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 C₁₁, C₁₂, C₄₄ 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
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 \( c_B \ll c_A \), 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]

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

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

\[\gamma_B = 4(\gamma_{1B} + \gamma_{2B}), (3)\]

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

\[\gamma_{2B} = \frac{6}{48} \sum_{i=1}^{4} \left( \frac{\partial^4 \varphi_{AB}}{\partial u_{2B}^4} \right)_{eq} = \frac{1}{2r_{1B}} \frac{d^3 \varphi_{AB}(r_{1B})}{dr_{1B}^3} + \frac{3}{4r_{1B}^3} \frac{d^2 \varphi_{AB}(r_{1B})}{dr_{1B}^2} + \frac{3}{4r_{1B}^3} \frac{d \varphi_{AB}(r_{1B})}{dr_{1B}} + \frac{9}{54} \frac{d^4 \varphi_{AB}(r_{2B})}{dr_{2B}^4} + \frac{2}{3r_{2B}^2} \frac{d^3 \varphi_{AB}(r_{2B})}{dr_{2B}^3} + \frac{2}{3r_{2B}^2} \frac{d \varphi_{AB}(r_{2B})}{dr_{2B}}, (5)\]

\[u_{0A_1} = u_{0A} + \varphi_{AB}(r_{1A_1}), (6)\]

\[k_{A_1} = k_A + \frac{1}{2} \sum_{i=1}^{4} \left[ \frac{\partial^2 \varphi_{AB}}{\partial u_{1A_1}^2} \right]_{r=r_{1A_1}} = k_A + \frac{d^2 \varphi_{AB}(r_{1A_1})}{dr_{1A_1}^2}, (7)\]

\[\gamma_{A_1} = 4(\gamma_{1A_1} + \gamma_{2A_1}), (8)\]

\[\gamma_{1A_1} = \gamma_{1A} + \frac{1}{48} \sum_{i=1}^{4} \left[ \frac{\partial^4 \varphi_{AB}}{\partial u_{1A_1}^4} \right]_{r=r_{1A_1}} = \gamma_{1A} + \frac{1}{24} \frac{d^4 \varphi_{AB}(r_{1A_1})}{dr_{1A_1}^4}, (9)\]
\[ \gamma_{2A_1} = \gamma_{2A} + \frac{6}{48} \sum_i \left[ \left( \frac{\partial^2 \varphi_{AB}}{\partial u^2_{\alpha i} \partial u^2_{\beta i}} \right)_{eq, j=1} \right] = \]

\[ = \gamma_{2A} + \frac{1}{4r_{1A_i}} \frac{d^3 \varphi_{AB}(r_{1A_i})}{dr^3_{1A_i}} - \frac{1}{2r^2_{1A_i}} \frac{d^2 \varphi_{AB}(r_{1A_i})}{dr^2_{1A_i}} + \frac{1}{2r^3_{1A_i}} \frac{d \varphi_{AB}(r_{1A_i})}{dr_{1A_i}}, \quad (10) \]

\[ u_{0A_2} = u_{0A} + \phi_{AB}(r_{1A_2}), \quad \text{(11)} \]

\[ k_{A_2} = k_A + \frac{1}{2} \sum_i \left[ \left( \frac{\partial^2 \varphi_{AB}}{\partial u^2_{\beta i}} \right)_{eq, j=1} \right] = k_A + \frac{1}{6} \frac{d^2 \varphi_{AB}(r_{1A_2})}{dr^2_{1A_2}} + \frac{23}{6r^3_{1A_2}} \frac{d \varphi_{AB}(r_{1A_2})}{dr_{1A_2}}, \quad (12) \]

\[ \gamma_{A_2} = \frac{1}{4} \left( \gamma_{1A_2} + \gamma_{2A_2} \right), \quad \text{(13)} \]

where \( \varphi_{AB} \) is the interaction potential between atoms A and B, \( r_{1X} = r_{01X} + y_{0}(T) \) 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, \( u_{0X}, y_{0}(T) \) 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]

