Mechanical and Electronic Properties of DNTF Crystals under Different Pressure

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Abstract: In the present study, the effects of pressure on the structure, elastic properties and electronic structure of DNTF compounds are studied using the first principles method. It is found that pressure has a great influence on lattice constants. When the pressure reaches 80 GPa, the structure of DNTF changes suddenly. The variation trend of C_{11}, C_{22} and C_{33} values is consistent with that of pressure. In addition, pressure can improve the compressibility and shear resistance of the DNTF compound. The pressure can reduce the bandgap and further increases the charge density, causing DNTF to decompose and explode.

1. Introduction

Furoxan derivatives are a class of important energetic materials, which have attracted extensive attention due to their high density, good oxygen balance, good detonation performance and high thermal stability [1–6]. 3, 4-bis (3-nitrofurazan-4-yl) furoxan (DNTF) is a compound of furoxan derivatives, with high energy, low melting point and excellent comprehensive properties. As a promising high energy density material (HEDM), DNTF has become the focus of energetic materials researchers in recent years [7–11]. It is of great significance to study the properties of DNTF since the properties of this material directly affect its use, transportation and storage.

In order to further improve the comprehensive performance of DNTF, domestic and foreign researchers have carried out continuous exploration. Sinditskii V P et al. [12] performed thermal decomposition under isothermal conditions. The final study found that the thermal stability of DNTF was close to 1, 3, 5, 7-tetranitro-1, 3, 5, 7-tetrazocane (HMX), and the combustion rate was close to that of 2, 4, 6, 8, 10, 12-hexanitro-2, 4, 6, 8, 10, 12-hexaazaisowurtzitane (CL-20). Song et al. [13] studied the effect of methanol and acetic acid/aqueous solution on the crystal morphology of DNTF. The results showed that (001), (111), and (111) crystal faces were mainly exposed, while (011), (101), and (110) faces disappeared or occupied small areas. These results can provide theoretical support for the crystallization process of DNTF. Kazakov et al. [14] have meticulously researched the thermochemical and energy characteristics of DNTF and DNFF as composite solid rocket propellants. When used for aluminum-free and active binder-containing components, DNTF can provide a specific impulse of 254.5 s at 40 and 1 atm pressure at the combustion chamber and nozzle exit, respectively. Gu et al. [15] studied the thermal decomposition kinetics of DNTF using differential scanning calorimetry (DSC) test. The results showed that the decomposition mainly consisted of exothermic peaks P1, P2 and P3, which could be described by the N-order reaction model.

Furthermore, Wu et al. [16] studied the effects of high pressure on the structure, electron and absorption properties of 2, 6-diamino-3, 5-dinitropyrazine-1-oxide (LLM-105)
by using first principles. The density of states analysis demonstrates that the interaction between valence electrons is enhanced under pressure. The p orbital plays an important role in the chemical reaction of LLM-105. Wang et al. [17] studied the structure, electron and thermodynamic properties of 4, 4′, 6, 6′-tetra (azido) azo-1, 3, 5-triazine (TAAT) under pressure by using the first principles method. The study shows that the bandgap is almost zero when the pressure is 70 GPa. This indicates that TAAT has metallic properties at this time. The density of states shows that electron delocalization generally increases in TAAT under the influence of pressure. This result indicates that the impact sensitivity can be improved by applying pressure.

However, the effect of pressure on DNTF performance has not been reported. In addition, it is of great significance to study the mechanical and electronic properties of DNTF under different pressures. Therefore, in this study, the effects of different pressures on the crystal structure, mechanical properties and electronic properties of DNTF were studied using first principles.

2. Materials and Methods

In this paper, the study of DNTF performance was conducted by using the Cambridge serial total energy package (CASTEP) software package based on density functional theory [18,19]. In order to obtain the most stable structure, the Broyden–Flecher–Goldfarb–Shanno (BFGS) [20] method was used for the geometric optimization of the crystal structure. Perdew–Burke–Ernzerhof (PBE) [21] in the generalized gradient approximation (GGA) can be selected for the commutative association. The ultrasoft pseudopotentials (USP) were selected as pseudopotentials. When optimizing the crystal structure, the convergence precision was set as: SCF $5.0 \times 10^{-5}$ eV/atom, the total energy $1.0 \times 10^{-7}$ eV/atom, the force on each atom $0.03$ eV/Å, the maximum displacement $0.001$Å and the maximum stress deviation $0.05$ GPa. After the convergence test and considering the computational efficiency, the energy cut-off was $480$ eV and the k-point was $5 \times 3 \times 2$.

