the SMM

T (K)	c_C(%)	0	1	2	3	4	5
100	C_{11}	16.4547	15.9306	15.7698	15.9436	16.4261	17.1942
	C_{12}	10.0851	9.7639	9.6654	9.7719	10.0676	10.5384
	C_{44}	3.1848	3.0833	3.0522	3.0858	3.1792	3.3279
300	C_{11}	15.4501	15.0964	15.0570	15.3073	15.8248	16.5886
	C_{12}	9.4694	9.2527	9.2285	9.3819	9.6990	10.1672
	C_{44}	2.9903	2.9219	2.9143	2.9627	3.0629	3.2107
500	C_{11}	14.2888	14.0839	14.1417	14.4407	14.9604	15.6814
	C_{12}	8.7576	8.6321	8.6675	8.8507	9.1693	9.6112
	C_{44}	2.7656	2.7259	2.7371	2.7950	2.8956	3.0351
700	C_{11}	12.9724	12.8964	13.0309	13.3567	13.8555	14.5091
	C_{12}	7.9508	7.9043	7.9867	8.1864	8.4921	8.8927
	C_{44}	2.5108	2.4961	2.5221	2.5852	2.6817	2.8082
900	C_{11}	11.5194	11.5559	11.7521	12.0918	12.5590	13.1381
	C_{12}	7.0603	7.0826	7.2029	7.4111	7.6975	8.0524
	C_{44}	2.2296	2.2366	2.2746	2.3403	2.4308	2.5429
1100	C_{11}	9.9701	10.1057	10.3546	10.7038	11.1407	11.6527
	C_{12}	6.1107	6.1938	6.3463	6.5604	6.8282	7.1420
	C_{44}	1.9297	1.9559	2.0041	2.0717	2.1563	2.2554
1300	C_{11}	8.3819	8.6054	8.9020	9.2625	9.6781	10.1398
	C_{12}	5.1373	5.2742	5.4560	5.6770	5.9317	6.2147
	C_{44}	1.6223	1.6656	1.7230	1.7927	1.8732	1.9626

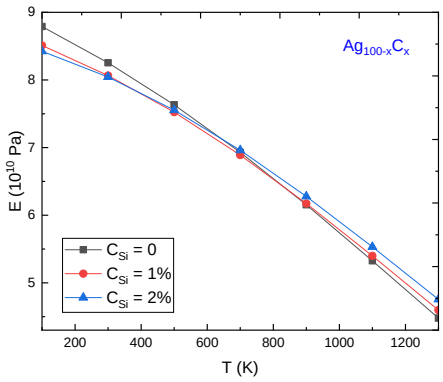

Figure 1. E (T,c_C)(10^{10} Pa) for AgC at P = 0 calculated by the SMM.

According to Table 4, Table 5 and Figure 1, for AgC at zero pressure and with the same concentration of interstitial atoms, when temperature increases, quantities E, G, K, C_{11}, C_{12}, C_{44} descrease. For AgC at zero pressure and at the same temperature, when the concentration of interstitial atoms increases, quantities E, G, K, C_{11}, C_{12}, C_{44} descrease.

We use the Voigt-Reuss-Hill conversion rule [19] for polycrystalline samples as follows:

$$E = \frac{9KG}{3K+G}, K = \frac{C_{11}^* + 2C_{12}^*}{3}, G = \frac{3\left(C_{11}^* - C_{12}^*\right)^2 + 38\left(C_{11}^* - C_{12}^*\right)C_{44}^* + 12C_{44}^{*2}}{30\left(C_{11}^* - C_{12}^*\right) + 40C_{44}^*}. \quad (30)$$

Note that the sign * is used to show elastic quantities of monocrystalline material.

Table 6. The dependence of elastic modulus E (10^{10} Pa) on temperature and concentration of interstitial atoms for FCC-AgC at P = 0, T < 300K calculated by the SMM, calculations (CAL)[20] and EXPT[21].

