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Ab-*initio* Calculations of the Physical Properties in Gallium Nitride at Equilibrium Phases: Rocksalt and Wurtzite

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Mechanical properties,
Electronic structure

Abstract: Ab-initio total energy calculations have been performed utilizing the Density Functional Theory (DFT) inside the generalized gradient approximation (GGA) parameterized by Perdew-Burke-Ernzerhof (PBE). Interactions of the ions and electrons with each other's was characterized via PAW potential within the valance electron configurations Ga-$4s^2 4p^1$ and N-$2p^2 2p^3$ to investigate the physical properties in the rocksalt B1 and wurtzite B4 phases. The equilibrium transition pressure (P_t) from B4 to B1 was estimated at about 33.66 GPa by using the common tangent construction. The DFT calculations indicate that the upper bands of wurtzite B4 between -0.256 eV and the Fermi level were mostly owing to N-p states. The lowest conduction bands were consisted of a mixture of N-s and Ga-s states. The valance band maximum and the conduction band minimum occured at the Γ symmetry point. Concordantly, B4 phase of GaN had a direct band gap at Γ-point, which calculated as 1.702 eV. The highest valance band of rocksalt B1 were consisted of with a major contribution of N-2p states. Although, the indirect band gap of the rocksalt B1 phase has been reported from the valance band maximum at the L-point to the conduction band minimum along the X direction [7], we observed the indirect energy band gap from the valance band maximum at the L-point to the conduction band minimum along the Γ direction. Our calculated value of indirect energy band gap for the rocksalt B1 phase was 0.777 eV and it was lower than the previous calculations.

Galyum Nitrür'ün Kararlı Rocksalt ve Wurtzite Fazlarının Fiziksel Özelliklerinin Ab-*initio* Hesabıyla Belirlenmesi

Anahtar Kelimeler
Yoğunluk fonksiyonel teorisi,
Ab-*initio* Hesabı,
Elastik sertlik katsayıları,
Faz geçiş basıncı,
Mekanik özellikler,
Elektronik Yapı

Özet: Perdew-Burke-Ernzerhof (PBE) tarafından parametrelize edilmiş, genelleştirilmiş eğim yaklaşımı (GGA) dahil olan Yoğunluk Fonksiyonel Teorisi (DFT) kullanılarak, ab-*initio* toplam enerji hesapları yapılmıştır. Rocksalt B1 ve wurtzite B4 fazlarının fiziksel özelliklerini araştırmak için PAW potansiyeli Ga-$4s^2 4p^1$ ve N-$2p^2 2p^3$ valans elektron konfigürasyonu ile iyonlar ve elektronlar arasındaki etkileşimi tanımlamak için kullanılmıştır. Ortak teğet yapımı kullanılarak, B4 yapısından B1 yapısına denge geçiş basıncı (P_t) 33.66 GPa olarak hesaplanmıştır. DFT hesapları wurtzite B4'ün en üst bandlarının -0.256 eV ile Fermi seviyesi arasında çoğunlukla N-p durumlarına bağlı olduğunu ortaya koymaktadır. En düşük iletim bandı N-s ve Ga-s durumlarının bir karışımından oluşmaktadır. Valans bandının maksimumu ve iletim bandının minimumu Γ simetri noktasında meydana gelmektedir. Buna paralel olarak, GaN'ün B4 fazı Γ noktasında 1.702 eV olarak hesaplanan bir dolaysız (direkt) band aralığına sahiptir. Rocksalt B1 fazının en yüksek valans bandı başlıca N-2p durumlarının katkılarından oluşmaktadır. Rocksalt B1 fazının dolaylı (in direkt) band aralığının valans bandının en üst bölgesi L-noktasından iletim bandının en alt bölgesi X yönünde olduğu rapor edilmesine rağmen [7], biz dolaylı (in direkt) band aralığını valans bandının en üst bölgesi L noktasından iletim bandının en alt bölgesi Γ yönünde olduğunun gözlemledik. Rocksalt B1 fazı için bizim hesapladığımız dolaylı (in direkt) band aralığı değeri 0.777 eV'dir ve önceki çalışmalardan daha düşüktür.

