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# Elastic and mechanical properties of Osmium Diboride under high pressure

## ABSTRACT

*The approach towards designing superhard materials incorporates the lighter elements like Boron, Carbon and Nitrogen. With the application of developed DFT theoretical formalism, the calculation of the single crystal elastic constants for Osmium Diboride $OsB_2$ under High Pressure from first principle calculations are described in this paper. The calculated mechanical properties using Voigt and Reuss approximation for Bulk (B), Young (E) and Shear Modulus (G) (in kbar) and Poisson ratio (n) for different pressure ranges (0to 200 GPa) have been reported.*
***Keywords**: DFT; $OsB_2$; Pressure*

## 1. INTRODUCTION

Osmium di-borides ($OsB_2$), a compound of Osmium (z=76) [Xe] $4f^{14}$ $5d^6$ $6s^2$ and Boron (z=5), is known for its high hardness as sapphire due to a combination of high $e^-$ density of Os with their covalent bonds. Some researchers classified it as superhard in hardness as like in Rhenium Diboride ($ReB_2$). However, it is still not a superhard material at normal conditions in comparison with hardest known Diamond or cubic-BN material [1]. $OsB_2$ can be manufactured in vacuum or having atmosphere with inert gases at high temperature of about 1000°C with mixture of Magnesium Diboride and Osmium tri-chloride [2]. Previously, it was seen as hexagonal in structure [3], but lateron some experiments verified that it is an orthorhombic [4]. However modern synthesis methods found that its hexagonal phase is similar to the hexagonal-$ReB_2$ [5].

With the application of developed DFT theoretical formalism and recent updated version of Quantum ESPRESSO (ver. 7.1) with efficient codes (thermo_pw, thermo_control and pw.x), the calculation for various properties specially elastic and mechanical properties of the single crystal elastic constants for Osmium Diboride $OsB_2$ under High Pressure from first principle calculations are described in this paper.

The elastic behavior of a completely asymmetric material is specified by 21 set of independent elastic constants, while for an isotropic material, the number is 2. With some limits, the necessary number is determined by the symmetry of the material, and it is 9 for orthorhombic crystals. These nine-independent elastic constants are usually referred to as $c_{11}$, $c_{22}$, $c_{33}$, $c_{44}$, $c_{55}$, $c_{66}$, $c_{12}$, $c_{13}$ and $c_{23}$. A theoretical treatment of the elasticity of orthorhombic systems is thus considerably more difficult than for cubic, hexagonal and tetragonal structures which have three, five, and six independent elastic constants, respectively. The task of calculating the elastic constants of orthorhombic crystals becomes even more costly when realizing that the strains needed to be calculated where some of them give rise to a geometry with very low symmetry. Due to the fact that very less theoretical work on elastic constants of orthorhombic systems are available and still unavailable for high pressure upto 200 GPa with the method adopted in this research. Hence, these properties at different pressure ranges from zero to upto 200 GPa are calculated and predicted.

Since the hardness of a material is directly related to its various properties viz incompressibility in its Mechanical Properties, elasticity and resistance tochange in shape, hence, the calculation of the Bulk modulus is essential tool to understand the hardness of the material. The bulk modulus is a tool to identify deformation in a solid crystal. Elements with small molar volumes and strong interatomic forces shows high order of bulk moduli.

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There is also a direct relationship between bulk modulus and valence electron density. This can be easily said that having the more electrons, greater the repulsions within the structure. The shear modulus 'G' is defined as ratio of shear stress to shear strain (G=stress/strain). The larger the shear modulus, the greater the ability for a material to resist shearing forces. It is the measure of rigidity. It's relation with bulk modulus (B) is given as 3/G=2B(1−2n)(1+n), where n is the Poisson's ratio. Fracture toughness also is a measure of material's ability to resist breakage from external force or pressure. Values of elastic constants provide valuable information about the bonding characteristic between adjacent atomic planes and the anisotropic character of the bonding and structural stability [6]. It has also been noticed that there is a correlation between the elastic constants and the melting temperature of a solid [7,8]. Pugh's ratio between the bulk and shear modulus, B/G, for polycrystalline phases as a measure of fracture/toughness in metals. A high or low B/G value is associated with ductility /brittleness[9,10].

## 2. COMPUTATIONAL METHOD

Osmium Diboride per unit cell contains eight formula units (Fig. 1) with hexagonal layers, which are stacked on top of each other in such a way that the Os atoms of adjacent layers avoid close contact. Structural optimization was carried out from total energy studies. Before performing calculations to obtain the elastic constants, firstly we optimized the structural parameters of $OsB_2$ using PBE type of the generalized gradient approximation -GGA for good approximations, which have been calculated. For this, using adopted experimental a, b and c parameters were used to optimized parameters and optimized equilibrium volume for corresponding pressure.

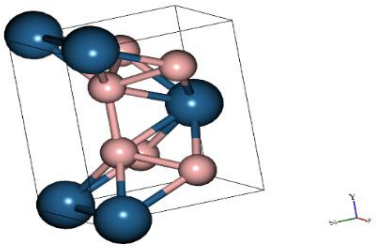


*Figure 1. Optimized Unit cell crystal structure of Osmium Diboride ($OsB_2$)(at 0 GPa) presented by XcrysDen and BURAI Graphical User Interface. Big balls represent for Os atoms and smaller one`s re for Boron*

For the structural optimization, total energy curves for iterations have been observed to calculate these parameters for $OsB_2$. The obtained data from this Perdew-Burke-Ernzerhof (PBE) type-GGA of exchange-correlational pseudo-potential (pp) approximations are shown. The equilibrium structural parameters wherever available obtained from our GGA calculations are in very good agreement with the corresponding experimental values.