In order to study the change of DNTF structure with pressure, optimization calculation was carried out in the range of 0–80 GPa with step size of 10 GPa. The molecular formula of DNTF is $\text{C}_6\text{N}_8\text{O}_8$ and its chemical structural formula is shown in Figure 1a. The crystal structure belongs to orthogonal crystal and the space group is $\text{P}2_1\text{2} \text{1} \text{2}_1$ (No.19), as shown in Figure 1b.

![Figure 1. The structure of DNTF. (a) The chemical structure; (b) The crystal structure.](image)

3. Results

3.1. Lattice Constants and Stability

The calculated lattice constants of DNTF in 0 K and 0 GPa ground state are listed in Table 1. It can be seen that the lattice constants calculated at the ground state are in good agreement with the experimental values [22], indicating that the calculation method and simulation results adopted are accurate and reasonable. As can be seen from Table 1, in the range of 0–80 GPa, the lattice constants (a and c) of DNTF decrease with increasing...
pressure. However, when the pressure is 80 GPa, the lattice constant (b) increases suddenly, suggesting that the structure of the compound changes at this time.

**Table 1.** The calculated lattice parameters of DNTF under different pressure.

| Pressure | a(Å) | b(Å) | c(Å) |
|----------|------|------|------|
| 0 GPa    | 6.821| 10.983| 15.410|
| Exp. [22]| 6.662| 10.740| 15.093|
| 10 GPa   | 5.847| 10.381| 14.132|
| 20 GPa   | 5.519| 10.154| 13.618|
| 30 GPa   | 5.311| 9.994 | 13.315|
| 40 GPa   | 5.164| 9.872 | 13.074|
| 50 GPa   | 5.039| 9.775 | 12.900|
| 60 GPa   | 4.922| 9.714 | 12.748|
| 70 GPa   | 4.820| 9.703 | 12.548|
| 80 GPa   | 4.760| 9.874 | 12.090|

With the aim to intuitively show the influence of pressure on the structure of the DNTF compound, the relationship between lattice constant changes and pressure is shown in Figure 2. As displayed in the figure, the change rate of the lattice constant of DNTF gradually decreases with the increase of pressure. When the pressure increases from 0 to 80 GPa, the change rate of lattice constant a (a/a₀) of DNTF changes most obviously, decreasing to 0.658. It means that the a-direction is more sensitive to pressure in the crystal structure of DNTF. Moreover, with the increase of pressure, the decreasing trend of a/a₀, b/b₀ and c/c₀ tends to be slower. This is because the distance between atoms in DNTF crystal decreases with the increase of pressure, which leads to the increasing of interatomic repulsion force. In particular, when the pressure reaches 80 GPa, the value of b/b₀ increases suddenly from 0.843 at 70 GPa to 0.858. On the contrary, the decreasing degree of c/c₀ suddenly increased, demonstrating that the structure of DNTF changed at this point.

![Figure 2. The lattice constant changes of DNTF under different pressure.](image-url)
range of pressure is selected as 0–70 GPa. The fitting curves are shown in Figure 2 and the fitting formulas are as follows:

\[
\begin{align*}
a/a_0 & = 1.02231 \times P^{-0.09919}, \\
b/b_0 & = 0.98313 \times P^{-0.03672}, \\
c/c_0 & = 1.01770 \times P^{-0.05940},
\end{align*}
\]

3.2. Mechanical Properties

The elastic constants play an important role in the mechanical and thermodynamic properties of materials. It is well known that orthogonal crystals have nine independent elastic constants, which are \(C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13} \) and \(C_{23}\). The mechanical stability of compounds with orthorhombic structure can be judged according to formula (4) [23]

\[
\begin{align*}
C_{11} & > 0, C_{22} > 0, C_{33} > 0, C_{44} > 0, C_{55} > 0, C_{66} > 0, \\
[ C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23}) ] & > 0, \\
(C_{11} + C_{22} - 2C_{12}) & > 0, (C_{11} + C_{33} - 2C_{13}) > 0, \\
(C_{22} + C_{33} - 2C_{23}) & > 0.
\end{align*}
\]

where, \(C_{ij}\) is the elastic constant.

