Research Article

Study of Nonlinear Deformation of FCC-AuCuSi under Pressure by the Statistical Moment Method

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In this work, we build the model and derive the theory of nonlinear deformation for substitutional alloy AB with interstitial atom C and face-centered cubic structure under pressure from the statistical moment method. The calculation results for FCC-AuCuSi are presented. We obtain the values of density of deformation energy, maximum real stress, limit of elastic deformation, and the stress-strain curve and compare the calculated results with experiments and other calculations.

1. Introduction

The study of elastic and thermodynamic properties of perfect ternary and binary interstitial alloys has also been attractive such as the theory of interstitial alloy [1], calculations from first principles, many-body potentials and dynamical dynamics for defects in metals, alloys and solid solutions [2–4] and elastic and thermodynamic properties of perfect ternary and binary interstitial alloys. We have studied the elastic deformation for body-entered cubic (BCC) and face-centered cubic (FCC) ternary and binary interstitial alloys under pressure by the statistical moment method (SMM) in [5–10].

The dependence of elastic and nonlinear deformations of materials on temperature, pressure, and concentration of components has very important role in predicting and understanding their interatomic interactions, strength, mechanical stability, phase transition mechanisms, and dynamical response. Silicides such as AuCuSi have attracted a lot of attention in recent years because of their functional applications and unusual physical properties. Gold silicide or gold silicon is one of the numerous metal alloys sold by American Elements under the trade name AE AlloysTM.

The experimental data on the real stress and the limit of elastic deformation in the nonlinear deformation of pure metal Au are presented in [11–14].

Thermodynamic and mechanical properties of metals and interstitial alloys are studied by some theoretical methods and simulations. For example, Mehl and Papaconstantopoulos [15] applied a tight-binding (TB) scheme to extend first-principle calculations (ab initio) to regimes containing \(10^2\)–\(10^3\) atoms in a unit cell and used two-center, nonorthogonal tight-binding parameters and on-site terms. Numerical calculations for many metals are compared with ab initio calculations and experiments. Deformation mechanisms in the mechanical response of nanoporous gold are investigated by molecular dynamics simulations [16]. In addition, in recent years, some researchers have considered factors affecting the structure, the phase transformation, and the crystallization process of alloys AuCu [17], NiCu [18, 19], and AgCu [20].

In the present paper, we will study nonlinear deformation of FCC ternary alloy (substitutional alloy AB with interstitial atoms C) under pressure by the statistical moment method (SMM) [21–24]. In Section 2, we build the model and theoretical calculations, and in Section 3, we carry out numerical calculations for alloy AuCuSi.

2. Model and Theoretical Calculations

In our model, for interstitial alloy AC with FCC structure and concentration condition \(c_C << c_A\) (\(c_A = N_A/N\) is the
concentration of atoms $A$, $N_A$ is the number of atoms A, $c_C = N_C/N$ is the concentration of atoms C, $N_C$ is the number of atoms C, and $N = N_A + N_C$ is the total number of atoms of the alloy AC), the cohesive energy $u_0$ and the alloy parameters $k, y_1, y_2, y$ ($k$ is called the harmonic parameter and $y_1, y_2, y$ are called anharmonic parameters) for the interstitial atom C in face centers of cubic unit cell in the approximation of two coordination spheres have the form [5–10]

\[ u_{0AC} = \frac{1}{2} \sum_{i=1}^{n} \varphi_{AC}(r_i) = 3\varphi_{AC}(r_{1C}) + 4\varphi_{AC}(r_{2C}), \]
\[ r_{2C} = \sqrt[3]{r_{1C}}, \]
\[ k_C = \frac{1}{2} \sum_{i} \left( \frac{\partial^2 \varphi_{AC}}{\partial u_i^2} \right)_{eq} = \frac{d^2 \varphi_{AC}(r_{1C})}{dr_{1C}^2} + \frac{2}{r_{1C}} \frac{d \varphi_{AC}(r_{1C})}{dr_{1C}} + \frac{4}{3} \frac{d^2 \varphi_{AC}(r_{2C})}{dr_{2C}^2} + \frac{8}{3r_{2C}} \frac{d \varphi_{AC}(r_{2C})}{dr_{2C}}, \]
\[ y_{1C} = 4(y_{1A} + y_{2C}), \]
\[ y_{1C} = \frac{1}{48} \sum_{i} \left( \frac{\partial^3 \varphi_{AC}}{\partial u_i^3} \right)_{eq} \]
\[ \quad = \frac{1}{24} \frac{d^3 \varphi_{AC}(r_{1C})}{dr_{1C}^3} + \frac{1}{4r_{1C}} \frac{d^2 \varphi_{AC}(r_{1C})}{dr_{1C}^2} \]
\[ + \frac{1}{54} \frac{d^3 \varphi_{AC}(r_{2C})}{dr_{2C}^3} + \frac{2}{9r_{2C}} \frac{d^2 \varphi_{AC}(r_{2C})}{dr_{2C}^2} \]
\[ y_{2C} = \frac{6}{48} \sum_{i} \left( \frac{\partial^3 \varphi_{AC}}{\partial u_i^3} \right)_{eq} \]
\[ \quad = \frac{1}{2r_{1C}} \frac{d^3 \varphi_{AC}(r_{1C})}{dr_{1C}^3} + \frac{3}{4r_{1C}^2} \frac{d^2 \varphi_{AC}(r_{1C})}{dr_{1C}^2} \]
\[ + \frac{3}{9} \frac{d^3 \varphi_{AC}(r_{2C})}{dr_{2C}^3} + \frac{3}{4r_{2C}^2} \frac{d^2 \varphi_{AC}(r_{2C})}{dr_{2C}^2} \]

