ELASTIC DEFORMATION OF BINARY AND TERNARY INTERSTITIAL ALLOYS WITH FCC STRUCTURE AT ZERO PRESSURE: DEPENDENCE ON TEMPERATURE, CONCENTRATION OF SUBSTITUTION ATOMS AND CONCENTRATION OF INTERSTITIAL ATOMS

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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, the bulk modulus, the rigidity modulus and the elastic constants for interstitial alloy AC and interstitial alloy ABC (substitution alloy AB with interstitial atom C) with FCC structure at zero pressure are derived using the statistical moment method. We apply the theoretical results to the interstitial alloys AuLi and AuCuLi at zero pressure and at different temperatures, concentrations of substitution atoms and interstitial atoms. Calculated results for the main metal in these alloys are compared with the experimental data and other calculations.

Keywords: Binary and ternary interstitial alloy, statistical moment method, Young modulus, bulk modulus, rigidity modulus, elastic constant.

1. Introduction

The elastic deformation of metals and alloys has attracted the attention of many researchers [1-16]. In this paper the authors have used the statistical moment method (SMM) [1, 2, 16] to derive 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 $G$ and the rigidity modulus $K$, and the elastic constants $C_{11}, C_{12}, C_{44}$ depending on temperature, concentration of substitution atoms and concentration of interstitial atoms for interstitial alloy AC and interstitial alloy ABC (substitution alloy AB with interstitial atom C) with FCC structure at zero pressure. We applied the theoretical results to the interstitial alloys AuLi and AuCuLi at zero pressure and at different temperatures, concentration of substitution atoms and interstitial atoms. Some of the calculated results for the main metals in the alloys are compared with the experimental data and the other calculations.
2. Content

2.1. Elastic deformation of interstitial alloy AC with FCC structure

The bound energy of atom C (in the body center of a cubic unit cell) with atoms A (in the face centers and peaks of the cubic unit cell) in the approximation of three coordination spheres with a center C and radii \( r_1, r_1\sqrt{3}, r_1\sqrt{5} \) is determined by [1, 2]

\[
u_{0C} = \sum_{i=1}^{n_C} \varphi_{AC}(r_i) = 6\varphi_{AC}(r_1) + 8\varphi_{AC}(r_1\sqrt{3}) + 24\varphi_{AC}(r_1\sqrt{5}), \tag{2.1} \]

where \( \varphi_{AC} \) is the interaction potential between atom A and atom C, \( r_1 \equiv r_{1C} = r_{01C} + y_{0A_1}(T) \) is the nearest neighbor distance between interstitial atom C and metallic atom A at temperature \( T \), \( r_{01C} \) is the nearest neighbor distance between interstitial atom C and metallic atom A at 0 K and is determined from the minimum condition of the bound energy \( u_{0C}, y_{0A_1}(T) \) is the displacement of atom \( A_1 \) (atom A stays in the face center of cubic unit cell) from equilibrium position at temperature \( T \). The alloy’s parameters for atom C in the approximation of three coordination spheres have the form [1, 2]