The pseudopotential form of rrkjus have been used in BURAI of QE for the calculation of optimized structure corresponding to the pressure within combination of non-linear core-correction and semi-core state-sp in valence for Os (Osmium).

Then with the scf calculation by pw.x code of QE, with high order of iteration processes, the gound state energy at absolute temperature and corresponding pressure other electronic and physical properties of $OsB_2$ have been calculated. With the Equation of states under stress-strain relations, the desired properties have been calculated by thermo_pw under thermo_control script and pw.x codes of QE. The structure in the point group 100 D_2h (mmm) is compatible with the Bravais lattice. Crystal is orthorhombic (ibrav=8, in input cif) type of structure. The kinetic energy cut-off (ecutwfc) of 53.7933 Ry and charge density cutoff (ecutrho) is 484.140 Ry for the calculation for best and high order approximations with plain mixing mode. Self-Consistency scf convergence threshold limit was set to $10^{-12}$ Ry. Spin polarization is taken as collinear. Monkhorst k-point mesh [11] is taken as 8x5x6 to 9x5x6 and as per pressure requirement and 21 number of Bands selected for calculation at High Symmetry IBZ. The pseudopotential type is taken as Ultrasoft PP, Exchange Correlation Function of PBE. The present first-principle optimization procedure and calculations of properties from the optimization of atomic positions was carried through the forces and energy minimization process considered during structural relaxation. This algorithm method is applied to pressure control to allow the variation in shape and the volume of the fully relaxed cell in all directions. A smearing width of $10^{-2}$ Ry is taken for the start unit cell. After running the pw.x for checking a self-consistency, an optimized relaxed structure at 0 GPa is obtained. Having the obtained parameter and further run pw.x command in BURAI with setting pressure at 10 GPa with subsequently step-up, the required lattice parameter in output of scf file can be generated. All pseudopotentials are taken from online references [12]. In order to find the accurate energy cut-off and k-point mesh, the scf convergence test was performed for all par ameters and considered to be achieved with the minimum consecutive iterative steps with sufficient energy difference.

## 3. RESULTS AND DISCUSSION

The calculated Elastic Constants ($C_{ij}$) for Osmium Diboride under pressure ranging from 0 to 200 GPa are presented in table 1. The Cauchy pressure calculated from ($C_{12}$–$C_{44}$) is -ve upto 170 GPa for Osmium Diboride and it is interesting to observe +ve Cauchy Pressure above 170 GPa. It indicates the covalent bonding and brittleness upto 170 GPa and positive Cauchy's Pressure at 180 GPa and above denotes strong and metallic bonding in $OsB_2$ crystal.

The variation of Elastic Constants ($C_{ij}$) in kbar with respect to Pressure (in GPa) shows increasing effect of Elastic Constants with Pressure. Here, in figure 2, it is visible that $c_{33}$ is highest in all elastic constants and $c_{55}$ is lowest susceptible to pressure. All these elastic constants expand linearly with respect to pressure in Osmium Diboride. It has clearly appeared in the variation curve in figure 3 that the change with longitudinal stains along $c_{33}$, $c_{11}$ and $c_{22}$ are more responsive to applied pressure comparative to $c_{13}$ and $c_{55}$. So, it can be said that longitudinal elastic constants along Z-axis and X-axis are more influenced towards the change in pressure while elasticity towards shape expressed by $c_{13}$ and $c_{55}$ differs to a small extent under pressure. All increases linearly as the pressure increases up. The elastic constants possess the trend $c_{33}>c_{11}>c_{22}>c_{12}>c_{66}>c_{13}>c_{55}$, which implies that change. mechanically stability criteria can be determined by the elastic constant in this orthorhombic crystal $OsB_2$ also. The generalized elastic stability criteria for the crystal,

$C_{11} + C_{22} + C_{33} + 2\,(C_{12} + C_{13} + C_{23}) > 0$;

$C_{11} + C_{22} - 2\,C_{12} > 0$;

$C_{11} + C_{33} - 2\,C_{13} > 0$;

$C_{22} + C_{33} - 2\,C_{23} > 0$

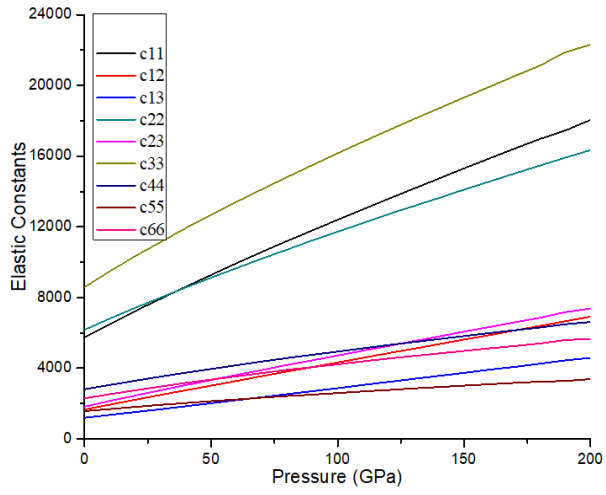



*Figure 2. Variations of Elastic Constants of Osmium Diboride under pressure*

*Table 1. Calculated values of Elastic Constants of Osmium Diboride under pressure*

