NONLINEAR DEFORMATION OF BCC METAL Fe AND BCC INTERSTITIAL ALLOY FeSi: DEPENDENCE ON TEMPERATURE, PRESSURE AND SILICON CONCENTRATION

N.Q. Hoc1, B.D. Tinh1*, N.D. Hien2, G. Coman3
1Hanoi National University of Education, 136 Xuan Thuy, Hanoi, Vietnam
2Mac Dinh Chi High School, Chu Pah, Gia Lai, Vietnam
3“Dunarea de Jos” University of Galati, Romania
*e-mail: tinhbd@hnue.edu.vn

Abstract. Based on our model and theory of nonlinear deformation for BCC binary interstitial alloy built by the statistical moment method, we perform numerical calculations for characteristic quantities of nonlinear deformation such as the density of deformation energy, the maximum real stress, the limit of elastic deformation together with the stress-strain curve for metal Fe and alloy FeSi with the BCC structure at temperature up to 1100K, pressures up to 10 GPa, and silicon concentrations up to 4%. The calculated results of Fe are compared with experiments and the calculated results of FeSi are our new predictions.

Keywords: nonlinear deformation, interstitial alloy, the density of deformation energy, maximum real stress, limit of elastic deformation, stress-strain curve, statistical moment method

1. Introduction
Iron and its alloys are widely used in structural, electrical, and other technological applications. The dependence of elastic and nonlinear deformations of materials on temperature and pressure has a very important role in order to predict and understand their interatomic interactions, strength, mechanical stability, phase transition mechanisms, and dynamical response.

Iron silicides have paid attention in recent decades due to their unusual physical properties and functional applications [1-10]. β-FeSi2 is a semiconducting phase and has been studied as a material for thermoelectric conversion, solar cells, and optoelectronic applications [1]. Si has been proposed to be a potential light element in the Earth's core based on density, velocity, isotopic and geochemical data [2,3]. In order to assess Si as a constituent of the core, it is necessary to determine the physical properties of the Si-bearing iron phase under extreme conditions. The compressibility of silicides β-FeSi2 and ε-FeSi (B20 structure) at high pressures has been reported [4,5]. The pressure dependence of the structural, optical and elastic properties for β-FeSi2 is described by some works [5,6]. The thermodynamic and elastic properties depending on temperature and pressure of ε-FeSi have also been investigated [7-9]. Iron silicides have also been reported in the field of magnetic application [10].

In [11], silicon does form genuine interstitial compounds when in association with the larger transition-metal atoms of Groups IV and V. Therefore, we proposed a model of interstitial alloy FeSi with the BCC structure in our previous papers [12-21], where in our
model of interstitial alloy AB with the BCC structure in the concentration condition $c_A << c_B$, the main metal atoms A stay in the vertices and the body center of the cubic unit cell and the interstitial atom B stays in the face centers of the cubic unit cell. In that concentration condition, the interstitial atoms B only stay in the face centers of the cubic unit cell. In our numerical results, $c_B = 0 \pm 5\%$. This means that the interstitial atoms B only stay in the face centers of some cubic unit cells and all other cubic unit cells only have the metal atoms A. We have many published papers [12-21], where the main metal atoms A = Fe, W, Ta and the interstitial atoms B = Si, C, H are in the alloys FeSi, FeH, FeC, WSi, TaSi. We still proposed a model of interstitial and substitutional alloy FeCrSi with the BCC structure in our previous papers [22-25], where in our model of interstitial and substitutional alloy ABC with the BCC structure in the concentration condition $c_A << c_B << c_C$, the main metal atoms A stay in the vertices, the substitutional atom B substitutes the main metal atoms A in the body center of the cubic unit cell and the interstitial atom B stays in the face centers of the cubic unit cell. We have some published papers [22-25], where the main metal atoms A = Fe, V, the substitutional atom B = Cr, W, and the interstitial atoms C = Si are in the alloys FeCrSi, VWSi. The above mentioned model of interstitial alloy AB and model of interstitial and substitutional alloy ABC with BCC structure are approximate models for ternary and binary interstitial alloys. Many of our SMM numerical calculations in published papers based on these models are in good agreement with other calculations and data experiments. We have been considered the structural, elastic, thermodynamic, and melting properties of BCC-FeSi in the range of temperature from 0 to 1000K, the range of pressure from 0 to 70 GPa, and the range of interstitial atom from 0 to 5% by the way of SMM in [12,13,15,19].