The cohesive energy $u_0$ and the alloy parameters $k, y_1, y_2, y$ for main metal atom A1 in body center of cubic unit cell in the approximation of three coordination spheres have the form [5–10]

\[ u_{0A1} = u_{0A} + \varphi_{AC}(r_{1A1}), \]
\[ k_{A1} = k_A + \frac{1}{2} \sum_{i} \left( \frac{\partial^2 \varphi_{AC}}{\partial u_i^2} \right)_{eq} \]
\[ = k_A + \frac{d^2 \varphi_{AC}(r_{1A1})}{dr_{1A1}^2}, \]
\[ y_{A1} = 4(y_{1A1} + y_{2A1}), \]
\[ y_{1A1} = y_{1A} + \frac{1}{48} \sum_{i} \left( \frac{\partial^3 \varphi_{AC}}{\partial u_i^3} \right)_{eq} \]
\[ = y_{1A} + \frac{1}{24} \frac{d^3 \varphi_{AC}(r_{1A1})}{dr_{1A1}^3}, \]
\[ y_{2A1} = y_{2A} + \frac{6}{48} \sum_{i} \left( \frac{\partial^3 \varphi_{AC}}{\partial u_i^3} \right)_{eq} \]
\[ = y_{2A} + \frac{1}{4r_{1A1}} \frac{d^3 \varphi_{AC}(r_{1A1})}{dr_{1A1}^3} - \frac{1}{2r_{1A1}^2} \frac{d^2 \varphi_{AC}(r_{1A1})}{dr_{1A1}^2} + \frac{1}{2r_{1A1}^2} \frac{d \varphi_{AC}(r_{1A1})}{dr_{1A1}}. \]
The cohesive energy $u_0$ and the alloy parameters $k, y_1, y_2, y$ for the main metal atom $A_2$ in corners of cubic unit cell in the approximation of three coordination spheres have the form [5–10]

\[
\begin{align*}
\begin{aligned}
\frac{u_{OA_2}}{u_{OA}} &= \psi_{AC}(r_{1A_2}), \\
 k_{A_2} &= k_A + \frac{1}{2} \sum_i \left[ \left( \frac{\partial^2 \psi_{AC}}{\partial u_{ij}^2} \right)_{eq} \right]_{r=r_{1A_2}} = k_A + \frac{1}{6} \frac{d^2 \psi_{AC}(r_{1A_2})}{dr_{1A_2}^2} + \frac{23}{6r_{1A_2}} \frac{d \psi_{AC}(r_{1A_2})}{dr_{1A_2}}, \\
 y_{A_2} &= 4(y_{1A_2} + y_{2A_2}), \\
 y_{1A_2} &= y_{1A} + \frac{1}{48} \sum_i \left[ \left( \frac{\partial^4 \psi_{AC}}{\partial u_{ij}^2 \partial u_{kl}^2} \right)_{eq} \right]_{r=r_{1A_2}} = y_{1A} + \frac{1}{54} \frac{d^4 \psi_{AC}(r_{1A_2})}{dr_{1A_2}^4} + \frac{2}{9r_{1A_2}} \frac{d^3 \psi_{AC}(r_{1A_2})}{dr_{1A_2}^3}, \\
 &\quad - \frac{2}{9r_{1A_2}} \frac{d^2 \psi_{AC}(r_{1A_2})}{dr_{1A_2}^2} + \frac{2}{9r_{1A_2}^2} \frac{d \psi_{AC}(r_{1A_2})}{dr_{1A_2}}, \\
 y_{2A_2} &= y_{2A} + \frac{6}{48} \sum_i \left[ \left( \frac{\partial^4 \psi_{AC}}{\partial u_{ij}^2 \partial u_{kl}^2} \right)_{eq} \right]_{r=r_{1A_2}} = y_{2A} + \frac{1}{81} \frac{d^4 \psi_{AC}(r_{1A_2})}{dr_{1A_2}^4}, \\
 &\quad + \frac{14}{27r_{1A_2}} \frac{d^3 \psi_{AC}(r_{1A_2})}{dr_{1A_2}^3} + \frac{14}{27r_{1A_2}^2} \frac{d^2 \psi_{AC}(r_{1A_2})}{dr_{1A_2}^2} - \frac{14}{27r_{1A_2}^3} \frac{d \psi_{AC}(r_{1A_2})}{dr_{1A_2}}.
\end{aligned}
\end{align*}
\]