| Pressure (GPa) | Cauchy's Pressure (c12-c44) | Anisotropy factor (A) |
|---|---|---|
| 0 | -1,138.00 | 1.37 |
| 10 | -1,113.39 | 1.34 |
| 20 | -1,082.54 | 1.31 |
| 30 | -1,042.33 | 1.29 |
| 40 | -993.76 | 1.28 |
| 50 | -944.59 | 1.27 |
| 60 | -891.11 | 1.25 |
| 70 | -823.15 | 1.24 |
| 80 | -758.8 | 1.24 |
| 90 | -691.06 | 1.23 |
| 100 | -618.62 | 1.22 |
| 110 | -538.53 | 1.22 |
| 120 | -454.43 | 1.22 |
| 130 | -372.12 | 1.21 |
| 140 | -292.78 | 1.21 |
| 150 | -202.45 | 1.2 |
| 160 | -112.33 | 1.2 |
| 170 | -14.8 | 1.19 |
| 180 | 89.07 | 1.19 |
| 190 | 167.93 | 1.2 |
| 200 | 305.77 | 1.19 |

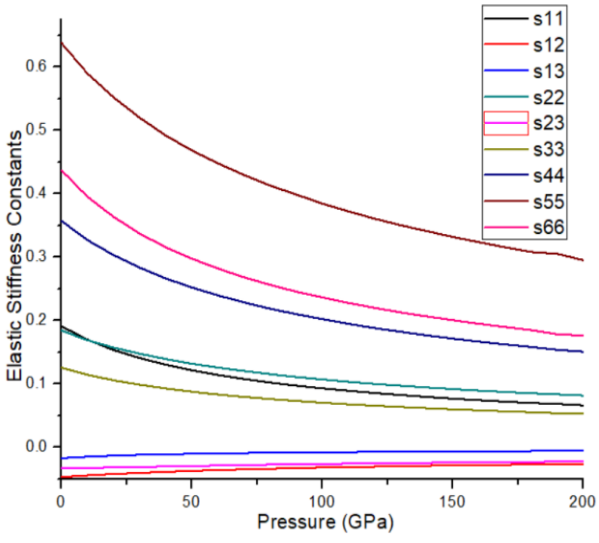



*Figure 3. Variations of Elastic Stiffness Constants of Osmium Diboride under pressure*

From table 2, the calculated mechanically stability criteria for hexagonal structure of Osmium Diboride crystal is given.It is analysed that the structure is stable under pressure. The stability

increases with pressure. Here, $C_{11}>C_{22}> C_{33}$, represents a comparative lower sensitivity towards pressure of lattice interactions along the crystallographic z-axis.

*Table 2. Calculated values of Elastic Stiffness Compliances of $OsB_2$ under pressure*

| Pressure (GPa) | s11 | s12 | s13 | s22 | s23 | s33 | s44 | s55 | s66 |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 0.191 | -0.046 | -0.017 | 0.184 | -0.033 | 0.126 | 0.357 | 0.638 | 0.437 |
| 10 | 0.170 | -0.044 | -0.014 | 0.169 | -0.032 | 0.115 | 0.327 | 0.589 | 0.395 |
| 20 | 0.154 | -0.042 | -0.013 | 0.158 | -0.031 | 0.106 | 0.303 | 0.552 | 0.363 |
| 30 | 0.141 | -0.040 | -0.011 | 0.148 | -0.031 | 0.099 | 0.284 | 0.520 | 0.337 |
| 40 | 0.131 | -0.038 | -0.011 | 0.140 | -0.030 | 0.093 | 0.267 | 0.492 | 0.316 |
| 50 | 0.122 | -0.037 | -0.010 | 0.132 | -0.029 | 0.088 | 0.252 | 0.468 | 0.298 |
| 60 | 0.114 | -0.035 | -0.009 | 0.126 | -0.028 | 0.084 | 0.240 | 0.448 | 0.282 |
| 70 | 0.108 | -0.034 | -0.009 | 0.121 | -0.028 | 0.080 | 0.229 | 0.430 | 0.268 |
| 80 | 0.103 | -0.033 | -0.008 | 0.116 | -0.027 | 0.076 | 0.219 | 0.413 | 0.256 |
| 90 | 0.098 | -0.032 | -0.008 | 0.111 | -0.026 | 0.073 | 0.210 | 0.399 | 0.246 |
| 100 | 0.093 | -0.031 | -0.007 | 0.107 | -0.026 | 0.071 | 0.202 | 0.385 | 0.237 |
| 110 | 0.089 | -0.031 | -0.007 | 0.104 | -0.025 | 0.068 | 0.195 | 0.372 | 0.228 |
| 120 | 0.086 | -0.030 | -0.007 | 0.100 | -0.025 | 0.066 | 0.188 | 0.361 | 0.220 |
| 130 | 0.083 | -0.029 | -0.007 | 0.097 | -0.024 | 0.064 | 0.183 | 0.351 | 0.213 |
| 140 | 0.080 | -0.029 | -0.006 | 0.095 | -0.024 | 0.062 | 0.177 | 0.341 | 0.207 |
| 150 | 0.077 | -0.028 | -0.006 | 0.092 | -0.024 | 0.060 | 0.172 | 0.332 | 0.201 |
| 160 | 0.075 | -0.028 | -0.006 | 0.090 | -0.023 | 0.059 | 0.167 | 0.324 | 0.195 |
| 170 | 0.072 | -0.027 | -0.006 | 0.088 | -0.023 | 0.057 | 0.163 | 0.316 | 0.190 |
| 180 | 0.070 | -0.027 | -0.006 | 0.086 | -0.022 | 0.056 | 0.159 | 0.308 | 0.185 |
| 190 | 0.069 | -0.026 | -0.005 | 0.084 | -0.022 | 0.054 | 0.154 | 0.305 | 0.179 |
| 200 | 0.067 | -0.026 | -0.005 | 0.082 | -0.022 | 0.053 | 0.151 | 0.295 | 0.176 |

