Effects of pressure on structural, electronic, and mechanical properties of $\alpha$, $\beta$, and $\gamma$ uranium

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Effects of pressure on structural, electronic, and mechanical properties of $\alpha$, $\beta$, and $\gamma$ uranium

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The first-principles methods have been employed to calculate the structural, electronic, and mechanical properties of the $\alpha$, $\beta$, and $\gamma$ phases of uranium under pressure up to 100 GPa. The electronic structure has been viewed in forms of density of states and band structure. The mechanical stability of metal U in the $\alpha$, $\beta$, and $\gamma$ phases have been examined. The independent elastic constants, polycrystalline elastic moduli, as well as Poisson’s ratio have been obtained. Upon compression, the elastic constants, elastic moduli, elastic wave velocities, and Debye temperature of $\alpha$ phase are enhanced pronouncedly. The value of $B/G$ illustrates that $\alpha$ and $\gamma$ phases are brittle in ground state.

Keywords: first-principles, structural parameters, electronic structure, elastic constants

PACS: 61.50.Ah, 61.50.Ks, 71.20.–b, 62.20.–x

1. Introduction

Actinide elements and their compounds exhibit many fascinating physical behaviors and play special role in nuclear applications, for example, the superconductivity of the $f$-electron system, the complex magnetic structure in neptunium dioxide, and the topological electronic states in actinide nitrides. Among them, element uranium has attracted many attentions.

At ambient condition, the itinerant nature of U-$5f$ electrons results in a complex arrangement of atomic structure, a low symmetrical crystal structure of face-centered orthohombic (fco). This phase, $\alpha$-U, is stable in wide temperature range of 0 K–935 K and wide pressure area up to at least 100 GPa. At ambient pressure and under a narrow temperature range of 935 K–1045 K, a much complex $\beta$ phase appears. Under further high temperature of 1045 K–1460 K, in analogy to the transition metals of Ti, Zr, and Hf, $\beta$-U transits to a simple high-symmetry structure of body-centered cubic (bcc). The driving mechanism for this kind of transition has been attributed to the electron localization and/or the phonon-phonon interaction.

Concerning the physical properties, in experiments, the charge density wave (CDW) state below 43 K bulk modulus and equation of state, phonon-dispersion curves, and heat capacity of uranium were measured by ultrasonic technique, diamond anvil cell, x-ray diffraction, inelastic neutron scattering. In theory, the adiabatic compression curve up to 100 GPa effects of spin-orbit coupling, mechanical properties, melting, optical properties, work function, and phonon spectra CDW and electron–phonon coupling have been calculated in density-functional theory (DFT) level.

In this work, we use the first-principles DFT to carry out studies on the structural, electronic, and mechanical properties of uranium in its $\alpha$, $\beta$, and $\gamma$ phases under pressure up to 100 GPa. Specific details can be divided into four parts: (i) optimizing all lattice parameters and the internal degrees of freedom at selected volumes and then at our obtained pressures; (ii) comparing the enthalpy of the three phases to see the thermodynamic stability under pressure; (iii) analyzing the electronic structure; and (iv) calculating elastic constants and elastic moduli under different pressures.

2. Computational methods

We performed our first-principles DFT calculations within the Vienna ab initio simulation package (VASP). The Perdew–Burke–Ernzerhof form of the generalized gradient approximation was selected to described the exchange and correlation effects. A cutoff energy of 500 eV was set for the plane wave integration. All atoms were fully relaxed when Hellmann–Feynman forces become less than 0.01 eV/Å. The $k$-point meshes in the full wedge of the Brillouin zone (BZ) were sampled by 11 $\times$ 7 $\times$ 7, 7 $\times$ 7 $\times$ 13, and 13 $\times$ 13 $\times$ 13 grids, respectively for $\alpha$, $\beta$, and $\gamma$ phases according to the Monkhorst–Pack (MP) scheme. The U $6s^27s^26p^65d^{10}f^2$
orbits were treated as valence electrons.

To avoid the Pulay stress trouble, the geometry optimization was performed on the basis of fixed volumes rather than constant pressures. As shown in Fig. 1, we calculated the total energy versus volume data for the three phases in the first step, then performed the seventh-order polynomial fitting and obtained the \( E-V \) relation. Then, one can deduce the \( P-V \) relation by the thermodynamic derivative \( P = -\partial E/\partial V \). Using this \( P-V \) relation, we performed the second-step calculations at a series of volumes corresponding to some integer pressures. Note that these pressure values are different from the pressure values directly computed from DFT with the Hellmann–Feynman theorem.

