Pressure-dependent mechanical and thermodynamic properties of newly discovered cubic Na$_2$He

Md. Zahidur Rahaman$^1$

Department of Physics
Pabna University of Science and Technology, Pabna-6600, Bangladesh
Bangladesh University of Engineering and Technology, Dhaka, Bangladesh
zahidur.physics@gmail.com

Md. Lokman Ali$^2$

Department of Physics
Pabna University of Science and Technology, Pabna-6600, Bangladesh
lokman.cu12@gmail.com

Md. Atikur Rahman$^3^*$

Department of Physics
Pabna University of Science and Technology, Pabna-6600, Bangladesh
atik0707phy@gmail.com

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Abstract

Recently for the first time, a stable compound of He and Na (Na$_2$He) is predicted at high pressure. We explore the pressure-dependent elastic, mechanical and thermodynamic properties of this newly discovered Na$_2$He by using *ab initio* technique. The calculation presents good accordance between the theoretical and experimental lattice parameters. Though the most stable structure of Na$_2$He is found at 300 GPa, present study ensures the mechanical stability of this compound up to 500 GPa. The study of Cauchy pressure, Pugh’s ratio, and Poisson’s ratio implies the ductile manner of Na$_2$He up to 500 GPa. According to the value of Poisson’s ratio the bonding force exists in Na$_2$He is central. The study of Zener anisotropy factor indicates that Na$_2$He is an anisotropic material but near at 300 GPa approximately isotropic nature of Na$_2$He is revealed. The study of the bulk modulus, shear modulus, Young’s modulus and Vickers hardness implies that the hardness of Na$_2$He can be improved by applying external pressure. However, the Debye temperature, melting temperature and minimum thermal conductivity of Na$_2$He are also calculated and discussed at different pressures.

**Keywords:** Na$_2$He, Structural properties, Mechanical properties, Thermodynamic properties.
I. Introduction

Helium (He) is chemically inert because of its closed-shell electronic configuration. For this reason, helium is very unwilling to form any stable compound in normal condition. However, helium possesses many attractive chemical properties such as it has highest ionization potential (24.59 eV) \cite{1} and zero electron affinity \cite{2}. On the other hand, helium is available in large quantities in the universe. For this reason, many scientists have tried to discover a stable compound of helium in recent decades. For the first time in 2015, Xiao Dong et al predicted a stable compound of sodium (Na) and helium (He) at pressure 300 GPa \cite{3}. Though the predicted compound Na$_2$He is stable above 113 GPa. They carried out both experimental and theoretical investigation for ensuring the dynamical stability of Na$_2$He. However, the mechanical stability of Na$_2$He is still vague. They also showed that Na$_2$He is not an inclusion material. The formation of Na$_2$He is strongly exothermic and a wide bandgap appears when helium is inserted into sodium \cite{3}. They also studied the electronic structure and pressure-dependent bandgap of Na$_2$He.

It is well known that pressure has a significant effect on the physical properties as well as chemical properties of materials. When a material is compressed it is generally deformed. This deformation behavior helps to understand the nature of solid-state theories \cite{4}. High pressure can also lead to the phase transition of a material \cite{5,6,7}. Therefore, it is very important to investigate the pressure effect on the mechanical and thermodynamic properties of newly reported Na$_2$He. In this paper, we study the elastic, mechanical and thermodynamic properties of Na$_2$He by using the DFT (Density Functional Theory) based first principles code CASTEP under different pressure up to 500 GPa. In this present letter, we also ensure the mechanical stability of Na$_2$He by theoretical means.

II. Method of computation

The first principles calculations were performed in the CASTEP computer code with generalized gradient approximation (GGA) using the PBE (Perdew, Burke, and Ernzerhof) exchange-correlation functional \cite{8,12}. The structural relaxation was obtained by using
the BFGS minimization scheme \cite{13}. In this case, the convergence criteria were set to 
\(0.5 \times 10^{-5} \text{ eV/atom}\) for energy, \(0.05 \text{ GPa}\) for stress and \(0.03 \text{ eV/Å}\) for the force. The energy cutoff was set at 1000 eV with \(10 \times 12 \times 10\) grids in primitive cells of Na\(_2\)He through
the investigation. Stress-strain method \cite{13} was used for obtaining the elastic stiffness 
constants at different pressures. In this case, the maximum value of strain amplitude was 
set to 0.003 through the whole elastic constant calculations at various pressures.