\[ u_{0A} = 6\varphi_{AA}(r_{1A}) + 3\varphi_{AA}(r_{2A}), \quad r_{2A} = \sqrt{2r_{1A}}, \quad \text{(16)} \]

\[ k_A = 2 \left[ \frac{d^2 \varphi_{AA}(r_{1A})}{dr^2_{1A}} + \frac{d \varphi_{AA}(r_{1A})}{dr_{1A}} + \frac{d^2 \varphi_{AA}(r_{2A})}{dr^2_{2A}} + \frac{2 \varphi_{AA}(r_{2A})}{dr_{2A}} \right], \quad \text{(17)} \]

\[ \gamma_{1A} = \frac{1}{24} \frac{d^4 \varphi_{AA}(r_{1A})}{dr^4_{1A}} + \frac{1}{4r^2_{1A}} \frac{d^3 \varphi_{AA}(r_{1A})}{dr^3_{1A}} + \frac{1}{8r^4_{1A}} \frac{d^2 \varphi_{AA}(r_{1A})}{dr^2_{1A}} + \frac{1}{8r^8_{1A}} \frac{d \varphi_{AA}(r_{1A})}{dr_{1A}}, \quad \text{(18)} \]
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 \[16\]

\[
\psi = U_{0X} + \psi_{0X} + 3N \left\{ \frac{\theta^3}{(k \theta)^2} \left[ \frac{1}{2} \gamma_{2X} \left( Y_X \right)^2 - \frac{2}{3} \gamma_{1X} \left( 1 + \frac{Y_X}{2} \right) \right] + \frac{2 \theta^3}{(k \theta)^2} \left[ \frac{4}{3} \gamma_{2X} \left( Y_X \right)^2 - 2 \gamma_{1X} \gamma_{2X} \left( 1 + \frac{Y_X}{2} \right) \left( 1 + Y_X \right) \right] \right\},
\]

where $\psi_X$ 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.

From \(21\), we can calculate the nearest neighbor distance $r_{1X}(P,0)$ ($X = A, A_1, A_2, B$), the parameters $k_X(P,0), \gamma_{1X}(P,0), \gamma_{2X}(P,0), \gamma_{3X}(P,0)$, 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 $r_{1A}(P,T)$ as follows: \[10-16\]

\[
r_{1B}(P,T) = r_{1B}(P,0) + y_B(P,T) + r_{1A}(P,T) = r_{1A}(P,0) + y_A(P,T),
\]

\[
r_{1A_1}(P,T) = r_{1B}(P,T) + r_{1A_2}(P,T) = r_{1A_2}(P,0) + y_{A_1}(P,T),
\]

\[
r_{1A}(P,T) = r_{1A}(P,0) + y(P,T),
\]

\[
r_{1A}(P,0) = (1 - c_B) r_{1A}(P,0) + c_B r_{1A}'(P,0), r_{1A}'(P,0) = \sqrt{2} r_{1B}(P,0),
\]

\[
y(P,T) = (1 - 15c_B) y_A(P,T) + c_B y_B(P,T) + 6c_B^2 y_{A_2}(P,T) + 8c_B y_{A_1}(P,T).
\]
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]

$$
E = \frac{1}{\pi t_A A_{1A}} \left( 1 - 15c_B + c_B \right) \left( 1 - \frac{\partial^2 \varphi_B}{\partial \varepsilon^2} + \frac{6}{c_B} \frac{\partial^2 \varphi_A}{\partial \varepsilon^2} + 8 \frac{\partial^2 \varphi_A}{c_B \partial \varepsilon^2} \right),
$$

$$
A_{1A} = \frac{1}{k_A} \left[ 1 + \frac{2g_A^2 \partial^2}{k_A} \left( 1 + \frac{Y_A}{Y_B} \right) \left( 1 + Y_A \right) \right],
$$

$$
K_{AB} = \frac{E_{AB}}{3(1 - 2\nu_A)},
$$

$$
G_{AB} = \frac{E_{AB}}{2(1 + \nu_A)},
$$

$$
C_{11AB} = \frac{E_{AB}(1 - \nu_A)}{(1 + \nu_A)(1 - 2\nu_A)},
$$

$$
C_{12AB} = \frac{E_{AB}\nu_A}{(1 + \nu_A)(1 - 2\nu_A)},
$$

$$
C_{44AB} = \frac{E_{AB}}{2(1 + \nu_A)},
$$

where $\nu_A, \nu_B$ 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]