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1. Introduction

Gallium Nitride (GaN) is a two-component semiconductor. In recent years, it has become more popular to enormous potential fabrication of various semiconductor for high-power and frequency devices such as short wavelength or blue light emitting diodes (LEDs), laser diodes (LD), optical detectors and ultra violet (UV) photo detectors since GaN provides very high breakdown voltages and electron mobility. Besides, Gallium nitride as RF power amplifiers is also an ideal candidate for high-power and temperature microwave applications. As a conclusion, it is very important that to decide the physical properties of GaN material as accurately as possible which has various superior features.

In recent years, many of the theoretical and experimental studies have been related to GaN semiconductor material. Achour et al. investigated the structural properties of GaN for different crystal structures such as NaCI, CsCI, wurtzite, zincblende, β-tin, Cinnabar and NiAs by using FPLMTO method [1]. Yao et al. studied the mechanisms of the wurtzite-rocksalt phase transformation of GaN semiconductor by DFT based metadynamics method [2]. Also, the thermodynamics properties for B4 and B1 phases of GaN by carrying out the first-principles calculations within the DFT and DFPT were investigated by Zhou et al. [3]. Qian et al. reconstructed the solid solid phase transformations of GaN material from B4 to B1 and from B3 to B1 by applying the nudged elastic band (NEB) [4]. On the other hand, the theoretical study for the structural parameters and phase transformation for Gallium nitride under pressure up to 100 GPa pressure were reported by Saoud et al. [5]. Xiao et al. carried out the pressure-induced B4 and B3 to B1 phase transformation for AlN and GaN by using first-principle total energy calculations [6]. The physical properties of GaN semiconductor as a theoretical study were presented used the first-principles full-potential PAW approach implemented GGA by Arbouche et al. [7]. Researchers focused on the B4 to B1 phase transformation of the group-III nitrides by means of using ab-initio calculation [8]. Moreover, under high pressure phase transitions of GaN-InN by applying the LDA and GGA for exchange-correlation potential were calculated by Said and Bouarissa [9].

They were considered as the B4, B3 and B1 phases of GaN and InN crystal structures. Furthermore, Zapol et al. investigated the properties of the reproduced fourfold coordinated B4 and B3 structures along with the sixfold-coordinated B1 structure by using a set of interatomic pair potentials derived for GaN within the shell model approach [10]. The elastic parameters of GaN were calculated by using Brillouin-scattering by Polian et al. [11]. Structural, energetic, mechanical and electronic properties for the zinc-blende B3 and wurtzite B4 phases of the AlN, GaN and InN semiconductor materials were investigated by Zoroddu et al. using local and gradient-corrected density-functional theory [12]. According to this paper, AlN, GaN and InN crystal structures are nonideal with respect to both the axial ratio and the internal parameter. Deviation from ideality increases from GaN to InN to AlN. The binding energy, lattice constants and internal parameters are considerably well estimated by the GGA in the many materials and approximations [12]. In the light of the previous theoretical studies, generalized gradient approximations (GGA) for the exchange-correlation energy improve upon the local spin density (LSD) description of atoms, molecules and solids. Therefore, we preferred to use the GGA in order to be able to more specifically calculate the electronic features in our work.

To sum up, when previous and recent theoretical and experimental studies are reviewed, it was observed that these studies are focused on the structural parameters of potential phases and mechanisms of the phase transition. However, the studies on thermodynamics, mechanical and electronic properties in the wurtzite B4 and rocksalt B1 phases of GaN materials by using ab-initio methods based on the DFT are quite limited.

Especially, the elastic constants in B1 phase of GaN compound have not been investigated both experimentally and theoretically. In addition, electronic band gap values of B1 rocksalt phase and types (direct or indirect) of the band transitions and directions of them to the symmetry points are still unclear.

Therefore, in this study, ab-*initio* calculations have been performed based on DFT to introduce a complementary work of the physical properties of GaN semiconductor material in the B4 and B1 crystal phases.