![Fig. 1](color online) The total energy (\( E \))-volume (\( V \)) and the pressure (\( P \))-\( V \) relations of \( \alpha \), \( \beta \), and \( \gamma \) phases. The red solid circles are the first-step calculated \( E \). Then we do polynomial fitting to these data and obtain the solid red line. Using the polynomial fitted \( E-V \), we can deduce the \( P \) by the relation \( P = -\partial E/\partial V \). The integrated values of \( P \) used in the following calculations, are indicated by the black hollow circles.

In order to calculate elastic constants, we can apply stress tensors with a small strain onto the equilibrium structure. According to Hooke’s law, the crystal energy is expanded by Taylor,\(^{[40]}\)

\[
E(V, \varepsilon) = E(V_0, 0) + V_0 \sum_{i=1}^{6} \sigma \varepsilon_i + \frac{V_0}{2} \sum_{i,j=1}^{6} C_{ij} \varepsilon_i \varepsilon_j + O \left( \varepsilon_i^3 \right),
\]

where \( E(V_0, 0) \) is the energy of the unstrained system with the equilibrium volume \( V_0 \), \( \varepsilon \) is strain tensor which has matrix elements \( \varepsilon_{ij} \) (\( i, j = 1, 2, \) and 3) defined by

\[
\varepsilon_{ij} = \begin{pmatrix}
\varepsilon_1 & \frac{1}{2} \varepsilon_6 & \frac{1}{2} \varepsilon_5 \\
\frac{1}{2} \varepsilon_6 & \varepsilon_2 & \frac{1}{2} \varepsilon_4 \\
\frac{1}{2} \varepsilon_5 & \frac{1}{2} \varepsilon_4 & \varepsilon_3
\end{pmatrix}
\]

and \( C_{ij} \) are the elastic constants. For orthorhombic \( \alpha \) phase, there are nine independent elastic constants \( (C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, \) and \( C_{23} ) \). They can be achieved from nine different strains listed in the following:

\[
\varepsilon_1 = (\delta, 0, 0, 0, 0, 0), \quad \varepsilon_2 = (0, \delta, 0, 0, 0, 0), \\
\varepsilon_3 = (0, 0, \delta, 0, 0, 0), \quad \varepsilon_4 = (0, 0, 0, \delta, 0, 0), \\
\varepsilon_5 = (\delta, \delta, 0, 0, 0, 0), \quad \varepsilon_6 = (0, 0, 0, 0, \delta, 0), \\
\varepsilon_7 = (0, \delta, 0, \delta, 0, 0), \quad \varepsilon_8 = (\delta, 0, \delta, 0, 0, 0), \\
\varepsilon_9 = (0, \delta, \delta, 0, 0, 0).
\]

As for tetragonal \( \beta \) phase, there are six independent elastic constants \( (C_{11}, C_{33}, C_{44}, C_{66}, C_{12}, \) and \( C_{13} ) \) and can be obtained from six different strains listed in the following:

\[
\varepsilon_1 = (\delta, \delta, 0, 0, 0, 0), \quad \varepsilon_2 = (0, 0, \delta, 0, \delta, 0), \\
\varepsilon_3 = (\delta, 0, \delta, 0, 0, 0), \quad \varepsilon_4 = (0, 0, 0, 0, 0, \delta), \\
\varepsilon_5 = (0, \delta, 0, \delta, 0, 0), \quad \varepsilon_6 = (0, 0, 0, \delta, 0, 0).
\]

For cubic \( \gamma \) phase, there are three independent elastic constants \( (C_{11}, C_{44}, \) and \( C_{12} ) \) and can be gained from three different strains listed in the following:

\[
\varepsilon_1 = (\delta, \delta, 0, 0, 0, 0), \quad \varepsilon_2 = (0, 0, 0, \delta, 0, 0), \\
\varepsilon_3 = (\delta, 0, \delta, 0, 0, 0).
\]

where the small strain \( \delta \) was varied in steps of 0.006 from \( \delta = -0.036 \) to \( \delta = 0.036 \).