The anisotropy factor A was obtained from the relation $A = 2C_{44}/ (C_{11} – C_{12})$ for orthorhombic type of crystal. Anisotropy decreases with pressure in $OsB_2$.

The calculated values of elastic stiffness compliance for orthorhombic $OsB_2$ ($s_{ii}$, i = 1, 2 or 3, where $s_{ii}$ are the diagonal elements of the compliance matrix) (in 1/Mbar) are presented in table 2. In fig 3, variation in Elastic Stiffness Compliances with respect to pressure have been shown for this Diboride. It is illustrated that, $s_{55}$ is highest prone to pressure effect in this elastic compliance and $s_{33}$ the lowest. However, some compliances $s_{12}$, $s_{23}$ and $s_{23}$ does not increases with pressure.

In table 3, the calculated mechanical properties of Osmium Diboride under pressure using Voigt and Reuss approximation for Bulk (B), Young (E) and Shear Modulus (G) (in kbar) and Poisson ratio (n) for different pressure ranges (0 to 200 GPa) have been reported. These values linearly increase with pressure. In table 4, average of Voigt and Reuss approximation as per Hill (VRH approximation) have been reported for the mechanical properties B, E and G and Poisson Ratio n. Also, Pugh Ratio have been presented under pressure. It is observed that on the basis of the variation in Pugh Ratio (B/G) of Osmium Diboride under pressure, the structure is changed into ductile beyond the pressure range of 110 GPa (when B/G > 1.75). However, similar analysis on the basis of the Poisson ratio indicates that Osmium Diboride behaves ductile at about and above 90 GPa (n>0.26). The Fig 4 displays the variation in Poisson' ratio (n) with pressure.

In table 5, calculated sound velocity for Longitudinal, Bulk and Shear directional represented by $V_P$, $V_B$ and $V_G$ (in m/s) of $OsB_2$ have been presented. The Average Debye Sound Velocity (m/s) and Debye temperature (K) are also presented in the table upto 200 GPa which shows linear increased effect of these thermodynamical properties with respect to pressure. In table 6, the calculated values of Speed of Sound towards Compressional ($V_P$), Bulk ($V_B$) and Shear ($V_G$) from VRH approximation of Osmium Diboride under pressure have been reported. As per fig 5, the variations of Speed of Sound towards Compressional ($V_P$), Bulk ($V_B$) and Shear ($V_G$) from VRH approximation of Osmium Diboride under pressure have been presented. It is seen that Compressional sound speed effected higher than others.

*Table 3- Calculated Voigt and Reuss approximation of Bulk (B), Young (E) and Shear Modulus (G) in kbar and Poisson ratio (n) for different pressure ranges (0 to 200 GPa) of $OsB_2$*