2. Material and Method

The first principle calculations were performed within the GGA method [13] according to DFT using VASP code [14-21]. Interactions of the ions and electrons with each other's was characterized by PAW method [22]. The energy convergency criterion of the electronic self-consistency was chosen as 10^{-5} eV/A^{0}. The minimum total energy and ground state geometric properties were determined using the conjugate-gradient algorithm via minimizing stresses on atoms and Hellman-Feynman forces. During all relaxations Brillouin zone integration was accomplished by Gaussian broadening method for 0.1 eV. The Ga and N atom positions were Ga (0.000, 0.000, 0.000) and N (0.500, 0.500, 0.500) in the primitive unit cell for the rocksalt phase. Besides, the positions of Ga and N atoms in the primitive unit cell for the wurtzite B4 phase were Ga (0.333, 0.666, 0.000) and N (0.332, 0.667, 0.375), respectively. Since the plane wave energy cut-off of 500 eV were found to be sufficient and accurate for the rocksalt B1 and wurzite B4 phases, the Kohn-Sham orbitals were expanded. The Brillouin zone integrations were carried out by Monkhorst-Pack special points mesh with a grid size of 10x10x10 and 18x18x10 for the rocksalt and wurtzite phases, respectively [23]. The valence electron configurations are Ga-$4s^2 4p^1$ and N-$2s^2 2p^3$ atoms. In this paper, the number of meshes was increased up to 18x18x18 and 26x26x26 for the final total energy to evaluate the DOS for the rocksalt B1 and wurzite B4 phases of GaN material, respectively. The energy band structures were computed along the special lines associating the high symmetry points, for examples, $W \rightharpoonup L \rightharpoonup \Gamma \rightharpoonup X \rightharpoonup W$ and $\Gamma \rightharpoonup A \rightharpoonup K \rightharpoonup \Gamma \rightharpoonup M \rightharpoonup L \rightharpoonup H$ for the rocksalt B1 and wurtzite B4 phases in the k-space, respectively. The all calculations were implemented at a temperature of 0K without external stress. The total energies of crystal structure of its volume calculated so as to decide the lattice constants and bulk modulus B (GPa) and its pressure derivative $B^{'}$ by means of fitting the data to the Birch-Murnaghan equation of states (EOS). This equation of state are given as [24];

$$E(V) = E_0 + \frac{9}{16} V_0 B_0 \left\{ \begin{array}{c} \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1 \right]^3 . B_0^{'} \\ + \left[\left(\frac{V_0}{V}\right)^{\frac{2}{3}} - 1 \right]^2 \\ * \left[6 - 4 \left(\frac{V_0}{V}\right)^{\frac{2}{3}} \right] \end{array} \right\} \qquad (1)$$

where E_0, V_0, B_0 and $B^{'}$ are defined as the total energy, equilibrium volume, bulk modulus and its pressure derivative at the zero pressure, respectively. These calculated structural parameters are given in Table 1 and Table 2 as well as previous related theoretical and experimental studies. The linear response method used to determine mechanical behavior of GaN material by using the calculated elastic constants. Some flags in the VASP code allowed determining the Hessian matrix and the only zone centered Γ- point vibrational frequencies of a crystal phase. The Hessian matrix can be estimated from the second derivative of the energy by way of the atomic positions used finite differences method. Finally, the elastic tensor was calculated using the six-finite deformation of the crystal lattice, where rigid ions and allowing for relaxation of the ions, and using strain-stress relationship of the elastic constants [25]. The ionic contributions was obtained by multiplying the reverse of Hessian matrix with the internal strain tensor [26]. By this approximation, the final elastic constants was included by compounding the distortions of the rigid ions with the effect of ionic relaxations. The effect of strain on the crystal structure is also important in terms of getting some information of the mechanical behaviours of the materials. The cubic crystals have just three independent elastic constants, called C_{11}, C_{12} and C_{44}, which have been calculated to reveal the mechanical stability of GaN in the B1 structure at zero pressure. Besides, the wurtzite B4 structure has six independent elastic constants, called C_{11}, C_{12}, C_{13}, C_{33}, C_{44} and C_{66}. The equation of state straightforwardly yields the conduct under a isotropic volumetric strain. It can be utilized to decide the bulk modulus of rocksalt B1 phase described as;

$$B = \frac{C_{11} + 2C_{12}}{3} \qquad (2)$$

The bulk modulus B is related to the independent elastic constants for B4 phase by

$$B = \frac{-2C_{13}^2 + C_{33}(C_{11} + C_{12})}{C_{11} + C_{12} + 2C_{33} - 4C_{13}} \qquad (3)$$

Using the values and the bulk modulus are reported in the Table 4.