In this work, the elastic constants of DNTF compounds under different pressures are calculated. According to formula (4), it can be judged that DNTF is mechanically stable at 0 GPa, as shown in Table 2. In order to show the influence of pressure on the elastic constant more intuitively, the variation trend of the elastic constant with pressure was plotted, as shown in Figure 3. Based on the previous results of lattice constant, the structure of DNTF changes when the pressure is 80 GPa. Therefore, the influence of pressure on performance in the range of 0–70 GPa is discussed in the following research. As can be seen from Figure 3, \(C_{11}, C_{22}\) and \(C_{33}\) show the same trend of change and their values increase with the enhancement of pressure. With the increase of pressure, the value of \(C_{66}\) is consistent with its change trend, but the trend of \(C_{44}\) and \(C_{55}\) is different. When the pressure is 50 GPa, the values of \(C_{44}\) and \(C_{55}\) reach 35.99 GPa and 17.78 GPa, respectively. As the pressure continues to increase, these value decreases. The increase in elastic constants \(C_{12}, C_{13}\) and \(C_{23}\) is the same as the change in the trend of pressure. When the pressure is greater than 50 GPa, the value of \(C_{13}\) increases more slowly than that of \(C_{12}\) and \(C_{23}\).

![Figure 3](image-url)
Table 2. The calculated elastic constants of DNTF at 0 GPa.

| Phase | Species | \(C_{11}\) | \(C_{12}\) | \(C_{13}\) | \(C_{22}\) | \(C_{23}\) | \(C_{33}\) | \(C_{44}\) | \(C_{55}\) | \(C_{66}\) |
|-------|---------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| DNTF  | Present | 8.70      | 1.75      | 1.09      | 3.39      | 0.70      | 7.40      | 1.72      | 0.63      | 0.07      |

The bulk modulus (B), shear modulus (G), Young’s modulus (E) and Poisson’s ratio (\(\nu\)) of DNTF compound can be calculated by the following equations [24,25]:

\[
B_H = \frac{1}{2}(B_V + B_R) \tag{5}
\]

\[
G_H = \frac{1}{2}(G_V + G_R) \tag{6}
\]

\[
E = \frac{9B_H G_H}{(3B_H + G_H)} \tag{7}
\]

\[
\sigma = \frac{(3B_H - 2G_H)}{2(3B_H + G_H)} \tag{8}
\]

For orthorhombic materials [26,27]:

\[
B_V = \frac{1}{9}(C_{11} + C_{22} + C_{33}) + \frac{2}{9}(C_{12} + C_{13} + C_{23}) \tag{9}
\]

\[
B_R = 1/\left[\left(S_{11} + S_{22} + S_{33}\right) + 2(S_{12} + S_{13} + S_{23})\right] \tag{10}
\]

\[
G_V = \frac{1}{15}(C_{11} + C_{22} + C_{33}) - \frac{1}{15}(C_{12} + C_{13} + C_{23}) + \frac{3}{15}(C_{44} + C_{55} + C_{66}) \tag{11}
\]

\[
G_R = 1/\left[\left(\frac{4}{15}(S_{11} + S_{22} + S_{33}) - \frac{4}{15}(S_{12} + S_{13} + S_{23}) + \frac{3}{15}(S_{44} + S_{55} + S_{66})\right)\right] \tag{12}
\]

where, \(B_V\) and \(B_R\) are bulk moduli calculated by Voigt and Reuss methods, which limit the maximum and minimum values of bulk moduli respectively. \(B_H\) is the bulk modulus calculated by the Hill method and is the average value of \(B_V\) and \(B_R\). The shear moduli \(G_V\), \(G_R\) and \(G_H\) are defined in the same way. \(S_{ij}\) is the elastic compliances constant.