The experimental data on elastic and nonlinear deformations of iron are presented in [26-28]. The elastic moduli of BCC-Fe under pressure and temperature are studied by the full-potential linear response and linear-muffin-tin orbital generalized gradient approximation (LMTO-GGA) method [29].

In the next section, we present the theory of nonlinear deformation for BCC binary interstitial alloy built by the statistical moment method (SMM) [30-33] and numerical results for metal Fe and alloy FeSi.

### 2. Content of research

**Theory of nonlinear deformation for BCC interstitial alloy AB under pressure.** In our model for interstitial alloy AB with BCC 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 called as the harmonic parameter and $\gamma_1, \gamma_2, \gamma$ are called as anharmonic parameters) for the interstitial atom B in face centers of the cubic unit cell, the main metal atom A in body center of the cubic unit cell and the main metal atom A in vertices of the cubic unit cell in the approximation of two coordination spheres have the form [12-25,30-33]

\[
\begin{align*}
\Phi_{AB}(r_i) &= \Phi_{AB}(r_{iB}) + 2\Phi_{AB}(r_{2B}),
\end{align*}
\]

\[
\begin{align*}
\frac{d^2\Phi_{AB}(r_i)}{dr_i^2} &= \frac{1}{r_{iB}} \frac{d\Phi_{AB}(r_{iB})}{dr_{iB}} + \frac{1}{r_{2B}} \frac{d\Phi_{AB}(r_{2B})}{dr_{2B}},
\end{align*}
\]

\[
\begin{align*}
\gamma_{AB} &= 4(\gamma_{1B} + \gamma_{2B}),
\gamma_{1B} &= \frac{1}{48} \sum_i \left( \frac{d^4\Phi_{AB}(r_i)}{dr_i^4} \right)_{eq} = \frac{1}{24} \frac{1}{8r_{iB}^2} \frac{d^3\Phi_{AB}(r_{iB})}{dr_{iB}^3} - \frac{1}{8r_{iB}^3} \frac{d^2\Phi_{AB}(r_{iB})}{dr_{iB}^2} + \frac{1}{48} \frac{d\Phi_{AB}(r_{iB})}{dr_{iB}} + \frac{1}{48} \frac{d\Phi_{AB}(r_{2B})}{dr_{2B}} + \frac{1}{48} \frac{d\Phi_{AB}(r_{2B})}{dr_{2B}}.
\end{align*}
\]
Nonlinear deformation of BCC metal Fe and BCC Interstitial alloy FeSi: dependence on temperature, pressure and...
where $\varphi_{AB}$ is the interaction potential between atoms A and B, $r_{iX} = r_{0iX} + y_{0X}(T)$ 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 $T$, $r_{0iX}$ 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. $u_{0A}, k_1, \gamma_1, \gamma_2, \gamma_3$ is the corresponding quantities in the clean metal A with BCC structure in the approximation of two coordination spheres [12-25,30-33].