After having obtained the elastic constants, the polycrystalline bulk modulus \( B \) and shear modulus \( G \) were calculated from the Voigt–Reuss–Hill (VRH) approximations.\(^{[41–43]}\) \( B = \frac{1}{3}(B_R + B_V) \) and \( G = \frac{1}{2}(G_R + G_V) \). The Young’s modulus \( E \) and Poisson’s ratio \( \nu \) were calculated through \( E = 9BG/(3B + G) \) and \( \nu = (3B - 2G)/[2(3B + G)] \). In the calculation of the Debye temperature (\( \Theta_D \)), we used the relation

\[
\Theta_D = \frac{\hbar}{k_B} \left( \frac{3n}{4\pi\Omega} \right)^{1/3} \upsilon_m,
\]

where \( \hbar \) and \( k_B \) are Planck and Boltzmann constants, respectively, \( n \) is the number of atoms in the molecule, \( \Omega \) is molecular volume, and \( \upsilon_m \) is the average sound wave velocity.
average wave velocity in the polycrystalline materials is approximately given by

$$\nu_m = \left[ \frac{1}{3} \left( \frac{2}{\nu_i} + \frac{1}{\nu_l} \right) \right]^{-1/3},$$  \quad (7)

in the above expression, $\nu_i = \sqrt{G/\rho}$ ($\rho$ is the density) and $\nu_l = \sqrt{(3B + 4G)/3\rho}$ are the transverse and longitudinal elastic wave velocity of the polycrystalline materials, respectively.

3. Results and discussion

3.1. Atomic structures and lattice parameters

$\alpha$-U crystallizes in the orthorhombic $Cmcm$ space group (No. 63) with 4 atoms in the unit cell located at 4e (0, y, 0.25) Wyckoff positions [see Fig. 2(a)]. $\beta$-U crystallizes in the tetragonal $Pnma$ space group (No. 136) with 30 atoms in the unit cell sited at 2h (0, 0, 0.5), 4j (x, x, 0), 8i (x, x, z), 8i (x1, y1, 0), and 8i (x2, y2, 0) Wyckoff positions [see Fig. 2(b)]. $\gamma$-U crystallizes in the simple bcc structure [see Fig. 2(c)].

Table 1. Optimized lattice constants ($a$, $b$, and $c$), the fractional coordinate of the atoms ($y$), atomic volume ($V$) under pressures from 0 GPa to 100 GPa as well as bulk modulus ($B$) and its pressure derivative ($B'$) at 0 GPa for $\alpha$, $\beta$, and $\gamma$ phases of uranium. For comparison, experimental values and theoretical results from other calculations at 0 GPa are also listed.

<table>
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<tr>
<th>Phase</th>
<th>Method</th>
<th>Pressure/GPa</th>
<th>$a$/Å</th>
<th>$b$/Å</th>
<th>$c$/Å</th>
<th>$y$</th>
<th>$V/(\text{Å}^3$/atom)</th>
<th>$B$/GPa</th>
<th>$B'$</th>
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<td>0.098</td>
<td>20.101</td>
<td>142.2</td>
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</table>

The thermodynamic stabilities of $\alpha$, $\beta$, and $\gamma$ phases under pressure up to 100 GPa can be judged by comparing the Gibbs free energy values. At 0 K, the Gibbs free energy is equal to the enthalpy and can be obtained by $G = H = E + PV$. We plot in Fig. 3 the relative enthalpies of the $\alpha$ and $\gamma$ phases with respect to the $\beta$ phase as a function of pressure. In the whole pressure range, there are no crossing points for the three curves. The $\alpha$ phase is always thermodynamically stable up to 100 GPa. The pressure can reduce the $\Delta H$ between the $\gamma$ and $\beta$ phases, while increase the $\Delta H$ between the $\alpha$ and $\beta$ phases. As shown in Fig. 3, the curves of the relative enthalpies of the $\alpha$ and $\gamma$ phases with respect to the $\beta$ phase are almost parallel, which shows that the effect of pressure on the $\Delta H$ between the $\gamma$ and $\alpha$ phases is negligible. These facts are in good agree-
ment with experiments. Here, one may wish to stabilize the simple bcc structure at ambient conditions. However, according to our simulations as well as previous experiments, the bcc phase can only be stabilized by increasing temperature, at least in pressure range of 0 GPa–100 GPa.