3. Results

3.1. Structural parameters

Firstly, the lattice constants and bulk modulus B_0 and its pressure derivative $B^{'}$ were calculated by minimizing the total energy for different volumes around the equilibrium volume V_0 by the way of Birch Murhangan's equation of state (EoS) as given in Figure 1.

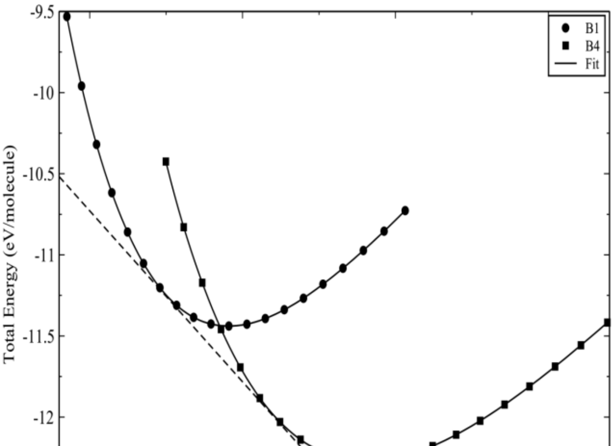

Figure 1. The total energy as a function of per formula unit volume for the rocksalt B1 and wurtzite B4 phases of GaN. Oblique dot line is the common tangent line.

The B4 crystal phase is the most stable phase at zero pressure and temperature conditions by connecting the total energy versus relative volume, which are given in Figure 1. Table 1 lists these EoS parameters and lattice constants. the calculated results compared for the B4 and B1 phases with previous theoretical studies and available experimental values.

Table 1. The calculated lattice parameters of a (A^0), b (A^0) and $c(A^0)$, bulk modulus $B(GPa)$ and its pressure derivative B' in the wurtzite (B4) phase with both other theoretical and experimental studies.

Structure	Methods	a(A⁰)	c(A⁰)	B(GPa)	B'	Ref.
B4 Wurtzite	Our Cal.	3.233	5.280	181.299	4.596	
	Exp.	3.190	5.190	237 ± 31	4.3 ± 2	[27]
		3.180	5.166	204.1	4.5	[28]
		3.192	5.178	210	3.2	[29]
		3.186	5.185	220	4.3	[30]
		3.190	5.19	188	3.2	[31]
	Other Cal.	3.189	5.153	175.794	3.950	[1]
		3.247	5.166			[3]
		3.123	5.088	170.6	4.34	[4]
		3.205	5.220	196.210	4.199	[5]
		3.220	5.242			[6]
		3.221	5.205	176.54	4.37	[7]
		3.145	5.136			[8]
		3.250	5.298	167.07	4.16	[9]
		3.230	5.160			[10]
		3.199	5.226			[12]
		3.190	5.188			[32]
		3.180	5.190	196	4.3	[33]
		3.170	5.135	207	4.5	[34]
		3.245	5.296	172	5.11	[35]
		3.162	5.141	202	3.2	[36]
		3.224	5.296	171.2	4.5	[37]
		3.245	5.250	196	5.11	[38]
		3.200	5.216	169		[39]
		3.150	5.110			[40]
		3.126	5.119	190	2.92	[41]
				251	2.7	[42]
		3.215	5.189	210.6	3.75	[43]
		3.155	5.170			[44]
				196		[45]

Table 2. The calculated lattice parameters of a (A^0), b (A^0) and $c(A^0)$, bulk modulus $B(GPa)$ and its pressure derivative B' in the rocksalt (B1) phase with both other theoretical and experimental studies.

Structure	Methods	a(A⁰)	c(A⁰)	B(GPa)	B'	Ref.
B1 Rocksalt	Our Cal.	4.276	4.276	225.629	4.994	
	Exp.	4.234		248	5.5	[31]
				323 ± 27	3.5 ± 0.8	[46]
		4.234				[47]
	Other Cal.	4.184	4.184	233.313	4.531	[1]
		4.278	4.278			[3]
		4.263	6.028	218.9	4.15	[4]
		4.252	4.252	238.505	4.250	[5]
		4.269				[6]
		4.260	4.260	224.70	3.99	[7]
		2.956	3.413			[8]
		4.310	4.310	202.08	4.36	[9]
		4.225		240	4.50	[33]
		4.263	4.63	211	5.415	[37]
		4.271	4.271	211.6	4.50	[38]
		4.098		223	3.69	[41]
				287	4.3	[42]
		4.268		236	4.23	[43]
		4.100				[44]
				243		[45]
				244		[48]
				269		[49]
				248	3.9	[50]