\[
k_C = \varphi_{AC}^{(2)}(r_1) + \frac{2}{r_1}\varphi_{AC}^{(1)}(r_1) + \frac{4}{3}\varphi_{AC}^{(2)}(r_1\sqrt{3}) + \frac{8\sqrt{3}}{9r_1}\varphi_{AC}^{(1)}(r_1\sqrt{3})
+ 4\varphi_{AC}^{(2)}(r_1\sqrt{5}) + \frac{8\sqrt{5}}{5r_1}\varphi_{AC}^{(1)}(r_1\sqrt{5}),
\gamma_C = 4(\gamma_{1C} + \gamma_{2C}),
\gamma_{1C} = \frac{1}{24}\varphi_{AC}^{(4)}(r_1) + \frac{1}{4r_1^2}\varphi_{AC}^{(2)}(r_1) + \frac{1}{4r_1}\varphi_{AC}^{(1)}(r_1) + \frac{1}{54}\varphi_{AC}^{(4)}(r_1\sqrt{3})
+ \frac{2\sqrt{3}}{27r_1}\varphi_{AC}^{(3)}(r_1\sqrt{3}) - \frac{2}{27r_1^2}\varphi_{AC}^{(2)}(r_1\sqrt{3})
+ \frac{2\sqrt{3}}{81r_1^3}\varphi_{AC}^{(1)}(r_1\sqrt{3}) + \frac{17}{150}\varphi_{AC}^{(4)}(r_1\sqrt{5}) + \frac{8\sqrt{5}}{125r_1}\varphi_{AC}^{(3)}(r_1\sqrt{5})
+ \frac{1}{25r_1^2}\varphi_{AC}^{(2)}(r_1\sqrt{5}) - \frac{\sqrt{5}}{125r_1^2}\varphi_{AC}^{(1)}(r_1\sqrt{5}),
\gamma_{2C} = \frac{1}{2r_1}\varphi_{AC}^{(3)}(r_1) - \frac{3}{4r_1^2}\varphi_{AC}^{(2)}(r_1) + \frac{3}{4r_1}\varphi_{AC}^{(1)}(r_1) + \frac{1}{4}\varphi_{AC}^{(4)}(r_1\sqrt{2})
+ \frac{\sqrt{2}}{8r_1}\varphi_{AC}^{(3)}(r_1\sqrt{2}) + \frac{7}{8r_1^2}\varphi_{AC}^{(2)}(r_1\sqrt{2})
- \frac{7\sqrt{2}}{16r_1^3}\varphi_{AC}^{(1)}(r_1\sqrt{2}) + \frac{4}{25}\varphi_{AC}^{(4)}(r_1\sqrt{5}) + \frac{26\sqrt{5}}{125r_1}\varphi_{AC}^{(3)}(r_1\sqrt{5})
- \frac{3}{25r_1^2}\varphi_{AC}^{(2)}(r_1\sqrt{5}) + \frac{3\sqrt{5}}{125r_1^3}\varphi_{AC}^{(1)}(r_1\sqrt{5}), \tag{2.2} \]
where $\varphi^{(k)}_{AC}(r_i) \equiv \frac{\partial^k \varphi_{AC}}{\partial r_i^k}(k = 1, 2, 3, 4)$.

The bound energy of atom $A_1$ (which contains interstitial atom C 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 $A_1$ is determined by [1, 2]

$$u_{0A_1} = u_0A + \varphi_{AC}(r_{1A_1}),$$

$$k_{A_1} = k_A + \varphi^{(2)}_{AC}(r_{1A_1}), \gamma_{A_1} = 4(\gamma_{1A_1} + \gamma_{2A_1}), \gamma_{1A_1} = \gamma_A + \frac{1}{24}\varphi^{(4)}_{AC}(r_{1A_1}),$$

$$\gamma_{2A_1} = \gamma_2 + \frac{1}{4r_{1A_1}}\varphi^{(3)}_{AC}(r_{1A_1}) - \frac{1}{2r_{1A_1}^2}\varphi^{(2)}_{AC}(r_{1A_1}) + \frac{1}{2r_{1A_1}^3}\varphi^{(1)}_{AC}(r_{1A_1}),$$

(2.3)

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

The bound energy of atom $A_2$ (which contains the interstitial atom C on the first coordination sphere) with the atoms in the crystalline lattice and the corresponding alloy’s parameters in the approximation of three coordination spheres with the center $A_2$ is determined by [1, 2]

$$u_{0A_2} = u_0A + \varphi_{AC}(r_{1A_2}),$$

$$k_{A_2} = k_A + \frac{1}{6}\varphi^{(2)}_{AC}(r_{1A_2}) + \frac{23}{6r_{1A_2}}\varphi^{(1)}_{AC}(r_{1A_2}), \gamma_{A_2} = 4(\gamma_{1A_2} + \gamma_{2A_2}),$$

$$\gamma_{1A_2} = \gamma_1 + \frac{1}{54}\varphi^{(4)}_{AC}(r_{1A_2}) + \frac{2}{9r_{1A_2}}\varphi^{(3)}_{AC}(r_{1A_2}) - \frac{2}{9r_{1A_2}^2}\varphi^{(2)}_{AC}(r_{1A_2}) + \frac{2}{9r_{1A_2}^3}\varphi^{(1)}_{AC}(r_{1A_2}),$$

$$\gamma_{2A_2} = \gamma_2 + \frac{1}{81}\varphi^{(4)}_{AC}(r_{1A_2}) + \frac{4}{27r_{1A_2}}\varphi^{(3)}_{AC}(r_{1A_2}) + \frac{14}{27r_{1A_2}^2}\varphi^{(2)}_{AC}(r_{1A_2}) - \frac{14}{27r_{1A_2}^3}\varphi^{(1)}_{AC}(r_{1A_2}),$$