| Pressure (GPa) | Voigt approximation B | Voigt approximation E | Voigt approximation G | Voigt approximation poisson ratio |
|---|---|---|---|---|
| 0.00 | 3,318.39 | 5,771.80 | 2,384.82 | 0.21 |
| 10.00 | 3,746.15 | 6,362.89 | 2,614.35 | 0.22 |
| 20.00 | 4,148.61 | 6,907.74 | 2,825.28 | 0.22 |
| 30.00 | 4,544.30 | 7,429.90 | 3,026.43 | 0.23 |
| 40.00 | 4,935.17 | 7,935.60 | 3,220.60 | 0.23 |
| 50.00 | 5,313.83 | 8,418.75 | 3,405.78 | 0.24 |
| 60.00 | 5,684.38 | 8,885.06 | 3,584.16 | 0.24 |
| 70.00 | 6,052.84 | 9,340.43 | 3,757.79 | 0.24 |
| 80.00 | 6,417.21 | 9,781.50 | 3,925.30 | 0.25 |
| 90.00 | 6,773.89 | 10,207.93 | 4,086.96 | 0.25 |
| 100.00 | 7,122.86 | 10,622.22 | 4,243.96 | 0.25 |
| 110.00 | 7,475.03 | 11,032.81 | 4,399.02 | 0.25 |
| 120.00 | 7,824.59 | 11,436.18 | 4,551.15 | 0.26 |
| 130.00 | 8,164.25 | 11,822.02 | 4,696.26 | 0.26 |
| 140.00 | 8,501.61 | 12,203.87 | 4,839.91 | 0.26 |
| 150.00 | 8,840.92 | 12,584.70 | 4,983.02 | 0.26 |
| 160.00 | 9,178.87 | 12,957.59 | 5,122.71 | 0.26 |
| 170.00 | 9,507.99 | 13,322.61 | 5,259.76 | 0.27 |
| 180.00 | 9,843.58 | 13,681.62 | 5,393.47 | 0.27 |
| 190.00 | 10,198.24 | 14,063.19 | 5,535.95 | 0.27 |
| 200.00 | 10,496.35 | 14,379.91 | 5,653.96 | 0.27 |
| Pressure (GPa) | Reuss approximation B | Reuss approximation E | Reuss approximation G | Reuss approximation poisson ratio |
| 0.00 | 3,233.64 | 5,466.94 | 2,243.81 | 0.22 |
| 10.00 | 3,660.25 | 6,017.84 | 2,454.29 | 0.23 |
| 20.00 | 4,062.31 | 6,522.70 | 2,646.36 | 0.23 |
| 30.00 | 4,457.68 | 7,006.34 | 2,829.60 | 0.24 |
| 40.00 | 4,848.25 | 7,474.39 | 3,006.46 | 0.24 |
| 50.00 | 5,226.57 | 7,921.23 | 3,175.08 | 0.25 |
| 60.00 | 5,597.03 | 8,348.53 | 3,335.68 | 0.25 |
| 70.00 | 5,965.98 | 8,766.57 | 3,492.39 | 0.26 |
| 80.00 | 6,329.43 | 9,171.25 | 3,643.72 | 0.26 |
| 90.00 | 6,685.89 | 9,561.38 | 3,789.23 | 0.26 |
| 100.00 | 7,034.69 | 9,943.09 | 3,931.86 | 0.26 |
| 110.00 | 7,386.98 | 10,319.11 | 4,071.69 | 0.27 |
| 120.00 | 7,736.92 | 10,689.24 | 4,209.24 | 0.27 |
| 130.00 | 8,076.06 | 11,040.49 | 4,339.28 | 0.27 |
| 140.00 | 8,413.45 | 11,387.15 | 4,467.56 | 0.27 |
| 150.00 | 8,753.53 | 11,736.07 | 4,596.81 | 0.28 |
| 160.00 | 9,091.09 | 12,074.28 | 4,721.52 | 0.28 |
| 170.00 | 9,420.65 | 12,407.57 | 4,844.85 | 0.28 |
| 180.00 | 9,755.97 | 12,734.10 | 4,964.73 | 0.28 |
| 190.00 | 10,100.96 | 13,038.01 | 5,073.66 | 0.28 |
| 200.00 | 10,409.12 | 13,361.17 | 5,194.59 | 0.29 |

*Table 4. Calculated Voigt-Reuss-Hill approximation of Bulk (B), Young (E) and Shear Modulus (G) in kbar and Poisson ratio (n) for different pressure ranges (0 to 200 GPa) of $OsB_2$*

| Pressure (GPa) | VR Hill average of the two approximation B | VR Hill average of the two approximation E | VR Hill approximation G | VR Hill average of the two approximation poisson ratio | Pugh Ratio (B/G) |
|---|---|---|---|---|---|
| 0.0 | 3,276.02 | 5,619.37 | 2,314.32 | 0.21 | 1.42 |
| 10.0 | 3,703.20 | 6,190.36 | 2,534.32 | 0.22 | 1.46 |
| 20.0 | 4,105.46 | 6,715.22 | 2,735.82 | 0.23 | 1.50 |
| 30.0 | 4,500.99 | 7,218.12 | 2,928.02 | 0.23 | 1.54 |
| 40.0 | 4,891.71 | 7,705.00 | 3,113.53 | 0.24 | 1.57 |
| 50.0 | 5,270.20 | 8,169.99 | 3,290.43 | 0.24 | 1.60 |
| 60.0 | 5,640.70 | 8,616.79 | 3,459.92 | 0.25 | 1.63 |
| 70.0 | 6,009.41 | 9,053.50 | 3,625.09 | 0.25 | 1.66 |
| 80.0 | 6,373.32 | 9,476.38 | 3,784.51 | 0.25 | 1.68 |
| 90.0 | 6,729.89 | 9,884.65 | 3,938.09 | 0.26 | 1.71 |
| 100.0 | 7,078.77 | 10,282.66 | 4,087.91 | 0.26 | 1.73 |
| 110.0 | 7,431.00 | 10,675.96 | 4,235.36 | 0.26 | 1.75 |
| 120.0 | 7,780.76 | 11,062.71 | 4,380.20 | 0.26 | 1.78 |
| 130.0 | 8,120.16 | 11,431.26 | 4,517.77 | 0.27 | 1.80 |
| 140.0 | 8,457.53 | 11,795.51 | 4,653.74 | 0.27 | 1.82 |
| 150.0 | 8,797.22 | 12,160.38 | 4,789.92 | 0.27 | 1.84 |
| 160.0 | 9,134.98 | 12,515.94 | 4,922.12 | 0.27 | 1.86 |
| 170.0 | 9,464.32 | 12,865.09 | 5,052.30 | 0.27 | 1.87 |
| 180.0 | 9,799.77 | 13,207.86 | 5,179.10 | 0.28 | 1.89 |
| 190.0 | 10,149.60 | 13,550.60 | 5,304.80 | 0.28 | 1.91 |
| 200.0 | 10,452.73 | 13,870.54 | 5,424.27 | 0.28 | 1.93 |