The equilibrium lattice parameter was computed as a=b=3.23352 A^0 and c=5.28017 A^0 for wurtzite B4 structure. One lattice parameter were compared well with other ab-initio theoretical calculations to a=b=3.250 A^0 and from c=5.110 A^0 to c=5.302 A^0. However, our results for lattice parameters of wurtzite B4 structure showed allowable ratio a deviation of ranging from 3% to 0.5% and from 3% to 0.4%.

Moreover, the bulk modulus and its pressure derivative calculated as 181.299 GPa and 4.596, respectively. Nevertheless our result of bulk modulus of B4 phase showed a deviation of 15% from the other experimental data, it is still comparable with those obtained from the previous calculations. Similarly, EoS parameters of rocksalt B1 structure are comparable to experimental and other calculations are given in Table 2.

The ground state structure of GaN material is the cubic B4 phase for ambient conditions. When focus on the previous studies to understand of the phase transition mechanism, were observed that in order to estimate the transition pressure, they have calculated the enthalpy energy of the possible phases for GaN material. Ueno et al. [27] experimentally have shown that stability of the B4 structure of GaN and InN by x-ray diffraction method and is observed the transition pressure as 52.2 GPa.

Xia et al. [31] researched the high pressure structure of GaN and determined the phase transition at about 37.00 GPa from wurtzite to rocksalt structures. The previous theoretically studies are calculated the phase transformation pressures from B4 to B1 structure as 32.4 GPa [3], 31.00 GPa [6], 37.69 GPa [9] and 33.70 GPa [33].

We tried to determine the equilibrium phase transformation pressure determined from the common tangent construction via numerical accuracy either on the total energy curve fitting. The equilibrium transition pressure (P_t) from B4 to B1 was calculated at about 33.66 GPa by way of the common tangent construction as shown in Table 3.

As shown in Table 3, while our obtained the phase transition pressure value, showing quantitative deviation from the experimental value of 52.2 ± 3.0[27] and theoretical values of 44.80 [2], 45.00 [5] and 40.00 [43], is comparable to that of other DFT within GGA and LDA calculation founded as 32.40 [3], 31.00 [6], and 33.7 [33], respectively.

3.2. Elastic and mechanical properties

Secondly, the elastic constants C_{ij}(GPa) calculated to determine mechanical behavior of GaN material by using the linear response method embedded in vasp code. The elastic constant results C_{ij}(GPa) and bulk modulus B of are presented in Table 4 with previous experimental and theoretical values. While our calculated elastic constants of C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66} and B for ambient condition for wurtzite B4 structure showed a deviation as 10.1%, 6.9%, 9.3%, 10.2%, 1.3%, 28.9% and 9.5% from the experiment [11] respectively, is comparable to previous ab-initio calculation studies [10, 51].

Besides, to our knowledge the elastic constants of C_{11}, C_{12}, C_{44} and B for rocksalt B1 structure has not been reported previously by experimentally and also by ab-initio calculations and in our study they are determined as 343.167, 157.377, 202.232 and 219.307 GPa, respectively.

The satisfy generalized elastic stability criteria for the hexagonal wurtize B4 and cubic rocksalt B1 were given by F. Mouhat and F. X. Couder [52], which indicates that B4 and B1 structures are mechanical stable. They can be written as$C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0, C_{44} > 0$ for B1 structure and $C_{11} > |C_{12}|, C_{33}(C_{11} + C_{12}) > 2(C_{13})^2$, $C_{44} > 0, C_{66} > 0$ for wurtzite B4 structure, respectively.

According to our knowledge, elastic constants of B1 phase of GaN compound have not been investigated previously both theoretically and experimentally. Therefore, the results of current study are first information belonging to B1 rocksalt phase of the compound.

This situation was stated by leaving the experimental and the other theoretical studies of B1 phase of Table 4 blank.