III. Results and discussion

A. Electronic structure

The first stable compound of helium Na\(_2\)He belongs to \textit{Fm}-3\textit{m} (225) space group with 
the cubic crystal structure, which retains four formula unit with 12 atoms per unit cell
\cite{3}. The experimentally evaluated lattice constant of Na\(_2\)He is 3.95 Å at 300 GPa \cite{3}. 
By minimizing the total energy the atomic positions and lattice parameters have been 
optimized as a function of normal pressure. Since Na\(_2\)He is more stable at 300 GPa, the 
crystal structure treated with 300 GPa is shown in Fig. 1. In the structure of Na\(_2\)He 
4\textit{a} atomic site is fully occupied by He atoms with fractional coordinates (0, 0, 0) and 
8\textit{c} atomic site is fully occupied by Na atoms with fractional coordinates (0.25, 0.25, 
0.25). The calculated structural parameters of Na\(_2\)He at 300 GPa are tabulated in Table
1 along with experimental values. The evaluated lattice constant at 300 GPa in this 
present study shows minor deviation (0.12\%) from the experimentally evaluated value 
bearing the reliability of the present investigation.

To investigate the effect of pressure on the structure of Na\(_2\)He, the variations of unit 
cell volume and lattice parameter of Na\(_2\)He have been studied under different pressure 
from 100 GPa to 500 GPa. Fig. 2(a) represents the change of lattice constant and unit cell 
volume of Na\(_2\)He with external pressure. It is evident that the normalized lattice constant 
and cell volume decreases with pressure. The compression of the crystal is not uniform 
over the whole range of pressure. With the increase of pressure, the relative compression 
of the structure is decreased due to the repulsive interaction among atoms. The more
the pressure is applied the nearer the atoms are and hence their repulsive interaction is strengthened, which leads to the above effect. Fig. 2(b) represents the pressure-volume plot of Na$_2$He from which we determine the pressure derivative bulk modulus $B'$ of Na$_2$He listed in Table 1.

**B. Mechanical properties**

In order to justify the mechanical stability and determine the different mechanical properties of solids, the single crystal elastic constants have been calculated by linear fitting of the calculated stress-strain function [14]. The cubic Na$_2$He belongs to three independent elastic constants $C_{11}$, $C_{12}$ and $C_{44}$. The evaluated elastic constants of Na$_2$He at different pressure are tabulated in Table 2. As shown in Table 2 it is clear that the studied compound is mechanically stable up to 500 GPa since the obtained values of $C_{ij}$ obey the well established Born stability criteria of solids [15] given below.

$C_{11} > 0$, $C_{44} > 0$, $C_{11} - C_{12} > 0$ and $C_{11} + 2C_{12} > 0$

The pressure-dependent elastic constants and different mechanical properties of Na$_2$He are demonstrated in Fig. 3. The value of $C_{11}$ implies the stiffness of compounds against (100)(100) uniaxial strain. We can see from Table 2 and Fig. 3(a) that Na$_2$He becomes stiffer with the increase of pressure. On the other hand, the value of $C_{12}$ and $C_{44}$ demonstrates the elasticity in shape. One can see from Fig. 3(a) that with the increase of pressure both the shear constants are increased implying that the compound becomes more resistant to shear deformation with pressure.

The Cauchy pressure is defined as $C_{12} - C_{44}$ which can be used to explain the atomic bonding character in a compound [16]. A compound will be nonmetallic (metallic) if $C_{12} - C_{44}$ is negative (positive) [17]. From Table 2 we see that the value of $C_{12} - C_{44}$ for Na$_2$He is positive over the pressure range studied indicating the metallic nature of Na$_2$He. However, the Cauchy pressure is increased with the increase in pressure [Fig. 3(b)]. Furthermore, the negative (positive) value of $C_{12} - C_{44}$ implies the brittle (ductile) manner of a compound [18]. As shown in Table 2 Na$_2$He is ductile and hence able to be drawn out into a thin wire. From Fig. 3(b) it is noticeable that the more the pressure is
applied the more ductile the compound is implying the increasing metallicity of Na$_2$He with pressure.