(2.4)

where $r_{1A_2} = r_{01A_2} + y_{0C}(T), r_{01A_2}$ is the nearest neighbor distance between atom $A_2$ and atoms in the crystalline lattice at 0 K and is determined from the minimum condition of the bound energy $u_{0A_2}, y_{0C}(T)$ is the displacement of 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 [1, 2].

The nearest neighbor distances $r_{1X}(0, T)(X = A, A_1, A_2, C)$ in the interstitial alloy at pressure $P = 0$ and temperature $T$ are derived from [16]

$$r_{1A}(0, T) = r_{1A}(0, 0) + y_A(0, T), r_{1C}(0, T) = r_{1C}(0, 0) + y_C(0, T),$$

$$r_{1A_1}(0, T) \approx r_{1C}(0, T), r_{1A_2}(0, T) = r_{1A_2}(0, 0) + y_C(0, T)$$

(2.5)

$r_{1X}(0, 0)(X = A, A_1, A_2, C)$ is determined from the equation of state or the minimum condition of bound energy. From the $r_{1X}(0, 0)$ obtained with the use of Maple software, we can determine the parameters $k_X(0, 0), \gamma_X(0, 0), \omega_X(0, 0)$ at 0 K. After that, we can calculate the displacements $y_{0X}(0, T)$

$$y_{0X}(0, T) = \sqrt{\frac{2\gamma_X(0, 0)\theta^2}{3k_X^2(0, 0)}}A_X(0, T), X = A, A_1, A_2, C,$$

(2.6)
where \( \theta = k_B T \), \( k_B \) is the Boltzmann constant and has the form as in [1, 2]. Then, we calculate the mean nearest neighbor distance in interstitial alloy \( AC \) using the expressions as follows [16]

\[
\overline{r_{1A}(0,T)} = \frac{1}{\pi} \frac{1}{r_1} = \frac{1}{\pi} \frac{1}{r_1(A)} \frac{1}{c_A} A \frac{1}{T} \frac{1}{r_1(A)} (1 - c_C) r_{1A}(0,0) + c_C r_{1A}'(0,0),
\]

\[
\overline{y(0,T)} = (1 - 15c_C) y_{A}(0,T) + c_C y_{C}(0,T) + 6c_C y_{A_1}(0,T) + 8c_C y_{A_2}(0,T),
\]

(2.7)

The Young modulus of interstitial alloy \( AC \) is determined by

\[
E_{AC}(c_C, T) = E_A(c_C, T) \left( 1 - 15c_C + c_C \frac{\partial^2 \psi_C}{\partial \epsilon^2} + 6 \frac{\partial^2 \psi_A}{\partial \epsilon^2} + 8 \frac{\partial^2 \psi_A}{\partial \epsilon^2} \right),
\]

(2.8)

\[
E_A(c_C, T) = \frac{1}{\pi} \frac{1}{r_1} \frac{1}{A_1(c_C, T)},
\]

\[
A_1(c_C, T) = \frac{1}{k_A(c_C, T)} \left[ 1 + \frac{2 \gamma_A^2(c_C, T) \theta^2}{k_A^2(c_C, T)} \left( 1 + \frac{1}{2} X_A \right) (1 + X_A) \right],
\]

\[
X_A \equiv x_A \coth x_A, x_A = \frac{h \omega_A(c_C, T)}{2 \theta},
\]

\[
\frac{\partial^2 \psi_X}{\partial \epsilon^2} = \left( \frac{1}{2} \frac{\partial^2 \psi_{X0}}{\partial r_1^2} + \frac{3}{4} \frac{h \omega_X}{k_X} \left[ \frac{\partial^2 k_X}{\partial r_1^2} - \frac{1}{2k_X} \left( \frac{\partial k_X}{\partial r_1} \right)^2 \right] \right) 4 \nu_{01}^2 + \frac{1}{2} \frac{\partial \psi_{X0}}{\partial r_1} + \frac{3}{2} \frac{h \omega_X \coth x_X}{2k_X} \frac{1}{2k_X} \frac{\partial k_X}{\partial r_1} 2 \nu_{01}, x_X = \frac{h \omega_X}{2 \theta}, \omega_X = \sqrt{\frac{k_X}{m}}.
\]