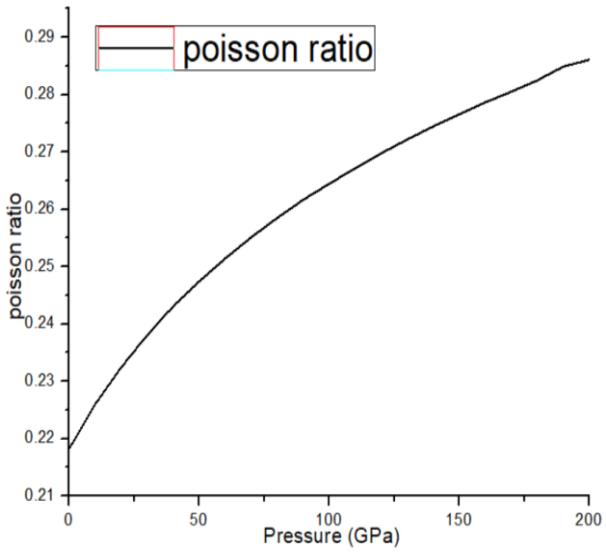



*Figure 4. Variations in Poisson's ratio (n) of Osmium Diboride under pressure*

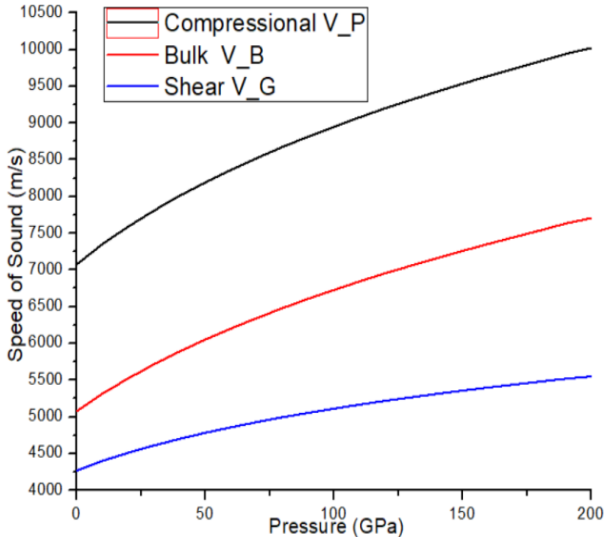
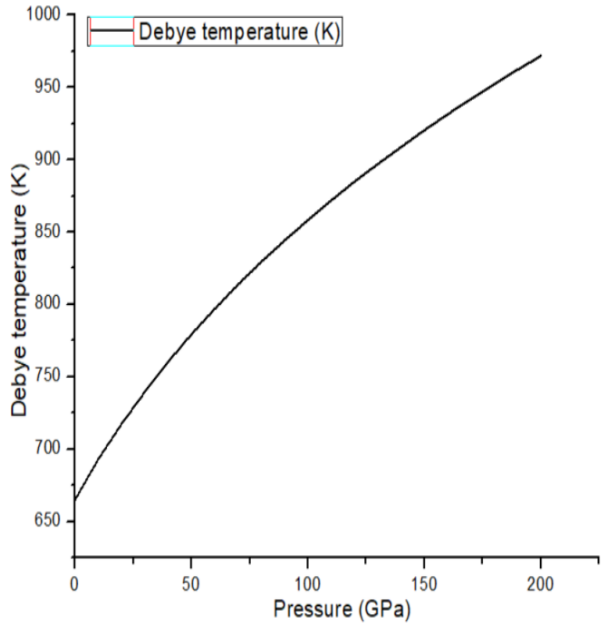



*Figure 5. Variations of Speed of Sound towards Compressional ($V_P$), Bulk ($V_B$) and Shear ($V_G$) from VRH approximation of OsB2 under pressure*

*Table 5. Calculated values of Speed of Sound towards Compressional ($V_P$), Bulk ($V_B$) and Shear ($V_G$) from VRH approximation of Osmium Diboride under pressure*

| Pressure (GPa) | Compressional V_P | Bulk V_B | Shear V_G |
|---|---|---|---|
| 0 | 7,075.19 | 5,077.17 | 4,267.37 |
| 10 | 7,352.99 | 5,316.98 | 4,398.53 |
| 20 | 7,590.67 | 5,523.57 | 4,509.03 |
| 30 | 7,807.99 | 5,713.79 | 4,608.47 |
| 40 | 8,009.70 | 5,890.99 | 4,699.85 |
| 50 | 8,193.21 | 6,052.52 | 4,782.44 |
| 60 | 8,362.62 | 6,202.46 | 4,857.69 |
| 70 | 8,523.44 | 6,345.40 | 4,928.36 |
| 80 | 8,674.51 | 6,480.48 | 4,993.78 |
| 90 | 8,815.94 | 6,607.42 | 5,054.41 |
| 100 | 8,948.27 | 6,725.96 | 5,111.24 |
| 110 | 9,077.72 | 6,842.70 | 5,165.93 |
| 120 | 9,201.75 | 6,954.67 | 5,218.10 |
| 130 | 9,316.23 | 7,058.93 | 5,265.25 |
| 140 | 9,427.01 | 7,159.64 | 5,310.93 |
| 150 | 9,536.21 | 7,258.69 | 5,356.11 |
| 160 | 9,641.02 | 7,354.57 | 5,398.58 |
| 170 | 9,740.38 | 7,444.81 | 5,439.43 |
| 180 | 9,838.47 | 7,535.45 | 5,478.08 |
| 190 | 9,940.42 | 7,630.95 | 5,516.82 |
| 200 | 10,020.93 | 7,704.06 | 5,549.77 |




*Figre 6. Variations of Debye temperature (in K) of Osmium Diboride under pressure*

In Table 6 the approximated values of Average Debye Sound Velocity (m/s) and Debye temperature (K) of Osmium Diboride under pressure have been tabulated. In fig. 6, variation of Debye temperature with pressure represents increasing Debye temperature.