T(K)	c_C = 0			c_C = 1%	c_C = 2%	c_C = 5%
	SMM	CAL[20]	EXPT[21]			
79	8.84	13.04	8.75	8.55	8.46	9.21
98	8.79	12.99	8.69	8.51	8.43	9.20
123	8.73	12.91	8.60	8.46	8.39	9.16
148	8.67	12.83	8.53	8.41	8.34	9.12
173	8.60	12.74	8.44	8.36	8.30	9.09
198	8.54	12.64	8.35	8.30	8.25	9.05
223	8.47	12.55	8.27	8.25	8.20	9.01
248	8.40	12.45	8.19	8.19	8.15	8.96
273	8.33	12.37	8.10	8.13	8.10	8.92
298	8.26	12.09	8.03	8.07	8.05	8.87

Table 7. The dependence of elastic modulus E (10^{10} Pa) on temperature and concentration of interstitial atoms for FCC-AgC at P = 0, T > 300K calculated by the SMM and CAL[22].

T(K)	c_C = 0		c_C = 1%	c_C = 3%	c_C = 5%
	SMM	CAL[22]			
300	8.253	9.245	8.064	8.177	8.862
500	7.633	8.306	7.524	7.714	8.377
750	6.742	6.872	6.717	6.974	7.576
1000	5.744	5.634	5.791	6.095	6.626

For the Young modulus of Ag at zero pressure and temperatures T < 300K, the SMM calculations in this paper are better than calculations in [20] in comparison with the experimental data in [21]. At temperatures T ≥ 750K, the SMM calculations are nearly the same as the calculations in [22] (see Table 6, Table 7, Figure 2 and Figure 3). Figure 4 and Figure 5 show the dependences of quantities E, G, K, C_{11}, C_{12}, C_{44} on the concentration of interstitial atoms for AgC at zero pressure and T = 500K.

According to Tables 8-10 and Figure 6, for AgC at T = 300K and under the same pressure, when the concentration of interstitial atoms increases, quantities E, G, K, C_{11}, C_{12}, C_{44} increase. For AgC at T = 300K and with the same concentration of interstitial atoms, when pressure increases, quantities E, G, K, C_{11}, C_{12}, C_{44} also increase. That agrees with the experimental rules.

When we use the Mie-Lennard-Jones potential, potential parameters for interactions Ag-Ag and C-C are taken from [14] and potential parameters for interaction Ag-C are determined approximately by

$$D_{Ag\text{-}Ci} = \sqrt{D_{Ag\text{-}Ag}.D_{C\text{-}C}}, r_{0Ag\text{-}C} = \frac{1}{2}\left(r_{0Ag\text{-}Ag} + r_{0C\text{-}C}\right) \quad (31)$$

and parameters m and n are fitted with the experimental data of Young modulus. In this paper, when we use the Morse potential [15] for interaction Ag-C, we do not apply the above-mentioned process of fitting.

However, both ways of using potential give the same law of elastic deformation in respect to temperature, pressure and concentration of interstitial atoms.

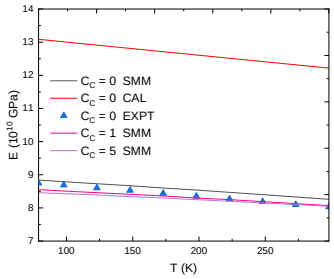

Figure 2. E (T,c_C)(10^{10} Pa) for AgC at P = 0, T < 300K calculated by SMM, CAL[20] and from EXPT[21]

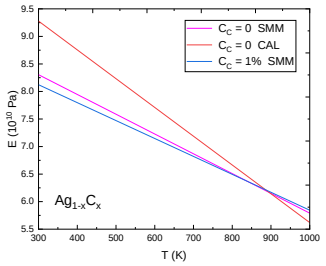

Figure 3. E (T,c_C)(10^{10} Pa) for AgC at P = 0, T > 300K calculated by SMM and CAL[22]