(2.9)

The bulk modulus and the rigidity modulus of interstitial alloy \( AC \) have the form

\[
K_{AC}(c_C, T) = \frac{E_{AC}(c_C, T)}{3(1 - 2 \nu_A)}, G_{AC}(c_C, T) = \frac{E(c_C, T)}{2(1 + \nu_A)}.
\]

The elastic constants of interstitial alloy \( AC \) have the form

\[
C_{11AC}(c_C, T) = \frac{E(c_C, T) (1 - \nu_A)}{(1 + \nu_A) (1 - 2 \nu_A)},
\]

\[
C_{12AC}(c_C, T) = \frac{E(c_C, T) \nu_A}{(1 + \nu_A) (1 - 2 \nu_A)}, C_{44AC}(c_C, T) = \frac{E(c_C, T)}{2(1 + \nu_A)}.
\]

(2.10)

The Poisson ratio of interstitial alloy \( AC \) has the form

\[
\nu_{AC} = c_A \nu_A + c_C \nu_C \approx \nu_A,
\]

(2.11)

where \( \nu_A \) and \( \nu_C \) are the Poisson ratio of the materials \( A \), \( C \) and \( c_A \) is the concentration of main atoms \( A \).
2.2. Elastic deformation of ABC interstitial alloy with FCC structure

The mean nearest neighbor distance between two atoms in the interstitial alloy ABC with FCC structure at temperature $T$ is given by

$$a_{ABC} = c_{AC}a_{AC}\frac{B_{TAC}}{B_T} + c_{B}a_{B}\frac{B_{TB}}{B_T}, B_T = c_{AC}B_{TAC} + c_{B}B_{TB}, c_{AC} = c_A + c_C, a_{AC} = \overline{r_{1A}}(0, T),$$

$$B_{TAC} = \frac{1}{\chi_{TAC}}, \chi_{TAC} = \frac{3\left(\frac{a_{AC}}{a_{0AC}}\right)^3}{2\sqrt{2}a_{AC} \frac{\partial^2 \psi_{AC}}{\partial a_{AC}^2} T},$$

$$\left(\frac{\partial^2 \psi_{AC}}{\partial a_{AC}^2}\right)_T = \left[\frac{\partial^2 \psi_{AC}}{\partial t_{1AC}^2(0, T)}\right]_T \approx (1 - 15c_C) \left(\frac{\partial^2 \psi_A}{\partial a_{A}^2}\right)_T$$

$$+ c_C \left(\frac{\partial^2 \psi_C}{\partial a_{C}^2}\right)_T + 6c_C \left(\frac{\partial^2 \psi_{A_1}}{\partial a_{A_1}^2}\right)_T + 8c_C \left(\frac{\partial^2 \psi_{A_2}}{\partial a_{A_2}^2}\right)_T,$$

$$\left(\frac{\partial^2 \psi_X}{\partial a_{X}^2}\right)_T = \left(\frac{\partial^2 \psi_{X}}{\partial r_{1X}^2(0, T)}\right)_T \frac{1}{3N} \left(\frac{\partial^2 \psi_{X}}{\partial a_{X}^2}\right)_T = \frac{1}{6} \frac{\partial^2 u_{0X}}{\partial a_{X}^2} + \frac{\hbar \omega_X}{4k_X} \left[\frac{\partial^2 k_X}{\partial a_{X}^2} - \frac{1}{2k_X} \left(\frac{\partial k_X}{\partial a_{X}}\right)^2\right].$$

(2.12)

The Young modulus of interstitial alloy ABC is determined by

$$E_{ABC} = E_{AB} - (c_A + c_B) E_A + E_{AC}, E_{AB} = c_A E_A + c_B E_B,$$

$$E_{AC} = E_A \left(1 - 15c_C + c_C \frac{\partial^2 \psi_C}{\partial a_{C}^2} + 6 \frac{\partial^2 \psi_{A_1}}{\partial a_{A_1}^2} + 8 \frac{\partial^2 \psi_{A_2}}{\partial a_{A_2}^2}\right),$$

(2.13)

where $E_{AB}$ is the Young modulus of substitution alloy AB and $E_{AC}$ is the Young modulus of interstitial alloy AC.

