

Structural and elastic properties of TiN and AlN compounds: first-principles study

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First-principles calculations of the lattice constants, bulk modulus, pressure derivatives of the bulk modulus and elastic constants of AlN and TiN compounds in rock-salt (B1) and wurtzite (B4) structures are presented. We have used the full-potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT) in the generalized gradient approximation (GGA) for the exchange-correlation functional. Moreover, the elastic properties of cubic TiN and hexagonal AlN, including elastic constants, bulk and shear moduli are determined and compared with previous experimental and theoretical data. Our results show that the structural transition at 0 K from wurtzite to rock-salt phase occurs at 10 GPa and -26 GPa for AlN and TiN, respectively. These results are consistent with those of other studies found in the literature.

Keywords: *N-compounds; elastic properties; first-principle calculations*

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1. Introduction.

In general, a nitride is a chemical combination of nitrogen with other element, often with a metal. Titanium nitride (TiN) ceramic coating, deposited by a process of physical vapor deposition (PVD), has a golden color and a gap near zero. It crystallizes in the face-centered cubic (fcc) rock-salt type structure. Its space group is $Fm\bar{3}m$ (225) with a lattice parameter $a = 0.4241$ nm [1]. The TiN coatings are widely used to improve the lifetime and performance of cutting tools or friction [2]. High hardness combined with low friction make the coating extremely cost effective in reducing general wear [3, 4]. Aluminum nitride (AlN) is a

semiconductor with a wide band gap (6.2 eV) [5–12]. It is a refractory material and an electrical insulator having a high thermal conductivity and high resistance to oxidation and abrasion. It crystallizes in the wurtzite structure which has a hexagonal symmetry, belonging to space group ($P6_3mc$). AlN has potential applications in optoelectronics within ultraviolet range, as a substrate for epitaxial growth, and power electronics for the manufacture of microwave power transistors [13, 14]. The present work is devoted to the study of the structural and elastic properties of TiN and AlN having rock-salt and wurtzite structures, respectively. It is also devoted to the study of the transition pressures of the structures of these materials. We have used the full-potential linearized augmented plane wave (FP-LAPW) within the density functional theory

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(DFT) and realized by the generalized gradient approximation (GGA) [15–18].

2. Calculation method

First-principles calculations were performed by WIEN2k [19]. R_{MT} $K_{Max} = 9$ was used to determine the matrix size (convergence), where K_{Max} is the plane wave cut-off and R_{MT} is the smallest of all atomic sphere radii; R_{MT} for Ti, Al and N were chosen equal to 1.80, 1.80 and 1.60 a.u., respectively. The exchange-correction functional was depicted by the GGA of Perdew-Burke-Ernzerhof (PBE) [15, 16]. The energy convergence criterion for electronic self-consistency was 10^{-4} eV per unit cell. The k -point meshes chosen in the present calculations were 72 and 84 for rock-salt and wurtzite structures of both TiN and AlN. In our calculations, we treated the states Ti ($1s^2 2s^2 3s^2 2p^6 3p^6$), Al ($1s^2 2s^2 2p^6$) and N ($1s^2$) as core states, and the states Ti ($3d^2 4s^2$), Al ($3s^2 3p^1$) and N ($2s^2 2p^3$) as valence states.

To calculate the elastic constants, we have used two different methods, Mehl method, [20] for the cubic system and the method developed by Shang et al. [21], for the hexagonal system, with deformation $\delta = 0.01$. Materials with cubic symmetry have only three independent elastic moduli C_{11} , C_{12} and C_{44} . These moduli were evaluated by calculating the total energy for a perturbed system. To calculate the coefficients C_{11} and C_{12} , a volume-conserving orthorhombic strain tensor was applied, given by the following expression:

$$\bar{\varepsilon} = \begin{bmatrix} \delta & 0 & 0 \\ 0 & -\delta & 0 \\ 0 & 0 & \frac{\delta^2}{(1-\delta^2)} \end{bmatrix} \quad (1)$$

The total energy has the following form:

$$E(\delta) = E(-\delta) = E(0) + (C_{11} - C_{12})V_0\delta^2 + O[\delta^4] \quad (2)$$

From the formula of the bulk modulus B , $B = (C_{11} + 2C_{12})/3$ and the value of $C_{11} - C_{12}$ we can determine the constants C_{11} and C_{12} .