\[
\begin{align*}
  u_{0A} &= 4\varphi_{AA}(r_{1A}) + 3\varphi_{AA}(r_{2A}), \\
  r_{2A} &= \frac{2}{\sqrt{3}} r_{1A},
\end{align*}
\]

\[
\begin{align*}
  k_A &= \frac{4}{3} \frac{d^2\varphi_{AA}(r_{1A})}{dr_{1A}^2} + \frac{8}{3r_{1A}} \frac{d\varphi_{AA}(r_{1A})}{dr_{1A}} + \frac{2}{r_{2A}} \frac{d\varphi_{AA}(r_{2A})}{dr_{2A}}, \\
  \gamma_{1A} &= \frac{1}{54} \frac{d^4\varphi_{AA}(r_{1A})}{dr_{1A}^4} + \frac{8}{9r_{1A}^2} \frac{d^3\varphi_{AA}(r_{1A})}{dr_{1A}^3} - \frac{20}{9r_{1A}^4} \frac{d^2\varphi_{AA}(r_{1A})}{dr_{1A}^2} + \frac{20}{9r_{1A}^3} \frac{d\varphi_{AA}(r_{1A})}{dr_{1A}},
\end{align*}
\]

\[
\begin{align*}
  \gamma_{2A} &= \frac{1}{54} \frac{d^4\varphi_{AA}(r_{2A})}{dr_{2A}^4} + \frac{5}{9r_{2A}^2} \frac{d^3\varphi_{AA}(r_{2A})}{dr_{2A}^3} - \frac{5}{18} \frac{d^2\varphi_{AA}(r_{2A})}{dr_{2A}^2} + \frac{5}{18} \frac{d\varphi_{AA}(r_{2A})}{dr_{2A}},
\end{align*}
\]

The equations of state for BCC interstitial alloy at temperature T and pressure P and at 0K and pressure P are written in the form [12,13,15-21,23,24,30-33]

\[
\begin{align*}
  P &\mathbf{V} = -r_{1A} \left( \frac{1}{6} \frac{\partial u_0}{\partial \mathbf{r}_{1A}} + \frac{\xi e^t}{2k} \frac{\partial k}{\partial \mathbf{r}_{1A}} \right), \\
  V &\mathbf{P} = -r_{1A} \left( \frac{1}{6} \frac{\partial u_0}{\partial \mathbf{r}_{1A}} + \frac{\hbar \omega_0}{4k} \frac{\partial \mathbf{r}_{1A}}{\partial \mathbf{r}_{1A}} \right),
\end{align*}
\]

From that, 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 $y_{0X}(P,T)$ of atom X from equilibrium position as in [29], the nearest neighbor distance $r_{iX}(P,T)$, and the mean nearest neighbor distance between two atoms in the alloy $r_{iA}(P,T)$ as follows [12,13,15-21,23,24,30-33]

\[
\begin{align*}
  r_{1b}(P,T) &= r_{1b}(P,0) + y_{A_1}(P,T), \\
  r_{IA}(P,T) &= r_{1A}(P,0) + y_A(P,T), \\
  r_{IA}(P,T) &\approx r_{1b}(P,T), \\
  r_{IA}(P,T) &= r_{1A}(P,0) + y_B(P,T), \\
  r_{IA}(P,T) &= r_{1A}(P,0) + y_{A_1}(P,0) + c_B y_B(P,T), \\
  (1 - c_B) r_{IA}(P,0) &+ c_B r_{IA}(P,0) = \sqrt{3} r_{1b}(P,0), \\
  y(P,T) &= (1 - c_B) y_A(P,T) + c_B y_B(P,T) + 2 c_B y_{A_1}(P,T) + 4 c_B y_{A_2}(P,T).
\end{align*}
\]

The Helmholtz free energy of BCC interstitial alloy AB with the condition $c_B << c_A$ is determined by [12-25,30-33]

\[
\begin{align*}
  \psi_{AB} &= (1 - 7c_B) \psi_A + c_B \psi_B + 2 c_B \psi_{A_1} + 4 c_B \psi_{A_2} - T S, \\
  N.Q. Hoc, B.D. Tinh, N.D. Hien, G. Coman
\end{align*}
\]
\[ \psi_X \approx U_{0X} + \psi_{0X} + 3N \left\{ \frac{2}{(k_X)^2} \left[ \gamma_{2X} Y_X \right] - \frac{2\gamma_{1X}}{3} \left(1 + \frac{Y_X}{2}\right) \right\} + \frac{20^3}{(k_X)^3} \left[ \frac{4}{3} \gamma_{2X} Y_X \left(1 + \frac{Y_X}{2}\right) - 2\left(\gamma_{1X}\right)^2 - 2\gamma_{1X} \gamma_{2X} \left(1 + \frac{Y_X}{2}\right) \right], \]