The bulk modulus and rigidity modulus of interstitial alloy ABC have the form

$$K_{ABC} = \frac{E_{ABC}}{3(1 - 2\nu_{ABC})}, G_{ABC} = \frac{E_{ABC}}{2(1 + \nu_{ABC})}.\quad (2.14)$$

The elastic constants of interstitial alloy ABC have the form

$$C_{11ABC} = \frac{E_{ABC}(1 - \nu_{ABC})}{(1 + \nu_{ABC})(1 - 2\nu_{ABC})}, C_{12ABC} = \frac{E_{ABC}\nu_{ABC}}{(1 + \nu_{ABC})(1 - 2\nu_{ABC})},$$

$$C_{44ABC} = \frac{E_{ABC}}{2(1 + \nu_{ABC})}.\quad (2.15)$$

The Poisson ratio of interstitial alloy ABC has the form

$$\nu_{ABC} = c_A\nu_A + c_B\nu_B + c_C\nu_C \approx c_A\nu_A + c_B\nu_B = \nu_{AB}.\quad (2.16)$$

where $c_B$ is the concentration of substitution atoms B and $\nu_{AB}$ is the Poisson ratio of substitution alloy AB.
2.3. Numerical results and discussion for alloys AuLi and AuCuLi

For metallic crystal, we can apply the n-m pair potential in the form as follows [1]

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

(2.17)

where the potential parameters and the Poisson ratio for materials Au, Cu and Li are presented in Table 1 [3].

<table>
<thead>
<tr>
<th>Material</th>
<th>m</th>
<th>n</th>
<th>D ((10^{-16})\ \text{erg})</th>
<th>r_0 ((10^{-19})\ \text{m})</th>
<th>\nu</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au</td>
<td>5.5</td>
<td>10.5</td>
<td>6462.54</td>
<td>2.8751</td>
<td>0.39</td>
</tr>
<tr>
<td>Cu</td>
<td>5.5</td>
<td>11</td>
<td>4693.518</td>
<td>2.5487</td>
<td>0.37</td>
</tr>
<tr>
<td>Li</td>
<td>1.66</td>
<td>3.39</td>
<td>6800.502</td>
<td>3.0077</td>
<td></td>
</tr>
</tbody>
</table>

For the interaction between the main atom A and the interstitial atom C in the interstitial alloy,

\[
\varphi_{AC}(a) \approx \frac{1}{2} \left[ \varphi_{AA}(a) + \varphi_{CC}(a) \right].
\]

(2.18)

According to Figures 1 and 2 at the same temperature when the concentration of interstitial atoms increases, the mean nearest neighbor distance in alloy AuLi increases. In the same concentration of interstitial atoms when the temperatures increases, the mean nearest neighbor distance in alloy AuLi increases. The increase in concentration of interstitial atoms is stronger than the increase with temperature (when the concentration of interstitial atoms increases from 0 to 5%, the mean nearest neighbor distance increases from 2.8402 to 2.9457 Å but when the temperature increases from 50 to 1000 K, the mean nearest neighbor distance increases from 2.8402 to 2.8848 Å). At zero concentration of interstitial atoms, we obtain the nearest neighbor distance of pure metal Au in [1].

According to Figures 3 and 4 at the same temperature when the concentration of interstitial atoms increases, the elastic moduli $E, K$ and the elastic constants of alloy AuLi decrease. In the same concentration of interstitial atoms, when the temperatures increases, the elastic moduli $E, K$ of alloy AuLi decrease. At zero concentration of interstitial atoms, we obtain the elastic moduli $E$ and $K$ of pure Au in [1].

According to Figures 5 and 6 at the same temperature when the concentration of interstitial atoms increases, the elastic constants $C_{11}, C_{12}, C_{44}$ of alloy AuLi decrease. At the same concentration of interstitial atoms when the temperatures increases, the elastic constants $C_{11}, C_{12}, C_{44}$ of alloy AuLi decrease. At zero concentration of interstitial atoms, we obtain the elastic constants $C_{11}, C_{12}$ and $C_{44}$ of pure Au in [1].