To calculate the elastic modulus C_{44} , a monoclinic deformation tensor retained volume is given

by the following matrix:

$$\bar{\varepsilon} = \begin{bmatrix} \frac{\delta}{2} & 0 & 0 \\ 0 & \frac{-\delta}{2} & 0 \\ 0 & 0 & \frac{\delta^2}{(4-\delta^2)} \end{bmatrix} \quad (3)$$

The total energy is then expressed as a function of deformation by:

$$E(\delta) = E(-\delta) = E(0) + \frac{1}{2}C_{44}V_0\delta^2 + O[\delta^4] \quad (4)$$

For crystals of hexagonal symmetry, the tensor of elastic constants is simplified by symmetry. The explanation and the results of these simplifications are given in Ref. [22] and take the following form:

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix} \quad (5)$$

$$C_{66} = \frac{C_{11} - C_{12}}{2} \quad (6)$$

For a hexagonal system, we imposed a deformation to the crystal and studied its response (stress and energy). Several different deformations must be fully applied to calculate the tensor of elastic constants.

2.1. Deformation by expansion (symmetry of the crystal unchanged):

$$X_1 = x_1 (1 + \delta)$$

$$X_2 = x_2 (1 + \delta)$$

$$X_3 = x_3 (1 + \delta)$$

$$E = \frac{9B_V V_0}{2} \delta^2$$

$$\varepsilon = \begin{pmatrix} \delta \\ \delta \\ \delta \\ 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow \sigma = \begin{pmatrix} (C_{11} + C_{12} + C_{13}) \delta \\ (C_{11} + C_{12} + C_{13}) \delta \\ (2C_{13} + C_{33}) \delta \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (7)$$

with

$$B_V = \frac{2C_{11} + 2C_{12} + 4C_{13} + C_{33}}{9} \quad (8)$$

2.2. Deformation by elongation along x-y (symmetry of the crystal unchanged):

$$\begin{aligned} X_1 &= x_1(1 + \delta) \\ X_2 &= x_2(1 + \delta) \\ X_3 &= x_3 \\ E &= V_0(C_{11} + C_{12})\delta^2 \\ \varepsilon &= \begin{pmatrix} \delta \\ \delta \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow \sigma = \begin{pmatrix} (C_{11} + C_{12})\delta \\ (C_{11} + C_{12})\delta \\ 2C_{13}\delta \\ 0 \\ 0 \\ 0 \end{pmatrix} \end{aligned} \quad (9)$$

2.3. Deformation by elongation along z (symmetry of the crystal unchanged):

$$\begin{aligned} X_1 &= x_1 \\ X_2 &= x_2 \\ X_3 &= x_3(1 + \delta) \\ E &= \frac{V_0 C_{33}}{2}\delta^2 \\ \varepsilon &= \begin{pmatrix} 0 \\ 0 \\ \delta \\ 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow \sigma = \begin{pmatrix} C_{13}\delta \\ C_{13}\delta \\ C_{33}\delta \\ 0 \\ 0 \\ 0 \end{pmatrix} \end{aligned} \quad (10)$$

2.4. Deformation by elongation along x (the crystal becomes monoclinic):

$$\begin{aligned} X_1 &= x_1(1 + \delta) \\ X_2 &= x_2 \\ X_3 &= x_3 \\ E &= \frac{V_0 C_{11}}{2}\delta^2 \\ \varepsilon &= \begin{pmatrix} \delta \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow \sigma = \begin{pmatrix} C_{11}\delta \\ C_{12}\delta \\ C_{13}\delta \\ 0 \\ 0 \\ 0 \end{pmatrix} \end{aligned} \quad (11)$$