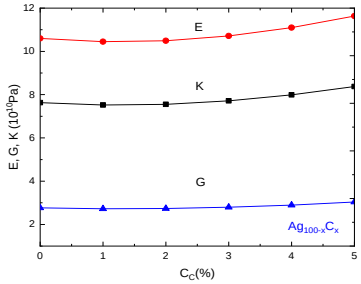

Figure 4. E(c_C), G(c_C), K (c_C) (10^{11}Pa) for AgC at P = 0, T = 500K calculated by SMM

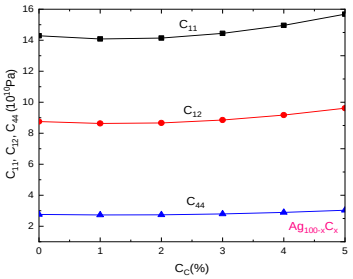

Figure 5. C_{11}(c_C), C_{12}(c_C), C_{44} (c_C) (10^{11}Pa) for AgC at P = 0, T = 500K calculated by SMM

Table 8. The dependence of mean nearest neighbor distance a_{AgC} (Å) on pressure and concentration of interstitial atoms for FCC-AgC at T = 300K calculated by the SMM

P (GPa)	c_C(%)	0	1	2	3	4	5
20	a_{AgC}(Å)	2.6936	2.7056	2.7177	2.7297	2.7417	2.7538
40		2.6200	2.6322	2.6445	2.6567	2.6690	2.6812
60		2.5702	2.5825	2.5949	2.6073	2.6196	2.6320
80		2.5325	2.5449	2.5573	2.5698	2.5822	2.5946
100		2.5021	2.5145	2.5270	2.5395	2.5520	2.5645
120		2.4766	2.4891	2.5016	2.5142	2.5267	2.5392
140		2.4547	2.4673	2.4798	2.4924	2.5049	2.5174
160		2.4355	2.4481	2.4607	2.4732	2.4858	2.4983

Table 9. The dependence of elastic moduli E, G, K (10^{10} Pa) on pressure and concentration of interstitial atoms for FCC-AgC at T = 300K calculated by the SMM

P (GPa)	c_C(%)	0	1	2	3	4	5
20	E	17.7977	17.9656	18.5129	19.4059	20.6143	22.1101
	K	24.7190	24.9522	25.7123	26.9527	28.6309	30.7085
	G	6.4484	6.5093	6.7076	7.0311	7.4689	8.0109
40	E	26.6268	27.1989	28.3459	30.0139	32.1543	34.7228

	K	36.9816	37.7763	39.3693	41.6860	44.6587	48.2261
	G	9.6474	9.8547	10.2703	10.8746	11.6501	12.5807
60	E	35.0413	36.0213	37.7652	40.1989	43.2554	46.8744
	K	48.6685	50.0296	52.4516	55.8317	60.0770	65.1034
	G	12.6961	13.0512	13.6830	14.5648	15.6723	16.9835
80	E	43.2174	44.6109	46.9540	50.1523	54.1206	58.7820
	K	60.0242	61.9595	65.2138	69.6559	75.1674	81.6416
	G	15.6585	16.1634	17.0123	18.1711	19.6089	21.2978
100	E	51.2338	53.0459	55.9914	59.9554	64.8344	70.5348
	K	71.1580	73.6748	77.7658	83.2714	90.0477	97.9650
	G	18.5630	19.2195	20.2867	21.7230	23.4907	25.5561
120	E	59.1336	61.3688	64.9200	69.6516	75.4414	82.1797
	K	82.1300	85.2345	90.1666	96.7383	104.7798	114.1385
	G	21.4252	22.2351	23.5217	25.2361	27.3339	29.7753
140	E	66.9437	69.6058	73.7656	79.2668	85.9685	93.7443
	K	92.9774	96.6748	102.4523	110.0927	119.4007	130.2004
	G	24.2550	25.2195	26.7267	28.7198	31.1480	33.9653
160	E	74.6819	77.7743	82.5455	88.8182	96.4329	105.2466
	K	103.7249	108.0199	114.6465	123.3586	133.9346	146.1758
	G	27.0587	28.1791	29.9078	32.1805	34.9395	38.1328