To calculate the elastic anisotropy, the orthorhombic Osmium Diboride crystal is assumed to be an elastically anisotropic type.The calculated shear anisotropic factors are presented in table 7. These shear anisotropic factors are a measure of the degree of anisotropy in the bonding between atoms in different planes. The shear anisotropic factor for the plane 1 0 0 ($A_1$), shear planes between the 0 1 1 and 0 1 0 directions ($A_2$ and $A_3$) are given and hence, can say that the crystal is almost isotropic towards the plane 0 1 0 and anisotropic towards the plane for the shear planes 0 0 1 between 1 1 0 and 0 1 0 directions and it increases its isotropic symmetry under high pressure towards the direction 0 1 0 as indicated in calculated values of the factors $A_1$, $A_2$, and $A_3$.

*Table 6. Calculated values of Average Debye Sound Velocity (m/s) and Debye temperature (K) n of Osmium Diboride under pressure*

| Pressure (GPa) | Average Debye sound velocity | The approximate Debye temperature VRH average | Debye temperature (K) |
|---|---|---|---|
| 0 | 4,685.92 | 669.67 | 665.16 |
| 10 | 4,834.18 | 697.81 | 693.16 |
| 20 | 4,959.11 | 722.25 | 717.48 |
| 30 | 5,071.70 | 744.62 | 739.73 |
| 40 | 5,175.17 | 765.43 | 760.41 |
| 50 | 5,268.76 | 784.57 | 779.45 |
| 60 | 5,353.91 | 802.33 | 797.08 |
| 70 | 5,433.95 | 819.16 | 813.80 |
| 80 | 5,508.10 | 834.98 | 829.50 |
| 90 | 5,577.01 | 849.84 | 844.27 |
| 100 | 5,641.40 | 863.97 | 858.29 |
| 110 | 5,703.53 | 877.62 | 871.84 |
| 120 | 5,762.84 | 890.75 | 884.89 |
| 130 | 5,816.39 | 902.93 | 896.98 |
| 140 | 5,868.24 | 914.77 | 908.71 |
| 150 | 5,919.62 | 926.45 | 920.31 |
| 160 | 5,967.90 | 937.59 | 931.36 |
| 170 | 6,014.23 | 948.37 | 942.05 |
| 180 | 6,058.30 | 958.73 | 952.32 |
| 190 | 6,101.26 | 968.92 | 962.23 |
| 200 | 6,139.56 | 978.26 | 971.62 |

The parameters α and β are defined as the relative change of the **b** and **c** axis as a function of the deformation of an a- axis. The linear bulk modulus $B_{relax}$is also obtained from the single crystal isotropic bulk modulus (table 8).

*Table 7. The calculated anisotropic factors $A_1$, $A_2$, and $A_3$ along different planes of Osmium Diboride*

| Pressure (GPa) | A1 | A2 | A3 |
|---|---|---|---|
| 0 | 1.09 | 0.57 | 0.82 |
| 10 | 1.08 | 0.56 | 0.84 |
| 20 | 1.07 | 0.56 | 0.86 |
| 30 | 1.07 | 0.56 | 0.87 |
| 40 | 1.07 | 0.56 | 0.88 |
| 50 | 1.06 | 0.56 | 0.89 |
| 60 | 1.06 | 0.56 | 0.89 |
| 70 | 1.06 | 0.56 | 0.90 |
| 80 | 1.07 | 0.56 | 0.91 |
| 90 | 1.07 | 0.56 | 0.91 |
| 100 | 1.07 | 0.56 | 0.92 |
| 110 | 1.07 | 0.56 | 0.92 |
| 120 | 1.08 | 0.56 | 0.93 |
| 130 | 1.08 | 0.56 | 0.93 |
| 140 | 1.08 | 0.57 | 0.93 |
| 150 | 1.08 | 0.57 | 0.94 |
| 160 | 1.08 | 0.57 | 0.94 |
| 170 | 1.08 | 0.57 | 0.94 |
| 180 | 1.09 | 0.57 | 0.94 |
| 190 | 1.09 | 0.56 | 0.96 |
| 200 | 1.09 | 0.57 | 0.95 |

*Table 8. Calculated values of Bulk Modulus Along Crystallographic Axes of Osmium Diboride under pressure*