2.5. Shear deformation (the crystal is triclinic):

$$\begin{aligned} X_1 &= x_1 + \delta x_3 \\ X_2 &= x_2 + \delta x_3 \\ X_3 &= x_3 + \delta(x_1 + x_2) \\ E &= 4V_0 C_{44} \delta^2 \\ \varepsilon &= \begin{pmatrix} 0 \\ 0 \\ 2\delta \\ 2\delta \\ 0 \end{pmatrix} \rightarrow \sigma = \begin{pmatrix} 0 \\ 0 \\ 2C_{44}\delta \\ 2C_{44}\delta \\ 0 \end{pmatrix} \end{aligned} \quad (12)$$

The values of C_{12} and C_{13} have been obtained from the value of $C_{11} + C_{12}$ and the formula of the bulk modulus B , $B = \frac{2C_{11} + 2C_{12} + 4C_{13} + C_{33}}{9}$, respectively. To calculate C_{66} , we have used the formula $C_{66} = \frac{C_{11} - C_{12}}{2}$.

The elastic quantities such as, the shear modulus G , the Young modulus E , and the Poisson's ratio ν , were derived from our calculated elastic constants for both cubic and hexagonal crystals, using the following equations [23–25]:

$$G_{Cubic} = \frac{C_{11} - C_{12} + 3C_{44}}{5} \quad (13)$$

$$G_{Hexagonal} = \frac{M + 12C_{44} + 12C_{66}}{30} \quad (14)$$

where

$$M = C_{11} + C_{12} + 2C_{33} - 4C_{13} \quad (15)$$

$$\nu = \frac{3B - E}{6B} \quad (16)$$

$$E = \frac{9BG}{3B + G} \quad (17)$$

3. Results and discussion

3.1. Structural properties

The structural properties were determined using the Murnaghan equation of states [20]:

$$\begin{aligned} E_{Tot}(V) &= E_0(V) + \\ &+ \frac{B_0 V}{B'(B' - 1)} \left[B \left(1 - \frac{V_0}{V} \right) + \left(\frac{V_0}{V} \right)^{B'} - 1 \right] \end{aligned} \quad (18)$$

where V_0 is the volume of static equilibrium of the mesh, E_0 is the total energy per primitive cell at ground state, B and B' are the bulk modulus and its pressure derivative, respectively.

Optimization of the rock-salt phase is simpler because we can only optimize the lattice parameter and it is performed by calculating the evolution of the total energy in terms of volume. For wurtzite phase, the unit cell contains 4 atoms positioned at (0,0,0) and (2/3,1/3,1/2) for cation atoms (Ti, Al) and (0,0, u) and (2/3,1/3,1/2+ u) for anion atoms (N), where the internal parameter u is the separation of the atom (Ti, Al) and N along the c axis. The structural optimization was performed by calculating the total energy as a function of three variables u , c/a and V .

Fig. 1 shows the variation of the total energy for TiN and AlN compounds in both rock-salt and wurtzite structures. As shown, the most stable phases for TiN and AlN are the rock-salt and the wurtzite phases, respectively. Such calculations are consistent with previous theoretical predictions [26–30]. Our calculations indicate that the phase transition from wurtzite to rock-salt takes place at 10.48 GPa for AlN, compared with 13.3 GPa [26] and 14 GPa [31], whereas from rock-salt to wurtzite, the change transform occurs at -26.34 GPa for TiN, compared with -24.0 GPa [26] and -21 GPa [32], which proves the good stability of TiN in the cubic phase. The equilibrium lattice constants, bulk modulus and its pressure derivative are listed in Table 1 showing our results compared with previously published data. The maximum deviation between the values calculated by us and others is 0.04 % for lattice constants (a) [26, 33], 0.06 % for (c) [26], 20 % for B [34] and 1.8 % for B' [35].

3.2. Elastic properties

Elasticity is a response in form of a slight deformation when a material is exposed to external mechanical stress. The elastic constants of TiN and AlN have been calculated for their most stable phases. Table 2 shows the values of elastic constants for TiN in the rock-salt structure calculated using the Mehl method [20] compared with