Table 10. The dependence of elastic constants C_{11}, C_{12}, C_{44} (10^{10} Pa) on pressure and concentration of interstitial atoms for FCC-AgC at T = 300K calculated by the SMM

P (GPa)	c_C(%)	0	1	2	3	4	5
20	C_{11}	33.3169	33.6312	34.6557	36.3275	38.5895	41.3897
	C_{12}	20.4200	20.6127	21.2406	22.2653	23.6516	25.3679
	C_{44}	6.4484	6.5093	6.7076	7.0311	7.4689	8.0109
40	C_{11}	49.8448	50.9159	53.0630	56.1855	60.1922	65.0004
	C_{12}	30.5500	31.2065	32.5225	34.4363	36.8920	39.8390
	C_{44}	9.6474	9.8547	10.2703	10.8746	11.6501	12.5807
60	C_{11}	65.5967	67.4312	70.6957	75.2515	80.9733	87.7481
	C_{12}	40.2044	41.3288	43.3296	46.1219	49.6288	53.7811
	C_{44}	12.6961	13.0512	13.6830	14.5648	15.6723	16.9835
80	C_{11}	80.9022	83.5107	87.8969	93.8841	101.3126	110.0387
	C_{12}	49.5852	51.1840	53.8723	57.5418	62.0948	67.4431
	C_{44}	15.6585	16.1634	17.0123	18.1711	19.6089	21.2978
100	C_{11}	95.9086	99.3008	104.8148	112.2354	121.3687	132.0398
	C_{12}	58.7827	60.8618	64.2413	68.7894	74.3872	80.9276
	C_{44}	18.5630	19.2195	20.2867	21.7230	23.4907	25.5561
120	C_{11}	110.6970	114.8812	121.5290	130.3864	141.2249	153.8388
	C_{12}	67.8466	70.4111	74.4855	79.9142	86.5572	94.2883
	C_{44}	21.4252	22.2351	23.5217	25.2361	27.3339	29.7753
140	C_{11}	125.3174	130.3008	138.0879	148.3858	160.9313	175.4875
	C_{12}	76.8074	79.8618	84.6345	90.9462	98.6353	107.5569
	C_{44}	24.2550	25.2195	26.7267	28.7198	31.1480	33.9653
160	C_{11}	139.8032	145.5921	154.5236	166.2659	180.5206	197.0196
	C_{12}	85.6858	89.2338	94.7080	101.9049	110.6416	120.7539
	C_{44}	27.0587	28.1791	29.9078	32.1805	34.9395	38.1328

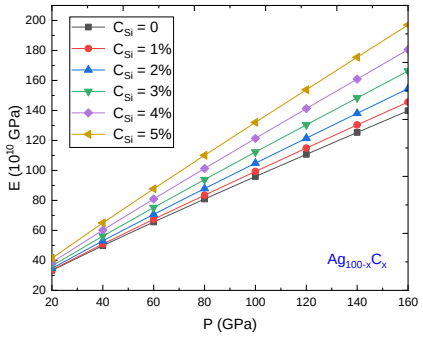

Figure 6. E(P)(10^{10} Pa) for FCC-AgC at T = 300 K calculated by the SMM.

3. Conclusion

From the obtained theoretical results and using the combination of the Mie-Lennard-Jones potential and the Morse potential, we calculated characteristic quantities for elastic deformation of FCC-AgC. We obtained the values of elastic moduli and elastic constants, and compared the calculated results with experiments and other calculations, and some of our calculated results were found to be in good agreement with available experiments and others suggest further experiment.

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