3.2. Electronic properties

In order to study the effects of pressure on electronic structure, the total and partial density of states (DOSs) of $\alpha$, $\beta$, and $\gamma$ uranium at 0, 40, 100 GPa are plotted in Fig. 4. Near the Fermi level, the main contribution is from the 5$f$ and 6$d$ orbitals. The occupations of the 5$f$ orbitals at the Fermi level for $\alpha$-U and $\gamma$-U decrease evidently under pressure. Even so, the main occupation near the Fermi level is still from the 5$f$ orbitals which should play a key role in many macroscopical properties, for example, the hardness, elasticity, and conductivity. For $\beta$-U, the occupations of the 5$f$ orbitals at the Fermi level behaves in an oscillation way under pressure. Since the $\beta$ phase only appears in a narrow pressure range in the $P$–$T$ phase diagram, we will focus our sight on the pressure effects on the $\alpha$ and $\gamma$ phases.

Fig. 3. (color online) Calculated enthalpy differences of the $\alpha$ and the $\gamma$ phases with respect to the $\beta$ phase as a function of pressure.

Fig. 4. (color online) Total and partial densities of states for $\alpha$, $\beta$, and $\gamma$ phases of uranium at (a) 0 GPa, (b) 40 GPa, and (c) 100 GPa.

Fig. 5. (color online) The band structures at 0, 40, and 100 GPa for (a) $\alpha$ and (b) $\gamma$ phases. The Fermi level is set at zero.
As shown in Fig. 5, a lot of bands cross the Fermi energy level in the Brillouin zone for both \( \alpha \) and \( \gamma \) phases. Upon compression, this kind of crossing never changes visibly. This means that the conductivity of uranium should not vary too much under pressure.

### 3.3. Elastic properties

#### 3.3.1. Elastic properties of \( \alpha \) phase under high pressure

The elastic constants can measure the resistance and mechanical properties of a crystal under external stress, thus describing the stability of crystals against elastic deformation. We present the calculated elastic constants (\( C_{ij} \)) and the Reuss bulk modulus (\( R_B \)), and Debye temperature (\( \theta_D \)) of \( \alpha \)-U in Table 2. At 0 GPa, our results are comparable with previous pseudopotential calculations by Taylor et al.,[32] full-potential calculations by Soderlind et al.,[16] as well as experiments at 298 K from Fisher and McSkimin.[45] The requirement of mechanical stability in an orthorhombic crystal lead to the following restriction on elastic constants[18]

\[
C_i(i = 1\sim6) > 0, \\
C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0, \\
(C_{11} + C_{22} - 2C_{12}) > 0, \\
(C_{11} + C_{33} - 2C_{13}) > 0, \\
(C_{22} + C_{33} - 2C_{23}) > 0. 
\]

From the calculated values of \( C_{ij} \), \( \alpha \)-U is mechanically stable under pressure up to at least 100 GPa, which is consistent with that of experiments.[12-15] Besides, the nine elastic constants increase almost linearly from 0 GPa to 100 GPa.

<table>
<thead>
<tr>
<th>Phase</th>
<th>( C_{11}/\text{GPa} )</th>
<th>( C_{33}/\text{GPa} )</th>
<th>( C_{44}/\text{GPa} )</th>
<th>( C_{66}/\text{GPa} )</th>
<th>( C_{23}/\text{GPa} )</th>
<th>( B/\text{GPa} )</th>
<th>( G/\text{GPa} )</th>
<th>( E/\text{GPa} )</th>
<th>( \nu )</th>
<th>( u_l/(\text{m/s}) )</th>
<th>( u_t/(\text{m/s}) )</th>
<th>( u_m/(\text{m/s}) )</th>
<th>( \theta_D/\text{K} )</th>
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</thead>
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<tr>
<td>0</td>
<td>287.2</td>
<td>219.5</td>
<td>352.3</td>
<td>151.2</td>
<td>117.4</td>
<td>101.2</td>
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<td>28.2</td>
<td>152.1</td>
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<td>367</td>
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<td>Calc.[45]</td>
<td>300</td>
<td>220</td>
<td>320</td>
<td>150</td>
<td>93</td>
<td>120</td>
<td>50</td>
<td>5</td>
<td>110</td>
<td>0.18</td>
<td>228</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Expt.[45]</td>
<td>215</td>
<td>199</td>
<td>267</td>
<td>124</td>
<td>73</td>
<td>74</td>
<td>46</td>
<td>22</td>
<td>108</td>
<td>0.2</td>
<td></td>
<td></td>
<td>251</td>
</tr>
</tbody>
</table>