where $\phi_{AC}$ is the interaction potential between atoms $A$ and $C$, $r_{1X} = r_{01X} + y_{0X}(T)$ is the nearest neighbor distance between the atom $X$ ($X = A_1, A_2, C$) (A in clean metal and $A_1, A_2$ and $C$ in interstitial alloy $AC$) and other atoms at temperature $T$, $r_{01X}$ is the nearest neighbor distance between the atom $X$ and other atoms at $T = 0 \text{ K}$ and is determined from the minimum condition of the cohesive energy $u_{0X}$, and $y_{0X}(T)$ is the displacement of atom $X$ from equilibrium position at temperature $T$. $u_{0A}, k_A, y_{1A}, y_{2A}$ are the corresponding quantities in the clean metal $A$ with FCC structure in the approximation of two coordination spheres and have the form [21, 22]

\[
\begin{align*}
\begin{aligned}
u_{0A} &= 6 \psi_{AA}(r_{1A}) + 3 \psi_{AA}(r_{2A}), \\
r_{2A} &= \sqrt{2}r_{1A}, \\
k_A &= 2 \frac{d^2 \psi_{AA}(r_{1A})}{dr_{1A}^2} + \frac{4}{r_{1A}} \frac{d \psi_{AA}(r_{1A})}{dr_{1A}} + \frac{2}{r_{2A}} \frac{d \psi_{AA}(r_{2A})}{dr_{2A}}, \\
y_{1A} &= \frac{1}{24} \frac{d^4 \psi_{AA}(r_{1A})}{dr_{1A}^4} + \frac{1}{4r_{1A}^2} \frac{d^3 \psi_{AA}(r_{1A})}{dr_{1A}^3} - \frac{1}{8r_{1A}^4} \frac{d^2 \psi_{AA}(r_{1A})}{dr_{1A}^2} + \frac{1}{8r_{1A}^6} \frac{d \psi_{AA}(r_{1A})}{dr_{1A}}, \\
&\quad + \frac{1}{24} \frac{d^4 \psi_{AA}(r_{2A})}{dr_{2A}^4} + \frac{1}{4r_{2A}^2} \frac{d^3 \psi_{AA}(r_{2A})}{dr_{2A}^3} + \frac{1}{4r_{2A}^4} \frac{d \psi_{AA}(r_{2A})}{dr_{2A}}, \\
y_{2A} &= \frac{1}{48} \frac{d^4 \psi_{AA}(r_{1A})}{dr_{1A}^4} + \frac{7}{8r_{1A}^2} \frac{d^3 \psi_{AA}(r_{1A})}{dr_{1A}^3} - \frac{31}{16r_{1A}^4} \frac{d^2 \psi_{AA}(r_{1A})}{dr_{1A}^2} + \frac{31}{16r_{1A}^6} \frac{d \psi_{AA}(r_{1A})}{dr_{1A}}, \\
&\quad + \frac{1}{2r_{2A}} \frac{d^3 \psi_{AA}(r_{2A})}{dr_{2A}^3} + \frac{9}{8r_{2A}^2} \frac{d^2 \psi_{AA}(r_{2A})}{dr_{2A}^2} + \frac{9}{8r_{2A}^4} \frac{d \psi_{AA}(r_{2A})}{dr_{2A}}.
\end{aligned}
\end{align*}
\]
The equations of state for FCC interstitial alloy at temperature \( T \) and pressure \( P \) and at 0 K and pressure \( P \) are written in the form [5, 6, 8–10, 23]

\[
P_v = -r_1 \left[ \frac{1}{6} \frac{\partial u_\theta}{\partial r_1} + \theta x c t h x \frac{1}{2k} \frac{\partial k}{\partial r_1} \right],
\]

\[
v = \sqrt{3} r_1^3,
\]

\[
P_v = -r_1 \left( \frac{1}{6} \frac{\partial u_\theta}{\partial r_1} + \frac{k_0}{4k} \frac{\partial k}{\partial r_1} \right).
\]

\[\text{(5)}\]