From the single crystal elastic constants, $C_{ij}$ the polycrystalline elastic moduli such as shear modulus $G$ and bulk modulus $B$ can be obtained according to Voigt-Reuss-Hill (VRH) approximation [19]. From the computed bulk modulus $B$ and shear modulus $G$ the Poisson’s ratio $\nu$ and Young’s modulus $E$ can be obtained by using the following relations [20],

$$\nu = \frac{3B - 2G}{2(3B + G)}$$  \hspace{2cm} (1) \\
$$E = \frac{9GB}{3B + G}$$  \hspace{2cm} (2)

The computed values of $B$, $G$, $\nu$, and $E$ under different pressure for Na$_2$He are listed in Table 3. It can be noted from Table 3 that the computed value of the bulk modulus $B$ matches well with that of obtained from fitting the third order Birch-Murnaghan Equation of State at 300 GPa. The bulk modulus $B$ is a measure of the ability of solids to defend compression. From Table 3 we see that at 300 GPa (more stable structure) the value of $B$ for Na$_2$He is 758.43 GPa which is comparatively so high than that of the well known hardest material diamond ($B = 443$ GPa) [21]. This high value of bulk modulus is indicating strong chemical bonding in Na$_2$He. A hard material possesses high bonding covalency. In Na$_2$He direct covalent interaction is found for Na-Na [3], showing good consistency with this study. With the increase in pressure, the bulk modulus also increases [Fig. 3(c)] indicating that the ability of the resist deformation of Na$_2$He is enhanced with pressure. The shear modulus $G$ is a measure of the ability of solids to defend plastic deformation. The value of $G$ depends upon the value of $C_{44}$. The large value of $C_{44}$ and $G$ at 300 GPa (see Table 2 and Table 3) implies a high level of resistant of Na$_2$He against the shear strain. It can also be noticed from Fig. 3(c) that with external pressure the value of $G$ is increased indicating the enhancement of the ability to resist shear deformation with the pressure of Na$_2$He. The Young’s modulus $E$ is a measure of the ability of solids to defend longitudinal stress. It is also used to judge the stiffness of a material. From Table 3 it can be seen that at 300 GPa the value of $E$ is quite
high for Na$_2$He and with the increase in pressure $E$ increases gradually indicating the enhancement of stiffness of Na$_2$He with external pressure.

Pugh’s ratio usually the ratio between bulk modulus and shear modulus ($B/G$) is a very useful index to detect the brittleness and ductility of materials [22]. $B/G < 1.75$ implies the brittle manner of a material and the value greater than 1.75 implies the ductile manner of a compound. From Table 3 one can see that Na$_2$He is ductile in nature shows good accordance with the result having from the analysis of Cauchy pressure. The pressure-dependent Pugh’s ratio of Na$_2$He is shown in Fig. 3(d). It can be noted that at 100 GPa the fabrication of this compound is easier. The Poisson’s ratio $\nu$ is another useful index to explain the plasticity and bonding nature of solids. For the covalent crystal, the value of $\nu$ is 0.10 and 0.25 for ionic crystal. The value from 0.25 to 0.50 implies the central force in a solid [23]. However, $\nu = 0.33$ indicates metallic material [24]. From Table 3 we notice that all over the pressure range the Poisson’s ratio is nearly similar and the value is around 0.39 implying the existence of the central force in Na$_2$He. The pressure-dependent Poisson’s ratio of Na$_2$He is shown in Fig. 3(e). We see a similar trend between the pressure-dependent curve of $B/G$ and $\nu$. Poisson’s ratio is also used to predict the brittleness and ductility of solids. If $\nu < 0.26$ for a compound then the compound will be brittle in the manner otherwise the compound will be ductile in the manner [25,26]. According to this condition, Na$_2$He is ductile in nature, accord well with other predictions.

To measure the rate of anisotropy in crystal the Zener anisotropy factor $A$ is a very useful index which is given as follows [28].

$$ A = \frac{2C_{44}}{(C_{11} - C_{12})} \quad (3) $$

For the complete isotropic crystal, the value of $A$ is unity. The value greater or smaller than unity implies the rate of anisotropy in solid. The calculated values of $A$ at various pressures are listed in Table 3. As shown in Table 3 the anisotropic nature of Na$_2$He has revealed. The pressure-dependent behavior of $A$ is illustrated in Fig. 3(f). With pressure up to 300 GPa the rate of anisotropy is decreased but after that, a strange behavior is
noticed. More theoretical work is required to understand this mysterious behavior of A for Na$_2$He.

The Vickers hardness $H_v$ is a very important property of compound used to measure the hardness of solids. Chen et al. developed a very useful formula to predict the hardness of solids given below [27],

$$H_v = 2 \left( K^2 G \right)^{0.585} - 3$$

(4)

Where, $K = G/B$. The values of $H_v$ computed from Eq. 4 under different pressures of Na$_2$He are tabulated in Table 3. Evidently $H_v$ of Na$_2$He increases gradually with applied pressure [Fig. 3(g)] implying that pressure has a significant effect on the hardness of Na$_2$He.