| Pressure (GPa) | B(relax) | α (Alpha) | β (Beta) | γ (Gamma) |
|---|---|---|---|---|
| 0 | 3,233.64 | 0.82 | 0.60 | 18,898.07 |
| 10 | 3,660.25 | 0.84 | 0.61 | 21,908.72 |
| 20 | 4,062.31 | 0.85 | 0.62 | 24,926.06 |
| 30 | 4,457.68 | 0.87 | 0.64 | 27,921.13 |
| 40 | 4,848.25 | 0.87 | 0.65 | 30,824.63 |
| 50 | 5,226.57 | 0.88 | 0.66 | 33,707.42 |
| 60 | 5,597.03 | 0.89 | 0.66 | 36,615.92 |
| 70 | 5,965.98 | 0.90 | 0.67 | 39,552.67 |
| 80 | 6,329.43 | 0.91 | 0.68 | 42,300.33 |
| 90 | 6,685.89 | 0.91 | 0.68 | 45,095.52 |
| 100 | 7,034.69 | 0.92 | 0.69 | 47,905.80 |
| 110 | 7,386.98 | 0.92 | 0.70 | 50,708.09 |
| 120 | 7,736.92 | 0.93 | 0.70 | 53,516.83 |
| 130 | 8,076.06 | 0.93 | 0.71 | 56,279.69 |
| 140 | 8,413.45 | 0.94 | 0.71 | 59,129.24 |
| 150 | 8,753.53 | 0.94 | 0.72 | 61,948.97 |
| 160 | 9,091.09 | 0.95 | 0.72 | 64,747.00 |
| 170 | 9,420.65 | 0.95 | 0.72 | 67,587.35 |
| 180 | 9,755.97 | 0.96 | 0.73 | 70,329.71 |
| 190 | 10,100.96 | 0.95 | 0.72 | 72,135.88 |
| 200 | 10,409.12 | 0.96 | 0.74 | 75,819.40 |

In Table 9, the calculated values of the Bulk moduli along the a,b and c axis of Osmium Diboride under pressure have been presented. The data shows higher Bulk Modulus along c axis comparative to a and b axes. It is also found that $B_c > B_b > B_a$.

*Table 9. Calculated values the bulk modulus along the a, b and c axis of Osmium Diboride under pressure*

| Pressure (GPa) | Ba | Bb | Bc |
|---|---|---|---|
| 0 | 7,817.26 | 9,520.03 | 13,108.75 |
| 10 | 8,954.97 | 10,720.89 | 14,649.98 |
| 20 | 10,062.67 | 11,808.86 | 16,101.44 |
| 30 | 11,156.31 | 12,881.16 | 17,524.17 |
| 40 | 12,224.80 | 13,972.70 | 18,906.89 |
| 50 | 13,273.07 | 15,012.47 | 20,251.86 |
| 60 | 14,315.73 | 16,016.07 | 21,562.94 |
| 70 | 15,361.34 | 17,024.83 | 22,841.12 |
| 80 | 16,362.68 | 18,034.49 | 24,138.26 |
| 90 | 17,363.87 | 19,013.28 | 25,391.69 |
| 100 | 18,357.62 | 19,955.86 | 26,617.77 |
| 110 | 19,354.06 | 20,929.90 | 27,834.96 |
| 120 | 20,348.35 | 21,901.56 | 29,029.66 |
| 130 | 21,319.44 | 22,810.35 | 30,232.11 |
| 140 | 22,304.28 | 23,705.12 | 31,409.14 |
| 150 | 23,286.74 | 24,648.55 | 32,545.30 |
| 160 | 24,261.51 | 25,552.87 | 33,731.72 |
| 170 | 25,233.25 | 26,438.54 | 34,848.12 |
| 180 | 26,194.17 | 27,354.17 | 36,013.42 |
| 190 | 26,993.36 | 28,274.80 | 37,612.08 |
| 200 | 28,092.94 | 29,145.92 | 38,221.40 |

## 4. CONCLUSION

In this paper, we outline descriptions of the structural features, relative stability via various parameters, crystal structure and mechanical properties of $OsB_2$ which were investigated via the first- principle techniques. Moreover, the elastic constants and elastic-dependent properties of Osmium Diboride (OsB2) are also successfully investigated. Our calculated hardness suggests that Osmium Diboride (OsB2) is potential hard materials.

In this manuscript we have given the valuable information of the structure unit of $OsB_2$. The equilibrium structural parameters are in good agreement (By GGA calculations) with the equation

of state under stress strain relation. The desired mechanical properties have been calculated by thermo_pw which are (a) Elastic constant $C_{ij}$ when observed from 0 to 200 GPa found $C_{33}$ is the highest and $C_{55}$ is the lowest. (b) The Cauchy pressure is negative below 170 and becomes positive when it is greater then 180 which shows strong metallic bonding (c) Elastic stiffness is the highest for $S_{55}$ and the lowest for $S_{33}$ (d) The research shows that Bulk, Young and Shear moduli and poisson ratio increase linearly with the increasing of pressure (e) With the help of Pugh ratio (B/G) the structural changed can be seen changing ductile beyond 110 GPa. This article shows the variation in sound velocity $V_P$, $V_B$ and $V_G$ (in m/s) from VRH approximations and is presented. In addition, it gives average Debye velocity at different temperature. Further we observed in general that increasing effect of Debye temperature accelerate the corrosion rate of materials.

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## IZVOD

### ELASTIČNA I MEHANIČKA SVOJSTVA OSMIJUM DIBORIDA POD VISOKIM PRITISKOM

*Pristup prema projektovanju supertvrdih materijala uključuje i upotrebu lakših elemenata kao što su bor, ugljenik i azot. Primena razvijenog teoretskog formalizma DFT je omogućila izračunavanje elastičnih konstanti u monokristalima osmijumdiborida $OsB_2$ pod.visokim pritiskom, što je ovde opisano. Izračunate mehaničke osobine korišćenjem Voigt i Reuss aproksimacijom za zapreminski (B), Jungov (E) i smicajni modul (G) (u kbar) kao i za Puasonov koeficijent (n) u rasponu različitih vrednosti pritiska ovde su prikazane.*

***Ključne reči:*** *DFT, $OsB_2$, pritisak*

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