The calculated (CAL) results from the SMM and the other calculations and the experimental data (EXPT) for the nearest neighbor distance, the elastic moduli and the elastic constants of main metal Au in interstitial alloys AuLi and AuCuLi are shown in Tables 2 and 3. Some calculated results from the SMM are in rather good agreement with experimental data and better than that obtained using other calculation methods.
Elastic deformation of binary and ternary interstitial alloys with fcc structure at zero pressure...

Table 2. The nearest neighbor distance and elastic moduli of Au at P = 0, T = 300 K from the SMM and the experimental data [5, 6]

<table>
<thead>
<tr>
<th>Method</th>
<th>a(Å)</th>
<th>E(10^10 Pa)</th>
<th>K(10^10 Pa)</th>
<th>G(10^10 Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SMM</td>
<td>2.8454</td>
<td>8.96</td>
<td>14.94</td>
<td>3.20</td>
</tr>
<tr>
<td>EXPT[5,6]</td>
<td>2.8838</td>
<td>2.8838</td>
<td>16.70</td>
<td>3.10</td>
</tr>
</tbody>
</table>
Table 3. The elastic constants of Au at $P = 0$, $T = 300$ K

from the SMM, other calculations [7-15] and experimental data [6]

<table>
<thead>
<tr>
<th>Elastic constant (10$^{10}$ Pa)</th>
<th>SMM</th>
<th>EXPT</th>
<th>Other calculations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}$</td>
<td>1.92</td>
<td>1.92</td>
<td>1.92</td>
</tr>
<tr>
<td>$C_{12}$</td>
<td>1.28</td>
<td>1.65</td>
<td>1.66</td>
</tr>
<tr>
<td>$C_{44}$</td>
<td>0.32</td>
<td>0.42</td>
<td>0.39</td>
</tr>
</tbody>
</table>

According to Figures 7-10 for alloy AuCuLi at the same temperature and concentration of substitution atoms when the concentration of interstitial atoms increases, the mean nearest neighbor distance increases (for example at 50 K and $c_{Cu} = 6\%$, $a$ increases from 2.8069 Å to 2.9162 Å when $c_{Li}$ increases from 0 to 5%). For alloy AuCuLi at the same concentration of substitution atoms and interstitial atoms when the temperature increases, the mean nearest neighbor distance increases (for example at $c_{Cu} = 6\%$, $c_{Li} = 5\%$, $a$ increases from 2.9162 Å to 2.9162 Å as the temperature increases from 0 to 1000 K).
to 3.6067 Å when \( T \) increases from 50 to 1000 K. For alloy AuCuLi at the same temperature and concentration of interstitial atoms when the concentration of substitution atoms increases, the mean nearest neighbor distance decreases (for example at 1000 K, \( c_{Li} = 0.6\% \), \( a \) decreases from 2.9743 to 2.9521 Å when \( c_{Cu} \) increases from 0 to 6\%). At zero concentration of substitution atoms, and interstitial atoms, the mean nearest neighbor distance of interstitial alloy AuCuLi becomes the mean nearest neighbor distance of metal Au in [1]. The change of mean nearest neighbor distance with temperature for interstitial alloy AuCuLi is similar to that for interstitial alloy AuLi. The change of mean nearest neighbor distance with temperature and concentration of substitution atoms for interstitial alloy AuCuLi is similar to that for substitution alloy AuCu [4].

**Figure 11.** \( E_{AuCuLi}(T), K_{AuCuLi}(T) \)

at \( P = 0, c_{Cu} = 10\%, c_{Li} = 5\% \)

**Figure 12.** \( E_{AuCuLi}(c_{Cu}), K_{AuCuLi}(c_{Cu}) \)

at \( P = 0, c_{Li} = 5\% \)

**Figure 13.** \( E_{AuCuLi}(c_{Li}), K_{AuCuLi}(c_{Li}) \)

at \( P = 0, c_{Cu} = 10\% \)