C. Thermodynamic properties

Debye temperature $\Theta_D$ is a very crucial thermodynamic parameter which is related to directly or indirectly many important thermal properties of solids such as specific heat of solid, melting point, thermal expansion etc. It is the temperature which is related to the highest normal mode of vibration of a crystal [29]. The Debye temperature can be obtained from different estimations. In this study, we have used the calculated elastic constants to compute the value of $\Theta_D$ for Na$_2$He. In this procedure, $\Theta_D$ can be computed directly by using the following equation [30],

$$\Theta_D = \frac{\hbar}{k_B} \left( \frac{3N}{4\pi V} \right)^{\frac{1}{3}} \times v_m$$

(5)

Where $v_m$ is the average sound velocity which can be calculated,

$$v_m = \left[ \frac{1}{3} \left( \frac{2}{v_t} + \frac{1}{v_l} \right) \right]^{-\frac{1}{3}}$$

(6)
Where \( v_l \) and \( v_t \) stands for longitudinal wave velocity and transverse wave velocity respectively which can be obtained as follows,

\[
v_l = \left( \frac{3B + 4G}{3\rho} \right)^{\frac{1}{2}} \tag{7}\]

And

\[
v_t = \left( \frac{G}{\rho} \right)^{\frac{1}{2}} \tag{8}\]

The computed values of \( v_l, v_t, v_m, \) and \( \Theta_D \) of Na\(_2\)He at different pressures are listed in Table 4. The pressure-dependent behavior of \( \Theta_D \) for Na\(_2\)He is illustrated in Fig. 4(a). It can be noticed from Fig. 4(a) that with the increase in pressure \( \Theta_D \) of Na\(_2\)He is increased gradually.

The thermal conductivity of the material is defined as the capacity to conduct heat energy through solid. The minimum thermal conductivity is a crucial thermodynamic parameter. With the increase in temperature, the thermal conductivity of solid is decreased and reaches a certain value generally defined as the minimum thermal conductivity \[31\]. The minimum thermal conductivity \( K_{min} \) can be obtained by using the following relation \[32\],

\[
K_{min} = K_B v_m \left( \frac{M}{n\rho N_A} \right)^{-2/3} \tag{9}\]

Where \( v_m \) stands for average sound velocity, \( K_B \) is the Boltzmann constant, \( n \) is the number of atoms per molecule, \( M \) is the molecular mass, and \( N_A \) is the Avogadro’s number. The calculated values of \( K_{min} \) at different pressures by using Eq. 9 are listed in Table 5 and plotted in Fig. 4(b). It can be noted from Fig. 4(b) that with the increase in pressure \( K_{min} \) of Na\(_2\)He is increased gradually.

The melting temperature of solid is another important thermodynamic parameter. The melting temperature \( T_m \) of cubic crystal can be computed as follows \[33\],

\[
T_m = 553 + 5.91C_{11} \pm 300 \ K \tag{10}\]
The calculated values of the melting temperature for Na\textsubscript{2}He at different pressures are listed in Table 5 and illustrated in Fig. 4(c). It can be seen from Fig. 4(c) that with the increase in pressure $T_m$ of Na\textsubscript{2}He is increased gradually. At high temperature, the anharmonic effect of the specific heat at constant volume is suppressed and close to a value known as Dulong-Petit limit \[34\]. The Dulong-Petit limit of solid can be evaluated as follows \[34\].

$$Dulong - Petit limit = 3nN_AK_B$$ (11)

Where $N_A$ is defined as the Avogadro’s constant and $K_B$ is the Boltzmann constant. The calculated Dulong-Petit limit of Na\textsubscript{2}He using Eq. 11 is listed in Table 5.

IV. Conclusions

In summary, a comprehensive investigation on the mechanical and thermodynamic properties of the first stable compound of helium and sodium Na\textsubscript{2}He has been carried out systematically by the theoretical method. The mechanical stability of cubic Na\textsubscript{2}He has been ensured through theoretical verification up to 500 GPa. Various mechanical properties (bulk modulus $B$, shear modulus $G$, Young’s modulus $E$, $B/G$ values, Poisson’s ratio $\nu$, anisotropy factor $A$ and Vickers hardness $H_v$) of Na\textsubscript{2}He under different pressure have also been reported. The study of the bulk modulus, shear modulus, Young’s modulus and Vickers hardness implies that the hardness of Na\textsubscript{2}He can be improved by applying external pressure. The study of Zener anisotropy factor indicates that Na\textsubscript{2}He is an anisotropic material but near at 300 GPa approximately isotropic nature of Na\textsubscript{2}He is revealed. The study of Cauchy pressure, Pugh’s ratio, and Poisson’s ratio implies the ductile manner of Na\textsubscript{2}He up to 500 GPa. The pressure-dependent behaviors of various thermal properties of Na\textsubscript{2}He have also been reported and discussed. We hope the predicted properties will have a good impact on comprehending the mechanical response of newly discovered Na\textsubscript{2}He.
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Figure 1: Crystal structure of Na$_2$He: (a) conventional unit cell and (b) primitive cell.