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

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

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

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

\[
r_{1A}(P, 0) = (1 - c_C) r_{1A}(P, 0) + c_C r_{1A}(P, 0), r_{1A_1}(P, 0) = \sqrt{3} r_{1C}(P, 0),
\]

\[
y(P, T) = (1 - 15c_C) y_A(P, T) + c_C y_C(P, T) + 6c_C y_{A_1}(P, T) + 8c_C y_{A_2}(P, T).
\]

\[\text{(6)}\]

\[
\psi_X = \psi_{0X} + 3N \left[ \frac{\theta^2}{k_X^2} y_{2X}^2 - \frac{2y_{1X}}{3} \left( 1 + \frac{Y_X}{2} \right) \right] + \frac{2\theta^2}{k_X^2} \left[ \left[ \frac{4}{3} y_{2X}^2 \left( 1 + \frac{Y_X}{2} \right) - 2 \left( \frac{Y_X}{2} \right)^2 \right] \left( 1 + \frac{Y_X}{2} \right) \right],
\]

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

\[
Y_X = x_X \coth x_X,
\]

\[\text{(7)}\]

From that, we can calculate the nearest neighbor distance \( r_{iX}(P, 0) \) \((X = A, A_1, A_2, C)\), the parameters \( k_X(P, 0), y_{1X}(P, 0), y_{2X}(P, 0), y_X(P, 0) \), the displacement \( y_{0X}(P, T) \) of atom \( X \) from equilibrium position as in [21], the nearest neighbor distance \( r_{iX}(P, T) \), and the mean nearest neighbor distance between two atoms \( A \) in alloy \( \bar{r}_{1A}(P, T) \) as follows [5, 6, 8–10]:

\[
\tilde{r}_{iX}(P, 0) = r_{iX}(P, 0) + y_{iX}(P, 0),
\]

\[
r_{iA}(P, 0) = (1 - c_C) r_{iA}(P, 0) + c_C r_{iA}(P, 0), r_{iA_1}(P, 0) = \sqrt{3} r_{iC}(P, 0),
\]

\[
y(P, T) = (1 - 15c_C) y_{iA}(P, T) + c_C y_C(P, T) + 6c_C y_{A_1}(P, T) + 8c_C y_{A_2}(P, T).
\]

\[\text{(8)}\]

The mean nearest neighbor distances between two atoms \( A \) in interstitial alloy \( AC \) at pressure \( P \) and temperature \( T \) after deformation have the form [9]

\[
\tilde{r}_{iX} = \tilde{r}_{iX} + e, \quad r_{iX}(P, 0) = r_{iX}(P, 0) + e, \quad r_{iX}(P, T) = r_{iX}(P, T) + e,
\]

\[
\tilde{r}_{iA}(P, 0) = \tilde{r}_{iA}(P, 0) + e, \quad r_{iA}(P, 0) = r_{iA}(P, 0) + e, \quad r_{iA}(P, T) = r_{iA}(P, T) + e,
\]

\[
\tilde{r}_{iA_1}(P, 0) = \tilde{r}_{iA_1}(P, 0) + e, \quad r_{iA_1}(P, 0) = r_{iA_1}(P, 0) + e, \quad r_{iA_1}(P, T) = r_{iA_1}(P, T) + e.
\]

\[\text{(9)}\]
The mean nearest neighbor distances between two atoms A in substitutional alloy AB with interstitial atoms C at pressure P and temperature T and at pressure P and temperature T = 0 K after deformation have the form [5, 6, 9]

\[
\psi_{ABC} = \psi_{AC} + c_B(\psi_B - \psi_A) + T S^{AC} - T S^{ABC},
\]

\[
\psi_{AC} = (1 - 15c_C)\psi_A + c_C\psi_C + 6c_C\psi_{A1} + 8c_C\psi_{A2} - T S^{AC},
\]

\[
\psi_{ABC} = \psi_{AC} + c_B(\psi_B - \psi_A) + T S^{AC} - T S^{ABC},
\]

\[
\psi_{AC} = (1 - 15c_C)\psi_A + c_C\psi_C + 6c_C\psi_{A1} + 8c_C\psi_{A2} - T S^{AC},
\]