**Figure 14.** \( C_{11AuCuLi}(T), C_{12AuCuLi}(T) \)

at \( P = 0, c_{Cu} = 10\%, c_{Li} = 5\% \)

According to Figures 11-13 for alloy AuCuLi in the same temperature and concentration of substitution atoms when the concentration of interstitial atoms increases, the elastic moduli \( E \) and \( K \) decrease (for example at 300 K, \( E \) decreases from 11.4259.10\(^{10}\) to 6.3259.10\(^{10}\) Pa when \( c_{Li} \) increases from 0 to 5\%). For alloy AuCuLi in the same concentration of substitution atoms
and concentration of interstitial atoms when the temperature increases, the elastic moduli $E$ and $K$ decrease (for example $c_{Cu} = 10\%$, $c_{Li} = 5\%$, at $E$ decreases from $6.7681.10^{10}$ to $5.2362.10^{10}$Pa when $T$ increases from 100 to 700 K). For alloy AuCuLi at the same temperature and concentration of interstitial atoms, when the concentration of substitution atoms increases, the elastic moduli $E$ and $K$ increase (for example at 300 K, $c_{Li} = 5\%$, $E$ increases from $5.97.10^{10}$ to $6.8597.10^{10}$Pa when $c_{Cu}$ increases from 0 to 25\%). At zero concentrations of substitution atoms and interstitial atoms, the elastic moduli $E$ and $K$ of metal Au in [1]. The change of elastic moduli $E$ and $K$ in temperature for interstitial alloy AuCuLi is similar to that for interstitial alloy AuLi. The change of elastic moduli $E$ and $K$ in temperature and concentration of substitution atoms for interstitial alloy AuCuLi is similar to that for substitution alloy AuCu [4].

![Figure 15. $C_{11AuCuLi}(c_{Li})$, $C_{12AuCuLi}(c_{Li})$ at $P = 0$, $c_{Cu} = 10\%$](image1.png)

![Figure 16. $C_{11AuCuLi}(c_{Cu})$, $C_{12AuCuLi}(c_{Cu})$ at $P = 0$, $c_{Li} = 5\%$](image2.png)

According to Figures 14-16 for alloy AuCuLi at the same temperature and concentration of substitution atoms, when the concentration of interstitial atoms increases, the elastic constants $C_{11}$, $C_{12}$ decrease (for example at 300 K and $c_{Cu} = 10\%$, $C_{11}$ decreases from $22.4909.10^{10}$ to $12.4519.10^{10}$ Pa when $c_{Li}$ increases from 0 to 5\%). For alloy AuCuLi with the same concentration of substitution atoms and concentration of interstitial atoms, when the temperature increases, the elastic constants $C_{11}$, $C_{12}$ decrease (for example at $c_{Cu} = 10\%$, $c_{Li} = 5\%$, $C_{11}$ decreases from $13.3223.10^{10}$ to $10.2952.10^{10}$Pa when $T$ increases from 100 to 700 K). For alloy AuCuLi at the same temperature and concentration of interstitial atoms, when the concentration of substitution atoms increases, the elastic constants $C_{11}$, $C_{12}$ increase (for example at 300 K, $c_{Li} = 5\%$, $C_{11}$ increases from $11.9089.10^{10}$ to $13.2435.10^{10}$Pa when $c_{Cu}$ increases from 0 to 25\%). At zero concentration of substitution atoms and interstitial atoms, the elastic constants of interstitial alloy AuCuLi become the elastic constants $C_{11}$, $C_{12}$ of metal Au in [1]. The change of elastic constants $C_{11}$, $C_{12}$ with temperature for interstitial alloy AuCuLi is similar to that for interstitial alloy AuLi. The change of elastic constants $C_{11}$, $C_{12}$ with temperature and concentration of substitution atoms for interstitial alloy AuCuLi is similar to that for substitution alloy AuCu [4].

56
3. Conclusion

Our results in using the elastic theory for interstitial alloys AC, ABC with FCC structure based on the SMM are applied to alloys AuLi and AuCuLi at zero pressure in the temperature intervals from 100 to 1000 K, in the range of concentration of substitution atoms from 0 to 25% and in the range of concentration of interstitial atoms from 0 to 5%. The calculated results for main metal Au in the interstitial alloys are in rather good agreement with experimental data and are compared with other calculated results.

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