\[ \psi_{0X} = 3N0\left[ x_X + \ln\left(1 - e^{-2x_X}\right) \right], \quad Y_X \equiv x_X \coth x_X, \quad (24) \]

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 BCC interstitial alloy AB.

The nearest neighbor distances between two atoms in alloy after deformation \( r_{1X}^F(P,0), r_{1X}^F(P,T) \) in alloy have the form

\[ r_{1X}^F(P,0) = r_{1X}(P,0)(1 + \varepsilon), \quad (25) \]

\[ r_{1X}^F(P,T) = r_{1X}(P,T) + \varepsilon r_{1X}(P,0)(2 + \varepsilon). \quad (26) \]

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

\[ \sigma_{AB} = \sigma_{oAB} \frac{\varepsilon_{AB}}{1 + \varepsilon_{F}}, \quad (27) \]

where \( \sigma_{oAB} \) and \( \alpha_{AB} \) are constants for every interstitial alloy.

The density of deformation energy can be written in the form

\[ f_{AB}(\varepsilon) = \frac{1}{N} (1 - 7c_B) \left\{ \psi_A \left( \frac{1}{v_{AB}} - \frac{1}{v_{AB}} \right) + 2\varepsilon \frac{\partial \psi_A}{\partial \varepsilon} \frac{\partial \psi_A}{\partial \varepsilon} + \varepsilon^2 \left[ \frac{\partial^2 \psi_A}{\partial \varepsilon^2} \left(2\varepsilon\right) + \frac{\partial \psi_A}{\partial \varepsilon} \left(2\varepsilon\right) \right] + \right\} + \]

\[ + \frac{c_B}{N} \left\{ \psi_B \left( \frac{1}{v_{AB}} - \frac{1}{v_{AB}} \right) + 2\varepsilon \frac{\partial \psi_B}{\partial \varepsilon} \frac{\partial \psi_B}{\partial \varepsilon} + \varepsilon^2 \left[ \frac{\partial^2 \psi_B}{\partial \varepsilon^2} \left(2\varepsilon\right) + \frac{\partial \psi_B}{\partial \varepsilon} \left(2\varepsilon\right) \right] + \right\} + \]

\[ + \frac{2c_B}{N} \left\{ \psi_A \left( \frac{1}{v_{AB}} - \frac{1}{v_{AB}} \right) + 2\varepsilon \frac{\partial \psi_A}{\partial \varepsilon} \frac{\partial \psi_A}{\partial \varepsilon} + \varepsilon^2 \left[ \frac{\partial^2 \psi_A}{\partial \varepsilon^2} \left(2\varepsilon\right) + \frac{\partial \psi_A}{\partial \varepsilon} \left(2\varepsilon\right) \right] + \right\} + \]

\[ + \frac{4c_B}{N} \left\{ \psi_A \left( \frac{1}{v_{AB}} - \frac{1}{v_{AB}} \right) + 2\varepsilon \frac{\partial \psi_A}{\partial \varepsilon} \frac{\partial \psi_A}{\partial \varepsilon} + \varepsilon^2 \left[ \frac{\partial^2 \psi_A}{\partial \varepsilon^2} \left(2\varepsilon\right) + \frac{\partial \psi_A}{\partial \varepsilon} \left(2\varepsilon\right) \right] + \right\}. \quad (28) \]

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

\[ f_{AB}(\varepsilon) = C_{AB} \sigma_{AB} \varepsilon, \quad (29) \]