The Helmholtz free energy of alloy ABC before and after deformation with the condition \(c_C << c_B << c_A\) is determined by [5, 6, 9]

\[
a^F_{ABC} = c_{AC}a^F_{AC}B^F_{TAC} + c_Ba^F_{B_TAC},
\]

\[
\bar{B}^F_T = c_{AC}B^F_{TAC} + c_BB^F_{TB},
\]

\[
c_{AC} = c_A + c_C,
\]

\[
a^F_{ABC} = r^F_{1A}(P, T),
\]

\[
a^F_{AC} = r^F_{1A}(P, T),
\]

\[
a^F_B = r^F_{1B}(P, T),
\]

\[
B^F_{TAC} = \frac{1}{\lambda_{TAC}}
\]

\[
B^F_{TB} = \frac{1}{\lambda_{TB}}
\]

\[
\left(\frac{\partial^2 \psi^F_X}{\partial \alpha_X^2}\right)_T = \left(1 - 15c_C\right)\left(\frac{\partial^2 \psi^F_A}{\partial \alpha_X^2}\right)_T + c_C\left(\frac{\partial^2 \psi^F_C}{\partial \alpha_X^2}\right)_T + 6c_C\left(\frac{\partial^2 \psi^F_{A1}}{\partial \alpha_X^2}\right)_T + 8c_C\left(\frac{\partial^2 \psi^F_{A2}}{\partial \alpha_X^2}\right)_T + 8c_C\left(\frac{\partial^2 \psi^F_{A3}}{\partial \alpha_X^2}\right)_T,
\]

\[
\frac{1}{3N}\frac{\partial^2 \psi^F_X}{\partial \alpha_X^2} = \frac{1}{6} \frac{\partial^2 \psi^F_{AX}}{\partial \alpha_X^2} + \frac{h a^F_X}{4 \kappa_X^2} \left[ \frac{\partial^2 \kappa^F_X}{\partial \alpha_X^2} + \frac{1}{2 \kappa_X^2} (\partial \kappa^F_X)^2 \right],
\]

\[
X = A, A_1, A_2, B, C
\]

\[
a^F_{0ABC} = c_{AC}a^F_{0AC}B^F_{0TAC} + c_Ba^F_{0TB},
\]

\[
\bar{B}^F_{0T} = c_{AC}B^F_{0TAC} + c_BB^F_{0TB},
\]

\[
a^F_{0ABC} = r^F_{01A}(P, 0),
\]

\[
a^F_{0AC} = r^F_{01A}(P, 0),
\]

The relationship between the stress and the deformation in nonlinear deformation is given by [9]

\[
\sigma^F_{ABC} = \sigma^F_{0ABC} \frac{e^{\alpha_{ABC}}}{1 + e^{\alpha_{ABC}}},
\]

where \(\sigma^F_{0ABC}\) and \(\alpha_{ABC}\) are constants for every alloy.

The density of deformation energy can be written in the form [9]
\[
\frac{f_{ABC}(\varepsilon)}{N} = (1 - c_A) \left\{ \psi_A \left( \frac{1}{\nu_{ABC}} - \frac{1}{\nu_{AB}} \right) + \frac{2e_{01A}^F}{\nu_{ABC}} \left( \sigma_{ABC}^{\varepsilon} - \lambda_{ABC} \sigma_{ABC}^{\varepsilon} \right) \right\} + 2e_{01A}^F \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) T + \frac{\varepsilon^2}{2V_{ABC}} \left[ \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) (2r_{01A}^F)^2 + \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) (2r_{01A}^F) \right] + \\
+ \frac{c_B}{N} \left\{ \psi_B \left( \frac{1}{\nu_{ABC}} - \frac{1}{\nu_{AB}} \right) + \frac{2e_{01B}^F}{\nu_{ABC}} \left( \sigma_{ABC}^{\varepsilon} - \lambda_{ABC} \sigma_{ABC}^{\varepsilon} \right) \right\} + \frac{\varepsilon^2}{2V_{ABC}} \left[ \left( \frac{\partial^2 \psi_B}{\partial r_{1B}^2} \right) (2r_{01B}^F)^2 + \left( \frac{\partial^2 \psi_B}{\partial r_{1B}^2} \right) \left( \frac{\partial^2 \psi_B}{\partial r_{1B}^2} \right) (2r_{01B}^F) \right] + \\
+ \frac{c_A}{N} \left\{ \psi_A \left( \frac{1}{\nu_{ABC}} - \frac{1}{\nu_{AB}} \right) + \frac{2e_{01A}^F}{\nu_{ABC}} \left( \sigma_{ABC}^{\varepsilon} - \lambda_{ABC} \sigma_{ABC}^{\varepsilon} \right) \right\} + \frac{\varepsilon^2}{2V_{ABC}} \left[ \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) (2r_{01A}^F)^2 + \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) (2r_{01A}^F) \right] + \\
+ \frac{c_A}{N} \left\{ \psi_A \left( \frac{1}{\nu_{ABC}} - \frac{1}{\nu_{AB}} \right) + \frac{2e_{01A}^F}{\nu_{ABC}} \left( \sigma_{ABC}^{\varepsilon} - \lambda_{ABC} \sigma_{ABC}^{\varepsilon} \right) \right\} + \frac{\varepsilon^2}{2V_{ABC}} \left[ \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) (2r_{01A}^F)^2 + \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) (2r_{01A}^F) \right] + \\
+ \frac{c_B}{N} \left\{ \psi_B \left( \frac{1}{\nu_{ABC}} - \frac{1}{\nu_{AB}} \right) + \frac{2e_{01B}^F}{\nu_{ABC}} \left( \sigma_{ABC}^{\varepsilon} - \lambda_{ABC} \sigma_{ABC}^{\varepsilon} \right) \right\} + \frac{\varepsilon^2}{2V_{ABC}} \left[ \left( \frac{\partial^2 \psi_B}{\partial r_{1B}^2} \right) (2r_{01B}^F)^2 + \left( \frac{\partial^2 \psi_B}{\partial r_{1B}^2} \right) \left( \frac{\partial^2 \psi_B}{\partial r_{1B}^2} \right) (2r_{01B}^F) \right] + \\
- \frac{c_B}{N} \left\{ \psi_A \left( \frac{1}{\nu_{ABC}} - \frac{1}{\nu_{AB}} \right) + \frac{2e_{01A}^F}{\nu_{ABC}} \left( \sigma_{ABC}^{\varepsilon} - \lambda_{ABC} \sigma_{ABC}^{\varepsilon} \right) \right\} + \frac{\varepsilon^2}{2V_{ABC}} \left[ \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) (2r_{01A}^F)^2 + \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) \left( \frac{\partial^2 \psi_A}{\partial r_{1A}^2} \right) (2r_{01A}^F) \right].
\]