experimental and theoretical data. The calculated C_{ij} of rock-salt TiN phase are in good agreement with experimental [36] and theoretical calculations [26, 37–39]. The maximum difference between the calculated and experimental values is 32 % for C_{12} and 24 % for C_{11} [36]. For wurtzite AlN structure, elastic constants have been calculated and compared with experimental [40] and theoretical data [26, 41]. The maximum discrepancy between the calculated values and the experimental ones is 31 % for C_{12} , 16 % for C_{11} and 17 % for C_{44} [40]. Fig. 2 summarizes the evolution of elastic energy as a function of deformation to determine $C_{11} - C_{12}$ and C_{44} for the rock-salt structure of TiN. Fig. 3 shows the direct correlation of the elastic energy as a function of deformation to determine $C_{11} + C_{12}$, C_{11} , C_{33} , and C_{44} for AlN in the wurtzite phase. The transition pressure from rock-salt to wurtzite for TiN is -26.34 GPa (compared to -21.0 GPa from theoretical results of Ref. [26]) whereas from wurtzite to rock-salt for AlN it is 10.48 GPa (compared to 13.3 GPa from theoretical results of Ref. [26]). These results are in good agreement with previous experimental and other theoretical data.

This gives us a good evaluation of the precision and accuracy of the elastic constants of the two binary TiN and AlN. A typical Poisson's ratio value for covalent materials is about 0.1, whereas for ionic materials is about 0.25 [50]. Our Poisson ratio is calculated to be equal to 0.24 in the rock-salt phase of TiN and 0.23 in the hexagonal phase of AlN, which means that these compounds are formed by covalent bonds. According to the Pugh's empirical formula [51], the critical value of the B/G , which separates the ductile and brittle behaviour of materials, is around 1.75; i.e., if $B/G > 1.75$, the material behaves in a ductile manner; otherwise the material behaves in a brittle manner. According to our calculations the values of B/G for TiN and AlN, are 1.62 and 1.6, respectively so we conclude that both materials are fragile.

To sum up, the calculated values of B , G and E for the binary TiN in rock-salt phase are as follows: 301 GPa, 185.4 GPa and 461.45 GPa, and for the binary AlN in the hexagonal phase are 196.73 GPa, 125.31 GPa and 310.09 GPa.

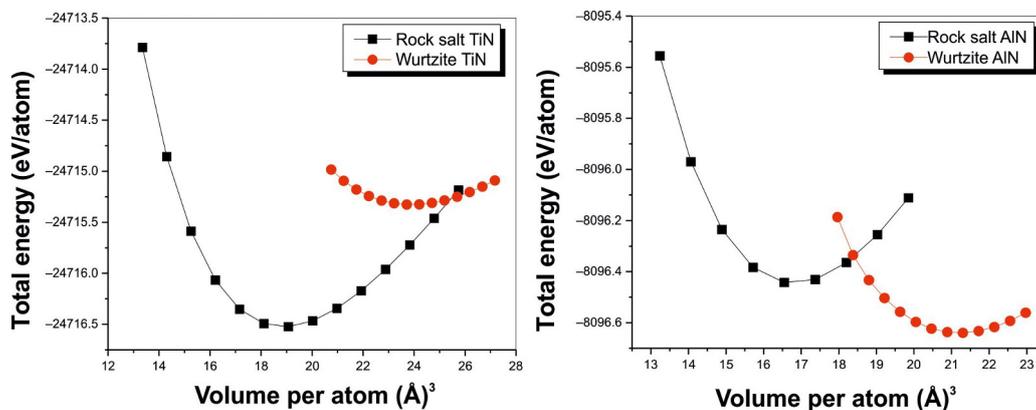


Fig. 1. Total energy optimization points (symbols) and Birch-Murnaghan fittings for TiN and AlN in rock-salt and wurtzite structures.

Table 1. The equilibrium lattice parameters a_0 (Å) and c_0 (Å), the bulk modulus B (GPa) and its pressure derivative B' of TiN and AlN in rock-salt and wurtzite structures using GGA.