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

\[ f_{AB}(\varepsilon_{AB}) = f_{AB}^{\text{max}} = C_{AB} \sigma_{AB}^{\text{max}} \varepsilon_{AB}, \quad (30) \]

The maximum value of stress \( \sigma_{AB}^{\text{max}} \) and the maximum real stress \( \sigma_{1AB}^{\text{max}} \) are

\[ \sigma_{AB}^{\text{max}} = \frac{f_{AB}^{\text{max}}}{\varepsilon_{AB}}, \quad \sigma_{1AB}^{\text{max}} = \frac{\sigma_{AB}}{1 + \varepsilon_{AB}^F} = \frac{f_{AB}^{\text{max}}}{\varepsilon_{AB}^F(1 + \varepsilon_{AB}^F)}. \quad (31) \]

From the maximum condition of stress \( \left(\frac{\partial \sigma_{AB}}{\partial \varepsilon}\right)_{\varepsilon_{AB}} = 0 \), we derive the deformation \( \varepsilon_{AB}^F \) corresponding to the maximum value of real stress as follows
\[ \varepsilon_{AB}^F = \frac{\alpha_{AB}}{1 - \alpha_{AB}}, \quad \sigma_{\text{max}} = \sigma_{0AB} \left( \frac{\varepsilon_{AB}^F}{\alpha_{AB}} \right)^{\alpha_{AB}}. \]  

(32)

\[ C_{AB} \] is determined from the experimental condition of stress \( \sigma_{0.2AB} \) in the alloy in the form

\[ C_{AB} = \frac{f_{AB}(\varepsilon_{0.2AB})}{\sigma_{0.2AB} \varepsilon_{0.2AB}}. \]  

(33)

From the obtained value of \( \varepsilon_{AB}^F \) we can calculate \( \sigma_{0AB} \) and \( \alpha_{AB} \). The limit of elastic deformation of interstitial alloy \( AB \) is determined by

\[ E_{\text{el}} = \sigma_{0AB} \frac{\varepsilon_{AB}^e}{1 + \varepsilon_{AB}^e}. \]  

(34)

**Numerical results for alloy FeSi.** To describe the interaction between atoms Fe and Si, we apply the Mie-Lennard-Jones pair interaction potential in the form [34]

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

(35)

where \( D \) is the depth of potential well corresponding to the equilibrium distance \( r_0 \), \( m \) and \( n \) are determined empirically. Then, the potential parameters for the interaction Fe-Si are determined by [35]

\[ D_{\text{Fe-Si}} = \sqrt{D_{\text{Fe-Fe}} D_{\text{Si-Si}}} \left( r_0^{\text{Fe-Fe}} + r_0^{\text{Si-Si}} \right) = \frac{1}{2} \left( r_0^{\text{Fe-Fe}} + r_0^{\text{Si-Si}} \right). \]  

(36)

We find \( n_{\text{Fe-Si}} \) and \( n_{\text{Fe-Si}} \) by fitting the theoretical result with the experimental data for the Young modulus of interstitial alloy FeSi \( 3\% \) at room temperature. The Mie-Lennard-Jones potential parameters for the interactions Fe-Fe, Si-Si, and Fe-Si are given in Table 1. The Poisson ratio of Fe is 0.29 [36].

<table>
<thead>
<tr>
<th>Interaction</th>
<th>D (eV)</th>
<th>( r_0 ) (nm)</th>
<th>m</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe-Fe [34]</td>
<td>0.401</td>
<td>2.4775</td>
<td>7</td>
<td>11.5</td>
</tr>
<tr>
<td>Si-Si [35]</td>
<td>2.32</td>
<td>2.351</td>
<td>2.48</td>
<td>4.0</td>
</tr>
<tr>
<td>Fe-Si (proposal)</td>
<td>0.965</td>
<td>2.4142</td>
<td>2.4</td>
<td>5.2</td>
</tr>
</tbody>
</table>

Our calculations for FeSi and Fe are shown in tables from Table 2 to Table 5 and figures from Fig. 1 to Fig. 7.