For the orthorhombic crystal system, the Voigt bulk modulus (\( B_V \)) and the Reuss bulk modulus (\( B_R \)) can be expressed by:

\[
B_V = (1/9)[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})], \\
B_R = \Delta[C_{11}(C_{22} + C_{33} - 2C_{23}) + C_{22}(C_{33} - 2C_{13}) - 2C_{33}C_{12} + 2(C_{23} - C_{13}) + C_{13}(2C_{12} - C_{13}) + C_{23}(2C_{13} - C_{23})]^{-1}, \\
\Delta = C_{13}(C_{12}C_{23} - C_{13}C_{22}) + C_{23}(C_{12}C_{13} - C_{23}C_{11}) + C_{33}(C_{11}C_{22} - C_{12}C_{12}), \\
\]

The Voigt shear modulus (\( G_V \)) and the Reuss shear modulus (\( G_R \)) are defined as:

\[
G_V = (1/15)[C_{11} + C_{22} + C_{33} + 3(C_{44} + C_{55} + C_{66}) - (C_{12} + C_{13} + C_{23})], \\
G_R = 15[4C_{11}(C_{22} + C_{33} + C_{23}) + C_{22}(C_{33} + C_{13}) + C_{33}C_{12} - C_{12}(C_{23} + C_{13}) - C_{23}(C_{13} + C_{21})]/\Delta + 3[1/(G_{14}) + 1/(G_{55}) + 1/(G_{66})]^{-1}. 
\]
It is very important to describe the elastic anisotropy behavior in engineering science and crystal physics. Crystal anisotropy reflects atomic arrangements along different directions. The shear anisotropic factors from our elastic constants are shown in Table 3. In the \{010\} shear planes between the \{011\} and \{010\} directions is written as \(A_1 = 4C_{44}/(C_{11} + C_{33} - 2C_{13})\). For the \{010\} shear planes between \{001\} and \{010\} directions, it is \(A_2 = 4C_{55}/(C_{22} + C_{33} - 2C_{23})\). And for the \{001\} shear planes between \{110\} and \{010\} directions is defined as \(A_3 = 4C_{66}/(C_{11} + C_{22} - 2C_{12})\). For an isotropic crystal, the factors \(A_1, A_2, \) and \(A_3\) must be one, while any value of them either smaller or greater than unity for orthorhombic structures. Our calculated results suggest that the shear anisotropic factor for the \{010\} shear planes between \{010\} and \{001\} directions show more anisotropic than the other two shear planes upon compression.

### Table 3. The anisotropic factors for \(\alpha\) and \(\beta\) phases.

<table>
<thead>
<tr>
<th>Phase</th>
<th>Pressure/GPa</th>
<th>(A_1)</th>
<th>(A_2)</th>
<th>(A_3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\alpha)</td>
<td>0</td>
<td>1.037</td>
<td>1.753</td>
<td>1.078</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.937</td>
<td>1.633</td>
<td>0.981</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>0.889</td>
<td>1.569</td>
<td>0.931</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>0.842</td>
<td>1.564</td>
<td>0.934</td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>0.842</td>
<td>1.564</td>
<td>0.936</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>0.767</td>
<td>1.326</td>
<td>0.834</td>
</tr>
<tr>
<td>(\beta)</td>
<td>0</td>
<td>1.198</td>
<td>1.019</td>
<td>0.701</td>
</tr>
</tbody>
</table>

3.3.2. Elastic properties of \(\beta\) and \(\gamma\) phases at ambient condition

For \(\beta\)-U and \(\gamma\)-U, we list their elastic constants, elastic moduli, elastic wave velocities, and Debye temperature in Table 4, in comparison with other theoretical results.\([28, 29, 32, 47]\) Here, the \(B_V\), \(B_R\), \(G_V\), and \(G_R\) of tetragonal and cubic structures are derived by the following formula:\([40]\)

\[
B_V = \frac{1}{9}[2(C_{11} + C_{12}) + 4C_{13} + C_{33}],  \\
B_R = \frac{C^2}{M},  \\
M = C_{11} + C_{12} + 2C_{33} - 4C_{13},  \\
C^2 = (C_{11} + C_{12})C_{33} - 2C_{13},  \\
G_V = \frac{1}{(M + 3C_{11} - 3C_{12} + 12C_{44} + 6C_{66})},  \\
G_R = \frac{15[(18B_V/C^2) + 6/(C_{11} - C_{12})] + (6/C_{44}) + (3/C_{66})}{7},  \\
\]