	TiN				AlN			
	a_0	c_0	B	B'	a_0	c_0	B	B'
Wurtzite								
Calc.	3.25 ^(a)	5.21 ^(a)	209 ^(a)	4.047 ^(a)	3.1179 ^(a)	5.0414 ^(a)	197 ^(a)	3.90 ^(a)
	3.29 ^(b)	5.27 ^(b)	204 ^(b)	4.31 ^(b)	3.12 ^(b)	5.00 ^(b)	194 ^(b)	3.99 ^(b)
					3.113 ^(f)	5.041 ^(f)	192 ^(f)	3.96 ^(f)
					3.1095 ^(g)	4.9938 ^(g)		
					3.135 ^(h)	5.022 ^(h)		
Exp.	3.29 [19]	5.26 [19]			3.11 [12]	4.978 [12]	185 [14]	5.7 [14]
							207 [15]	
Rock-salt								
Calc.	4.228 ^(a)		301 ^(a)	3.76 ^(a)	4.066 ^(a)		252 ^(a)	3.82 ^(a)
	4.256 ^(b)		294 ^(b)	4.52 ^(b)	4.07 ^(b)		251 ^(b)	4.06 ^(b)
	4.270 ^(c)		292 ^(c)					
	4.26 ^(d)		286 ^(d)					
	4.23 ^(e)		270 ^(e)					
Exp.	4.24 [46]		288 [44]	4.5 [48]	4.06 [49]		221 [31]	4.8 [31]
			318 [33]					

^(a) This work

^(b) GGA, plane-wave pseudopotential, Ref. [26]

^(c) GGA, plane-wave pseudopotential, Ref. [37]

^(d) GGA, FLAPW, Ref. [27]

^(e) GGA, FLMTO, Ref. [42]

^(f) GGA, plane-wave pseudopotential, Ref. [43]

^(g) GGA, plane-wave pseudopotential, Ref. [44]

^(h) GGA, FLMTO, Ref. [45]

Table 2. The calculated elastic constants C_{ij} (GPa) of TiN and AlN in rock-salt and wurtzite structures, respectively using GGA.

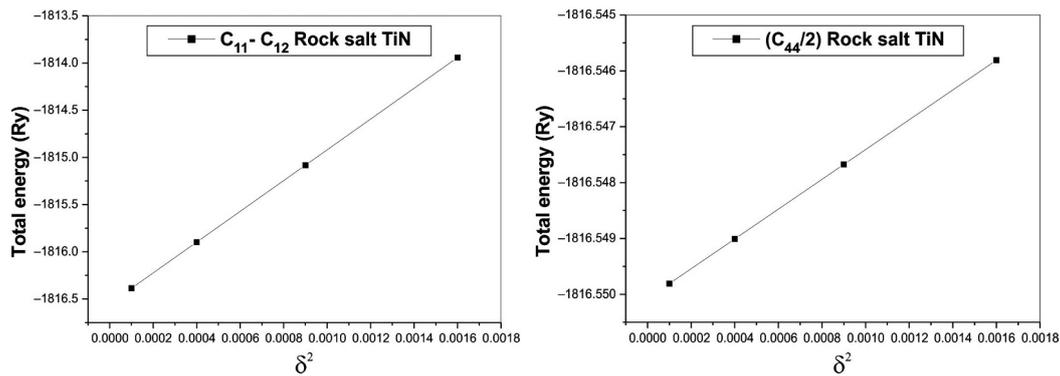
	TiN			AlN		
	Rock-salt			Wurtzite		
	This work	Exp.	Calc.	This work	Exp.	Calc.
C_{11}	601	625 [36]	610 ^(a) 604 ^(b) 610 ^(d)	378	394 [40]	376 ^(a) 376 ^(c)
C_{12}	133	165 [36]	137 ^(a) 136 ^(b) 100 ^(d)	103	134 [40]	127 ^(a) 121 ^(c)
C_{13}				99.4	95 [40]	97 ^(a) 93 ^(c)
C_{33}				412	402 [40]	355 ^(a) 354 ^(c)
C_{44}	153	163 [36]	158 ^(a) 162 ^(b) 168 ^(d)	104	121 [40]	112 ^(a) 115 ^(c)
C_{66}				137.5	130 [40]	124.5 ^(a) 127 ^(c)

^(a) GGA, plane-wave pseudopotential, Ref. [26]

^(b) GGA, VASP plane-wave pseudopotential, Ref. [37]

^(c) GGA, plane-wave pseudopotential, Ref. [41]

^(d) GGA, FPLMTO, Ref. [42]

Fig. 2. Calculated $(C_{11} - C_{12})$ (GPa) and C_{44} (GPa) of TiN in rock-salt structure using GGA.