Table 2. The maximum value of real stress \( \sigma_{\text{max}} \) and the limit of elastic deformation \( \varepsilon_{\text{e}} \) for FeSi alloys at \( P = 0 \) and \( T = 300 \text{K} \) calculated by SMM

<table>
<thead>
<tr>
<th>( \varepsilon_{\text{Si}} ) (%)</th>
<th>( \sigma_{\text{max}} ) (MPa)</th>
<th>( \varepsilon_{\text{e}} ) (%)</th>
<th>( \sigma_{\text{e}} ) (MPa)</th>
<th>( \varepsilon_{\text{e}} ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>243.10</td>
<td>6.6</td>
<td>200.31</td>
<td>0.11</td>
</tr>
<tr>
<td>2</td>
<td>250.46</td>
<td>6.8</td>
<td>206.53</td>
<td>0.12</td>
</tr>
<tr>
<td>3</td>
<td>258.70</td>
<td>7.0</td>
<td>213.56</td>
<td>0.14</td>
</tr>
<tr>
<td>4</td>
<td>279.37</td>
<td>7.0</td>
<td>233.30</td>
<td>0.16</td>
</tr>
<tr>
<td>5</td>
<td>296.44</td>
<td>7.0</td>
<td>250.28</td>
<td>0.19</td>
</tr>
</tbody>
</table>
Table 3. The limit of elastic deformation $\sigma_e$ and the maximum value of real stress $\sigma_{1max}$ for FeSi$_{2\%}$ at different pressures and $T = 300$K.

<table>
<thead>
<tr>
<th>P (GPa)</th>
<th>$c_{Si}(%)$</th>
<th>$\sigma_{1max}$ (MPa)</th>
<th>$\varepsilon_f(%)$</th>
<th>$\sigma_e$ (MPa)</th>
<th>$\varepsilon_e (%)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>0</td>
<td>247.43</td>
<td>6.5</td>
<td>203.17</td>
<td>0.09</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>243.34</td>
<td>7.0</td>
<td>197.98</td>
<td>0.11</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
<td>251.43</td>
<td>6.9</td>
<td>201.70</td>
<td>0.08</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>237.78</td>
<td>7.4</td>
<td>188.19</td>
<td>0.09</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>250.09</td>
<td>7.6</td>
<td>199.40</td>
<td>0.11</td>
</tr>
</tbody>
</table>

Fig. 1. The density of deformation energy $f(\varepsilon)$ for FeSi at different strains, $T = 300$K and $P = 0$ calculated by SMM.

Fig. 2. The real stress $\sigma_1(\varepsilon)$ for FeSi at different silicon concentration and strains, $T = 300$K and $P = 0$ calculated by SMM.
Figure 3. The density of deformation energy $f(\varepsilon)$ for FeSi at different temperatures and strains, $c_{Si} = 2\%$ and $P = 0$ calculated by SMM.

Figure 4. The real stress $\sigma_1(\varepsilon)$ for FeSi at different temperatures and strains, $c_{Si} = 2\%$ and $P = 0$ calculated by SMM.

Figure 5 shows the stress-strain relationship of alloys FeSi$_{1\%}$ at $P = 0$ and different temperatures from the SMM calculations. When $\varepsilon > 0.5\%$ the alloy FeSi is in the stage of nonlinear deformation and the $\sigma - \varepsilon$ dependence is described in the form of a complex curve. The stage of nonlinear deformation is an irreversible process. In the limit case, our obtained stress-strain curve of metal Fe is in relatively good agreement with the experimental curve of Singh et al. (2007) [26]. At a fixed strain $\varepsilon$, the stress $\sigma$ decreases when the concentration of
interstitial atoms increases. Adding silicon to iron to formulate steel will increase the strength and the hardness but will decrease the plasticity and toughness.