Figure 2: (a) Change of lattice parameter and cell volume as a function of pressure (b) Birch-Murnaghan equation of state for Na$_2$He.
Figure 3: Pressure-dependent mechanical properties of Na$_2$He.

Figure 4: Pressure-dependent thermodynamic properties of Na$_2$He.
**Table 1:** Calculated equilibrium Lattice constant “a”, unit cell volume “V”, bulk modulus “B” and its first pressure derivative “B’” of Na$_2$He at 300 GPa.

| Properties | Expt. [3] | This study | Deviation from Expt. (%) |
|------------|-----------|------------|--------------------------|
| a (Å )     | 3.950     | 3.955      | 0.12                     |
| V (Å$^3$)  | -         | 61.864     | -                        |
| B (GPa)    | -         | 747.32     | -                        |
| B’         | -         | 2.51       | -                        |

**Table 2:** Evaluated elastic constants $C_{ij}$ (GPa) and Cauchy pressure ($C_{12} - C_{44}$) of Na$_2$He under pressure.

| P (GPa) | $C_{11}$  | $C_{12}$  | $C_{44}$  | $C_{12} - C_{44}$ |
|---------|-----------|-----------|-----------|-------------------|
| 100     | 407.05    | 187.55    | 36.54     | 151.01            |
| 200     | 729.83    | 409.82    | 100.58    | 309.24            |
| 300     | 1018.20   | 628.55    | 170.20    | 458.35            |
| 400     | 1299.87   | 854.93    | 243.62    | 611.31            |
| 500     | 1575.16   | 1081.55   | 321.77    | 759.78            |
### Table 3: The evaluated bulk modulus $B$ (GPa), shear modulus $G$ (GPa), Young’s modulus $E$ (GPa), $B/G$ values, Poisson’s ratio $\nu$, anisotropy factor $A$ and Vickers hardness $H_v$ (GPa) of Na$_2$He under different pressures.

| $P$ (GPa) | $B$  | $G$  | $E$  | $B/G$ | $\nu$ | $A$  | $H_v$ |
|----------|------|------|------|-------|-------|------|-------|
| 100      | 260.71 | 57.82 | 161.51 | 0.396 | 0.332 | 0.68 |
| 200      | 516.49 | 121.23 | 337.29 | 0.391 | 0.628 | 3.07 |
| 300      | 758.43 | 179.65 | 499.51 | 0.390 | 0.873 | 4.72 |
| 400      | 1003.24 | 234.92 | 653.73 | 0.391 | 0.095 | 5.91 |
| 500      | 1246.08 | 289.34 | 805.66 | 0.392 | 1.303 | 6.97 |

### Table 4: The calculated density $\rho$ (in gm/cm$^3$), transverse ($v_t$), longitudinal ($v_l$), and average sound velocity $v_m$ (m/s) and Debye temperature $\Theta_D$ (K) of Na$_2$He.

| Pressure (GPa) | $\rho$ | $v_t$     | $v_l$     | $v_m$     | $\Theta_D$ |
|---------------|--------|-----------|-----------|-----------|-------------|
| 100           | 3.51   | 4058.68   | 9810.21   | 4592.46   | 688.69      |
| 200           | 4.60   | 5133.64   | 12141.64  | 5804.34   | 952.05      |
| 300           | 5.37   | 5783.97   | 13632.33  | 6538.80   | 1129.59     |
| 400           | 6.04   | 6236.50   | 14763.40  | 7051.52   | 1266.20     |
| 500           | 6.60   | 6621.13   | 15724.26  | 7487.27   | 1384.54     |

### Table 5: Calculated minimum thermal conductivity, $K_{min}$ (in Wm$^{-1}$K$^{-1}$), melting temperature, $T_m$ (in K) and the Dulong-Petit limit (in J/mole.K) of Na$_2$He at different pressures.

| Pressure (GPa) | $K_{min}$ | $T_m$          | Dulong-Petit limit |
|---------------|-----------|----------------|-------------------|
| 100           | 1.62      | 2958.66 ± 300  |                   |
| 200           | 2.45      | 4866.29 ± 300  |                   |
| 300           | 3.06      | 6570.56 ± 300  | 74.80             |
| 400           | 3.57      | 8235.23 ± 300  |                   |
| 500           | 4.02      | 9862.19 ± 300  |                   |