4. Conclusion

The FP-LAPW with GGA has been applied to evaluate the elastic properties of cubic TiN and hexagonal AlN compounds. We found that the most stable crystalline structures for TiN and AlN

are rock-salt and wurtzite, respectively. The transition pressure from rock-salt to wurtzite for TiN is -26.34 GPa whereas from wurtzite to rock-salt for AlN it is 10.48 GPa. These results are in good agreement with previous experimental and theoretical data. Compared to the literature data, the per-

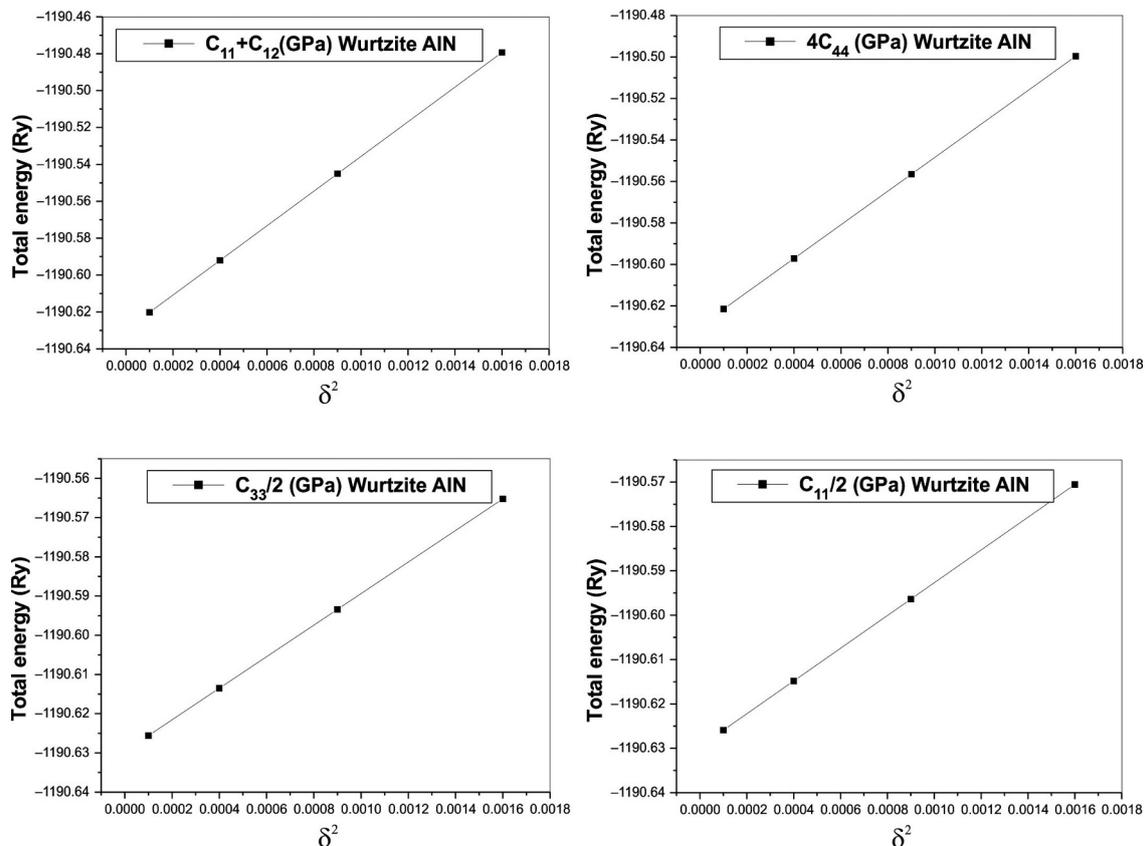


Fig. 3. Calculated ($C_{11} + C_{12}$) (GPa), $4C_{44}$ (GPa), $C_{33}/2$ (GPa) and $C_{11}/2$ of AlN in wurtzite structure using GGA.

centage discrepancy in the values of C_{11} and C_{12} for TiN rock-salt are 24 % and 32 %, respectively. Moreover, C_{12} for AlN phase wurtzite shows a difference of 31 % compared to previous data.

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