Our calculations for nonlinear deformation of clean metal Fe are shown in Table 4, Table 5, and Fig. 7. Table 4 shows the dependence of the density of deformation energy \( f(\varepsilon) \) and the maximum value of the real stress of Fe on the deformation \( \varepsilon \). The graph \( f(\varepsilon) \) exists one maximum point \( (\varepsilon_p, f_{\text{max}}) \). When the temperature increases, both \( \varepsilon_p \) and \( f_{\text{max}} \) decreases. Knowing \( \varepsilon_p \) and \( f_{\text{max}} \), we can determine the maximum value of real stress \( \sigma_{1\text{max}} \) when happens nonlinear deformation.

![Graph](image)

**Fig. 5.** The density of deformation energy \( f(\varepsilon) \) for FeSi at different pressure and strains, \( c_{Si} = 2\% \) and \( T = 300K \) calculated by SMM

<table>
<thead>
<tr>
<th>( \varepsilon )</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>6.2</th>
<th>6.4</th>
<th>6.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f(\varepsilon) )</td>
<td>2.04</td>
<td>5.24</td>
<td>8.85</td>
<td>12.32</td>
<td>15.22</td>
<td>17.13</td>
<td>17.30</td>
<td>17.34</td>
<td>17.15</td>
</tr>
<tr>
<td>( \sigma_{1\text{max}} )</td>
<td>193.79</td>
<td>246.31</td>
<td>274.53</td>
<td>283.78</td>
<td>277.93</td>
<td>258.12</td>
<td>251.86</td>
<td>244.12</td>
<td>233.67</td>
</tr>
</tbody>
</table>

Table 4. The dependence of the density of deformation energy \( f(\varepsilon) \) (GPa) and the real stress \( \sigma_{1} \) (MPa) on strain \( \varepsilon \) (%) for Fe at \( T = 300K \) and \( P = 0 \) calculated by SMM

Table 5 compares the SMM results and the experimental data for the maximum value of real stress and the limit of elastic deformation for Fe at \( P = 0 \) and room temperature.
Fig. 6. The real stress $\sigma_1(\varepsilon)$ for FeSi at different pressures and strains, $c_{Si} = 2\%$ and $T = 300K$ calculated by SMM.

Fig. 7. The real stress $\sigma_1(\varepsilon)$ for Fe at different strains, $T = 323K$ and $P = 0$ calculated by SMM (choose experimental stress $\sigma_{0.2} = 79$ MPa [26]) and from EXPT [26].

Table 5. The maximum value of real stress $\sigma_{1_{\text{max}}}$ and the limit of elastic deformation $\sigma_{\varepsilon}$ for Fe at $P = 0$ and $T = 300K$ calculated by SMM and from experiments [26,37,38]

<table>
<thead>
<tr>
<th></th>
<th>$\sigma_{1_{\text{max}}}$ (MPa)</th>
<th>$\sigma_{\varepsilon}$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SMM this work</td>
<td>244</td>
<td>201</td>
</tr>
<tr>
<td>EXPT [26]</td>
<td>240</td>
<td>180</td>
</tr>
<tr>
<td>EXPT [37]</td>
<td>296</td>
<td>204</td>
</tr>
<tr>
<td>EXPT [38]</td>
<td>230 - 345</td>
<td>110 - 220</td>
</tr>
</tbody>
</table>
3. Conclusions

From the obtained theoretical results and using the combination of the Mie-Lennard-Jones potential and our proposed potential or the Mie-Lennard-Jones potential, we calculated numerically characteristic quantities for nonlinear deformation of BCC-FeSi. We obtain the values of density of deformation energy, maximum real stress, the limit of elastic deformation, and the stress-strain curve and compare the calculated results with experiments for Fe. Some of our calculated results for Fe are in good agreement with available experiments and other calculated results predict experiments in the future.

Acknowledgements. No external funding was received for this study.

References