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

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].

| Interaction | D/kB (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]

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

where the parameters $\beta, \delta, r_w, N$ are given in Table 2.
Table 2. Morse potential parameters for interaction Ag-C [15]

| Interaction | \( \beta (eV) \) | \( \delta (\text{Å})^{-1} \) | \( r_o (\text{Å}) \) | \( N \) |
|-------------|-----------------|-----------------|-----------------|-------|
| 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 \( a_{AgC} (\text{Å}) \) for FCC-AgC at \( P = 0 \) calculated by the SMM

| \( T \) (K) | \( c_c(\%) \) | 0     | 1     | 2     | 3     | 4     | 5     |
|------------|--------------|-------|-------|-------|-------|-------|-------|
| 100        |              | 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        | \( a_{AgC}(\text{Å}) \) | 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} \text{ 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|
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 $E$, $G$, $K$, $C_{11}$, $C_{12}$, $C_{44}$ decrease. For AgC at zero pressure and at the same temperature, when the concentration of interstitial atoms increases, quantities $E$, $G$, $K$, $C_{11}$, $C_{12}$, $C_{44}$ decrease.

We use the Voigt-Reuss-Hill conversion rule [19] for polycrystalline samples as follows:
\[ E = \frac{9K_G}{3K + G}, \quad K = \frac{C_{11}^* + 2C_{12}^*}{3}, \quad G = \frac{3(C_{11}^* - C_{12}^*)^2 + 38(C_{11}^* - C_{12}^*)C_{44}^* + 12C_{44}^*}{30(C_{11}^* - C_{12}^*)^{11} + 40C_{44}^*}. \]  

(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] | SMM | CAL[20] | EXPT[21] | 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] | SMM | CAL[22] | SMM | CAL[22] | 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 \( \geq 750K \), 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

\[ D_{\text{Ag-C}} = \sqrt{D_{\text{Ag-Ag}} \cdot D_{\text{C-C}}} \cdot \pi_{\text{Ag-C}} = \frac{1}{2} \left( \sigma_{\text{Ag-Ag}} + \sigma_{\text{C-C}} \right) \]  

(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.

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) | cC (%) | 0    | 1    | 2    | 3    | 4    | 5    |
|---------|--------|------|------|------|------|------|------|
| 20      |        | 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) | cC (%) | 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  | 6.5993  | 6.7076  | 7.0311  | 7.4689  | 8.0109  |
| 40      | E      | 26.6268 | 27.1989 | 28.3459 | 30.0139 | 32.1543 | 34.7228 |
| P (GPa) | c11 (10^10 Pa) | c12 | c13 | c44 |
|---------|----------------|------|------|------|
| 20      | 33.3169        | 20.4200 | 6.4484 | 6.5932 |
| 40      | 49.8484        | 30.5500 | 9.6474 | 7.0920 |
| 60      | 65.5967        | 40.2044 | 12.6961 | 8.9510 |
| 80      | 80.9022        | 49.5852 | 15.6585 | 16.1634 |
| 100     | 95.9086        | 58.7827 | 18.5630 | 19.2195 |
| 120     | 110.6970       | 67.8466 | 21.4252 | 22.2351 |
| 140     | 125.3174       | 76.8074 | 24.2550 | 25.2195 |
| 160     | 139.8032       | 85.6858 | 27.0587 | 28.1791 |

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
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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