(11)

respectively. Our calculated elastic constants for \(\beta\)-U are well consistent with the values from Li et al.\([28]\) It is mechanically stable in the ground state because elastic constants satisfy the following mechanically stable criteria\([40]\) of tetragonal structure:

\[
C_{11} > 0, \quad C_{11} - C_{12} > 0, \quad C_{33} > 0,  \\
C_{44} > 0, \quad [2(C_{11} - C_{12}) + C_{33} + 4C_{13}] > 0,  \\
C_{66} > 0, \quad (C_{11} + C_{33} - 2C_{12}) > 0.  \\
\]

(13)

In fact, the \(C_{12}\) of \(\beta\)-U is much smaller than \(C_{11}\), the value of \(B, G, E, \) and \(\theta_D\) decrease from the \(\alpha\) phase to the \(\beta\) phase. The obtained bulk modulus value turns out to be accord with the result from the EOS fitting (see Table 1) at ambient pressure. Besides, the ratio of \(B/G\) (\(\sim 2.4\)) is above 1.75, which illustrates that tetragonal structure is ductile.

Furthermore, there are three elastic anisotropic factors in the tetragonal systems defined as \(A_1 = 2C_{66}/(C_{11} - C_{12}), \quad A_2 = 4C_{44}/(C_{11} + C_{33} - 2C_{13}), \) and \(A_3 = C_{44}/C_{66}\). The shear anisotropic factors \(A_1\) represents the \{001\} shear planes while the elastic anisotropic factors \(A_2\) for the \{011\} shear planes along the \{001\} direction. The \(A_3\) anisotropy relation corresponds to the shear along the \{010\} and \{100\} directions in the \{001\} and \{010\} planes, and their values are listed in Table 3. It is noted that anisotropy relation corresponds to the shear along the \{010\} and \{100\} directions in the \{001\} and \{010\} planes are more important than the other two shear planes.

Elastic constants unsatisfy the mechanically stable criteria\([40]\) of cubic structure, so the \(\gamma\) phase is mechanically unstable

\[
C_{11} > 0, \quad C_{44} > 0,  \\
C_{11} > |C_{12}|, \quad (C_{11} + 2C_{12}) > 0.  \\
\]

(14)

The calculations show that \(C_{11}\) is much smaller than \(C_{12}\), which is agreement with other theoretical calculations.\([29, 32, 47]\)
For bulk modulus, shear modulus, Young’s modulus, Poisson’s ratio, transverse, longitudinal, average sound velocities, as well as Debye temperature $\Theta_D$ at $0$ K. These results are compared with the values from Taylor and Shang [47] who employed the PW91-GGA exchange-correlation functional. Moreover, the value of the bulk modulus ($B=113$ GPa) slightly overestimates experimental calculation by Yoo et al. [13]. The ratio of $B/G$ ($\sim1.5$) of $\gamma$ phase demonstrates that bcc structure uranium is brittle in ground state.

4. Conclusion

In summary, the structural, electronic, and mechanical properties of the $\alpha$, $\beta$, and $\gamma$ phases of uranium under pressure up to 100 GPa have been studied by employing the first-principles DFT-GGA method. Our calculations show that the lowest energy structure of $U$ is $\alpha$-phase (orthorhombic $Cmcm$-type). By calculating the enthalpies of the three phases, we never find any phase transitions in pressure range of 0 GPa–100 GPa. According to our calculated elastic constants, $\alpha$ and $\beta$ phases are mechanically stable at ambient pressure. For $\gamma$ phase, however, it is mechanically unstable at 0 GPa. Under pressure, the bulk modulus $B$, shear modulus $G$, and Young’s modulus $E$ increase near linearly for $\alpha$ phase.

References

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[46] Pugh S F 1954 Philos. Mag. 45 823