When the deformation rate is constant, the density of deformation energy of alloy is determined by [9]

\[
f_{ABC}(\varepsilon) = C_{ABC} \cdot \sigma_{ABC} \cdot \varepsilon, \tag{14}
\]

where \(C_{ABC}\) is the proportional factor. At the maximum value of the density of deformation energy, we have

\[
f_{ABC}(\varepsilon_{ABC}^F) = f_{ABC,\text{max}} = C_{ABC} \sigma_{ABC,\text{max}} \varepsilon_{ABC}^F. \tag{15}
\]

The maximum value of stress \(\sigma_{ABC,\text{max}}\) and the maximum real stress \(\sigma_{1ABC,\text{max}}\) are [9]

\[
\sigma_{ABC,\text{max}} = \frac{f_{ABC,\text{max}}}{C_{ABC} \varepsilon_{ABC}^F},
\]

\[
\sigma_{1ABC,\text{max}} = \frac{\sigma_{ABC,\text{max}}}{1 + \varepsilon_{ABC}^F} = \frac{f_{ABC,\text{max}}}{C_{ABC} \varepsilon_{ABC}^F (1 + \varepsilon_{ABC}^F)}. \tag{16}
\]

From the maximum condition of stress \((\partial \sigma_{1ABC,\varepsilon}/\partial \varepsilon)_{ABC} = 0\), we derive the deformation \(\varepsilon_{ABC}^\alpha\) corresponding to the maximum value of real stress as follows [9]:

\[
\varepsilon_{ABC}^\alpha = \frac{\sigma_{ABC,\text{max}}}{1 - \sigma_{ABC,\text{max}}} \Rightarrow \sigma_{1ABC,\text{max}} = \sigma_{0ABC,\text{max}} \frac{(\varepsilon_{ABC}^\alpha)_{ABC}^{\sigma_{ABC}}}{1 + \varepsilon_{ABC}^\alpha}. \tag{17}
\]

\(C_{ABC}\) is determined from the experimental condition of stress \(\sigma_{0ABC,\text{ABC}}\) in alloy in the form [9]

\[
C_{ABC} = \frac{f_{ABC}(\varepsilon_{02})}{\sigma_{02ABC}}. \tag{18}
\]

From the obtained value of \(\varepsilon_{ABC}^\alpha\), we can calculate \(\sigma_{0ABC}\) and \(\sigma_{ABC,\text{ABC}}\). The limit of elastic deformation \(\sigma = E_{ABC} \varepsilon\) of alloy ABC is determined by [9]

\[
\sigma = E_{ABC} \varepsilon = \sigma_{0ABC} \frac{\varepsilon^\alpha}{1 + \varepsilon}. \tag{19}
\]

Here \(E_{ABC}\) is Young’s modulus of alloy ABC and has the form [5, 6]
Here $E_{AC}, E_{A}, E_{B}$ are Young’s moduli of alloy $AC$ and metals $A, B$, respectively.