Figure 4 exhibits the pressure dependence of the bulk modulus, shear modulus, Young’s modulus and Poisson’s ratio of the compound DNTF. It is reasonable to conclude that the bulk modulus and shear modulus increase with the rise of pressure. This result suggests that increasing pressure can improve the compressibility and shear resistance of a DNTF compound. When the pressure is less than 50 GPa, the Young’s modulus of the DNTF compound increases. However, when the pressure is greater than 50 GPa, the Young’s modulus decreases. This phenomenon indicates that the stiffness of the DNTF compound is the maximum when the pressure is 50 GPa but it is not beneficial to the increase of compound stiffness when the pressure continues to increase. As the pressure increased from 0 GPa to 70 GPa, the Poisson’s ratio of DNTF compound increases from 0.32 to 0.43. The result shows that increasing pressure can further improve the elasticity and reduce the brittleness of a DNTF compound. When the pressure reaches 30 GPa, the change of Poisson’s ratio becomes gentle and the influence of pressure becomes small.
3.3. Electronic Properties

In order to analyze the bonding properties between atoms in DNTF compounds and the effect of pressure on the chemical bonding in the structure, the total density of states (TDOS) and the partial density of states (PDOS) were calculated. The total density of states and the partial density of states at 0 GPa are shown in Figure 5. It can be observed from Figure 5, in the energy range from $-8$ to 0 eV and the conduction band part, the TDOS mainly comes from the p orbitals of O, N and C atoms. In addition, the TDOS is mainly derived from the s orbitals of O, N and C atoms in the low energy region.

The TDOS under different pressures is shown in Figure 6, from which it can be seen that the curve and trend of the TDOS under different pressures are similar. The results demonstrate that the structure of DNTF is stable and there is no structural change within the studied pressure range. As the pressure increases, the TDOS decreases, which is owing to the change of the interaction potential [28].

The bandgap is generally the energy difference between the bottom of the conduction band and the top of the valence band. As can be seen from Figure 6, the bandgap gradually decreases with the increase of pressure. In order to observe the change of the bandgap more intuitively, the change of the DNTF bandgap under different pressures is plotted in Figure 7. It can be clearly seen from Figure 7 that the bandgap gradually decreases as the pressure increases. When the pressure reaches 30 GPa, the decreasing trend

![Figure 4. The modulus and Poisson’s ratio of DNTF under different pressure.](image)

![Figure 5. The density of states of DNTF at 0 GPa.](image)

![Figure 6. The density of states of DNTF under different pressure.](image)

![Figure 7. The bandgap of DNTF under different pressure.](image)
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Figure 6. The density of states of DNTF under different pressure.

Figure 7. The bandgap of DNTF under different pressure.
In order to analyze the influence of pressure on the electron density in the DNTF compound in more detail, the electron density and electron density differences under different pressure are calculated. The electron density diagram can reflect the electron density around the atom in the DNTF compound. The influence of pressure on the charge density is shown in Figure 8, which is drawn in the range of 0–1 e/Å$^3$. With the increase of pressure, the electron density around the atom increases continuously. It can be seen that pressure promotes charge aggregation in DNTF compounds and increases electron density.

The electron density difference represents the gain and loss of electrons in a DNTF compound. The electron density difference of DNTF under different pressures is shown in Figure 9 and the plot range is $-0.8$–$0.8$ e/Å$^3$. In this figure, red means getting electrons and blue means losing electrons. In DNTF compounds, C atoms gain electrons and there is a shared electron between C-C bonds. With the increase of pressure, the degree of electron gain and loss does not change obviously. The degree of electron aggregation around N and O atoms increases. It leads to the further polarization of atomic binding bonds in DNTF compounds, which promotes the impact sensitivity of DNTF.

Figure 8. The electron density of DNTF under different pressure. (a) 0 GPa; (b) 20 GPa; (c) 40 GPa; (d) 60 GPa.

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Figure 9. The electron density difference of DNTF under different pressure. (a) 0 GPa; (b) 20 GPa; (c) 40 GPa; (d) 60 GPa.

4. Conclusions

In this work, the effect of pressure on the structure, elastic properties and electronic structure of DNTF compound is studied. The lattice constant of DNTF decreases with increasing pressure. When the pressure reaches 80 GPa, the structure of DNTF changes. As the pressure increases, the values of $C_{11}$, $C_{22}$ and $C_{33}$ increase. The bulk modulus and shear modulus increase with the increase of pressure. The results show that pressure is helpful to improve the compressibility and shear resistance of DNTF compounds. With the enhancement of pressure, the bandgap decreases gradually, which increases the possibility of material decomposition and explosion. The electron aggregation around N and O atoms increases, which improves the impact sensitivity of DNTF.

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