3. Numerical Results for Alloy AuCuSi

To describe the interaction between atoms Au and Si, we apply the Mie–Lennard-Jones pair interaction potential in the form [25]

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

where $D$ is the depth of potential well corresponding to the equilibrium distance $r_0$ and $m$ and $n$ are determined empirically. Then, the potential parameters for the interaction Au-Si are determined by [26]

$$
D_{Au-Si} = \sqrt{D_{Au-Au} D_{Si-Si}},
$$

$$
\frac{1}{2} (r_{0Au-Au} + r_{0Si-Si}).
$$

We find $m_{Au-Si}$ and $n_{Au-Si}$ by fitting the theoretical result with the experimental data for Young’s modulus of interstitial alloy AuSi$_{3\%}$ at room temperature. The Mie–Lennard-Jones potential parameters for the interactions Au-Au, Si-Si, and Au-Si are given in Table 1. The Poisson ratio is 0.42 for Au [28], 0.34 for Cu [29], and 0.21 for Si [30]. Our investigated range of temperature up to 900 K is below the melting temperature of Au, Cu, and Si in the range of pressure from zero to 6 GPa as studies on the melting curve for these materials [31–33].

$$
E = \frac{\sigma_{0.2}}{\epsilon_{0.2}} \Rightarrow \sigma_{0.2} = E \epsilon_{0.2} = E \times 0.2\%,
$$

the experimental value of Young’s modulus $E = 89.1 \times 10^9$ Pa for Au at $T = 300$ K and $P = 0$ [34]. From that, we obtain $\sigma_{0.2} = 89.1 \times 10^9 \times 0.002 = 178.2 \times 10^6$ Pa. Figure 1 shows the density of deformation energy $f(\epsilon)$ and the real stress $\sigma_1(\epsilon)$ of Au$_{99-x}$Cu$_x$Si$_{1\%}$ at $T = 300$ K and $P = 0$ calculated by the SMM. From that, we can find the maximum real stress $\sigma_{1\text{max}}$, the elastic limit $\sigma_e$, and the elastic strain $\epsilon_e$ for AuCuSi as shown in Table 2.

### Table 1: Mie–Lennard-Jones potential parameters for interactions Au-Au, Cu-Cu, and Si-Si.

| Interaction  | $D/k_B$ (K) | $r_0$ (10$^{-10}$ m) | $m$ | $n$ |
|-------------|-------------|----------------------|-----|-----|
| Au-Au [27]  | 7411.5      | 2.8751               | 1.96| 15.56|
| Cu-Cu [27]  | 6841.3      | 2.5487               | 3.03| 8.37 |
| Si-Si [25]  | 32701.7     | 2.295                | 6   | 12  |
When concentrations $c_{Cu}, c_{Si} \to 0$, we obtain the nonlinear deformation of main metal Au. Figure 2 shows the curve of real stress $\sigma_1(\varepsilon)$ for Au at $P = 0$ and $T = 300$ K where we have the comparison between the SMM and experiments [11, 12]. The maximum real stress $\sigma_{1\text{max}}$ and the elastic limit $\sigma_e$ calculated by the SMM in Table 3 are in good agreement with the molecular dynamics (MD) results [16] and experiments [13, 14]. The error of the maximum real stress between the SMM calculation and the experimental data [13] is 5.65%. Thus, the SMM calculations of the maximum real stress and the elastic limit for Au at $P = 0$ and $T = 300$ K are in good agreement with other calculations and experiments.

Figure 3 shows the density of deformation energy $f(\varepsilon)$ and the real stress $\sigma_1(\varepsilon)$ of AuCuSi at $T = 300$ K, $P = 0$, $c_{Cu} = 10\%$, and $c_{Si} = 0, 1, 2\%$ calculated by the SMM. For AuCuSi at the same temperature, pressure, and concentration of substitutional atoms, when the concentration of interstitial atoms increases, the maximum real stress and the elastic limit decrease strongly. We have the comparison on values of $\varepsilon_f$, $\sigma_{1\text{max}}$, $\varepsilon_e$, and $\sigma_e$ for alloys AuSi, AuCu, and AuCuSi in Table 4.

Figure 4 shows the density of deformation energy $f(\varepsilon)$ and the real stress $\sigma_1(\varepsilon)$ of AuCuSi at $T = 300$, 600, and 900 K, $P = 0$, $c_{Cu} = 10\%$, and $c_{Si} = 2\%$ calculated by the SMM. For AuCuSi at the same pressure, concentration of substitutional atoms, and concentration of interstitial atoms, when the temperature increases, the maximum real stress and the elastic limit increase. We have the comparison on values of $\varepsilon_f$, $\sigma_{1\text{max}}$, $\varepsilon_e$, and $\sigma_e$ for Au$_{99}$Cu$_1$Si$_1$ at $P = 0$ and $T = 300$ K in Table 5.

Figure 5 shows the real stress $\sigma_1(\varepsilon)$ of AuCuSi at $T = 300$, 600, and 900 K in Table 6.

### Table 2: Values of $\varepsilon_f (f(\varepsilon) = f_{\text{max}})$, $\sigma_{1\text{max}}$, $\sigma_e$, and $\varepsilon_e$ of Au$_{99}$Cu$_1$Si$_1$ at $P = 0$ and $T = 300$ K calculated by the SMM.

| $\sigma_{1\text{max}}$ (MPa) | $\varepsilon_e$ (%) |
|-----------------------------|-------------------|
| Au$_{99}$Cu$_1$Si$_1$ 8.0 | 231.79 0.21 190.84 |
| Au$_{96}$Cu$_3$Si$_1$ 8.0 | 230.38 0.21 189.40 |
| Au$_{94}$Cu$_5$Si$_1$ 8.0 | 227.06 0.20 186.38 |

### Table 3: Values of $\varepsilon_f (f(\varepsilon) = f_{\text{max}})$, $\sigma_{1\text{max}}$, $\varepsilon_e$, and $\sigma_e$ for Au$_{99}$Cu$_1$Si$_1$ at $P = 0$ and $T = 300$ K calculated by the SMM and from MD [16], EXPT [13], and EXPT [14].

| $\sigma_{1\text{max}}$ (MPa) | $\varepsilon_e$ (MPa) |
|-----------------------------|-------------------|
| SMM [16] MD | EXPT [13] EXPT [14] |
| $\varepsilon_f = 9.6\%$ 243.52 245 $\varepsilon_e = 0.19\%$ 188.70 200 45 300 |
Figure 3: The density of deformation energy $f(\varepsilon)$ (a) and the real stress $\sigma_1(\varepsilon)$ (b) of Au$_{99}$Si$_1$, Au$_{90}$Cu$_{10}$, and Au$_{89}$Cu$_{10}$Si$_1$ at $T = 300$ K and $P = 0$ calculated by the SMM.

Table 4: Values of $\varepsilon_F$, $\sigma_{1\text{max}}$, $\varepsilon_e$, and $\sigma_e$ for Au$_{99}$Si$_1$, Au$_{90}$Cu$_{10}$, and Au$_{89}$Cu$_{10}$Si$_1$ at $P = 0$ and $T = 300$ K calculated by the SMM.

| Alloy         | $\varepsilon_F$ (%) | $\sigma_{1\text{max}}$ (MPa) | $\varepsilon_e$ (%) | $\sigma_e$ (MPa) |
|---------------|---------------------|------------------------------|---------------------|-----------------|
| Au$_{99}$Si$_1$ | 9.6                 | 214.07                       | 0.18                | 165.49          |
| Au$_{90}$Cu$_{10}$ | 8.3             | 242.95                       | 0.19                | 196.75          |
| Au$_{89}$Cu$_{10}$Si$_1$ | 8.2            | 216.79                       | 0.19                | 175.98          |

Figure 4: The density of deformation energy $f(\varepsilon)$ (a) and the real stress $\sigma_1(\varepsilon)$ (b) of Au$_{88}$Cu$_{10}$Si$_2$ at $P = 0$ and $T = 300$, 600, and 900 K calculated by the SMM.
4. Conclusion

In our paper, we derive the analytic expressions of characteristic quantities for the nonlinear deformation such as the density of deformation energy, the maximum real stress, and the limit of elastic deformation depending on temperature, pressure, and concentration of components together with the strain-stress of substitutional alloy AB with interstitial atom C and FCC structure under pressure. We apply theoretical results to alloy AuCuSi. The maximum real stress $\sigma_{1\text{max}}$ and the elastic limit $\sigma_e$ calculated by the SMM are in good agreement with MD results [16] and experiments [13, 14]. For AuCuSi at the same temperature, concentration of substitutional atoms, and concentration of interstitial atoms, when the pressure increases, the maximum real stress increases and the elastic limit decreases. When the pressure increases from 2 to 4 GPa, the maximum real stress increases by 3% and the elastic limit decreases by 7.86%. When the pressure increases from 4 to 6 GPa, the maximum real stress increases by 11% and the elastic limit decreases by 10.56%. Our calculated results for alloy AuCuSi are compared with ones for alloys AuCu, AuSi, and metal Au. If we use more coordination spheres and we have exact experimental data for the stress $\sigma_0$ of alloy AuCuSi at different temperatures, pressures, and concentrations of components, we will obtain better calculations.

Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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Advances in Materials Science and Engineering 11

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