3.3. Electronic properties

Lastly, we presented the energy band structure and the relative total DOS for GaN in the B4 and B1 phases, in the Figure 2a)-b), respectively. The lowest valance band of wurtzite B4 located between -15.711 eV and -12.886 eV was exactly from N-2s electrons. The next four bands showing a very narrow peak of DOS centered roundly at -6.115 eV were referred to Ga-4s states. The next peak localized at about -1.154 eV was from a major contribution of N-2p states. The upper bands between -0.256 eV and the Fermi level were mostly owing to N-p states. The peak of N-p states on the conduction band of B4 structure situated at about 8.103 eV, while the lowest conduction band were consisted of a mixture of N-s and Ga-s states. Furthermore, the highest conduction band was mostly contributed by Ga-p states. Figure 3a)-b) displays the partial DOS (pDOS) which clarifies the contribution of the individual electronic states for the wurtzite B4 phase of the GaN.

The valance band maximum and the conduction band minimum occured at the $\Gamma -$ point. Concordantly, the B4 phase of GaN had a direct band gap at $\Gamma -$ point, which calculated as 1.702 eV, was clearly observed that our band gap result and previous calculations for energy band gap are compared with the theoretical calculation values of 1.88 eV [7] and 1.76 eV [35]. However, our calculated band gap 1.702 eV value were underestimated with comparison with other previous calculations of 2.3 eV [53], 1.9 eV [54], 3.47-3.50 eV [55], and 1.992 eV [56] as shown in Figure 2 a).

Table 3. The phase transition pressure of GaN material for the wurtzite (B4) to rocksalt (B1) structures with both experimental and other theoretical studies.

Phase Transition	Methods	Phase Transition Pressure $P_t(GPa)$	Ref.
$B4 \rightarrow B1$	Our Cal.	33.66	
	Exp.	52.2 ± 3.0	[27]
		37.00	[31]
	Other Cal.	44.80	[2]
		32.40	[3]
		45.00	[5]
		31.00	[6]
		37.69	[9]
		33.70	[33]
		40.00	[43]

Table 4. The calculated elastic constants and bulk modulus by linear respond method in the wurtzite (B4) and rocksalt (B1) phases with both experimental and other theoretical studies.

Structure	Methods	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	B	Ref.
B4 Wurtzite	Our Cal.	350.41	135.03	96.07	357.35	103.63	87.50	190.00	
	Exp.	390 ± 15	145 ± 20	106 ± 20	398 ± 20	105 ± 10	123 ± 10	210	[11]
								237 ± 31	[27]
								204.1	[28]
								210	[29]
								220	[30]
								188	[31]
		296.0	120.0	158.0	267.0	24.0	88.0	192.28	[57]
	Other Cal.							175.794	[1]
		322	115	83		92.43			[2]
								170.6	[4]
								196.210	[5]
								167.07	[9]
		386.3	159.8	141.3	391.2	115.0	113.2	227.57	[10]
				68	354				[12]
								196	[33]
								207	[34]
								172	[35]
								202	[36]
								171.2	[37]
								196	[38]
								190	[41]
								251	[42]
								210.6	[43]
		296	154			206		201.33	[51]
B1 Rocksalt	Our Cal.	343.167	157.377			202.232		219.307	
	Exp.							248	[31]
								323 ± 27	[46]
	Other Cal.							233.313	[1]
								218.9	[4]
								238.505	[5]
								224.70	[7]
								202.08	[9]
								211	[37]
								211.6	[38]
								223	[41]
								287	[42]
								236	[43]
								244	[48]
								269	[49]
								248	[50]

Besides, the lowest valance band of rocksalt B1 placed between -17.34 eV and -12.642 eV. One is mostly due to N-2s electrons. In this region the highest peak showing at -12.6 eV from N-2s states. The highest valance band consists of with a major contribution of N-2p states. While the lowest conduction band region were composed from Ga-s electrons, they were mostly occurred a mixture contribution to highest conduction band from Ga-p and N-p states, as shown in Figure 4a)-b). Although, the indirect band gap in the rocksalt B1 structure of GaN has been reported from the valance band maximum at the L – point to the conduction band minimum along the X direction [7], we observed the indirect energy band gap from the valance band maximum at the L −point to the conduction band minimum along the Γ direction as given in Figure 2b). Our calculated value of indirect energy band gap in the rocksalt B1 structure was 0.777 eV and it was lower than the previous calculations of 1.036 eV [7], 0.94 eV [58], and 1.9 eV [59], respectively. Our results and previous calculations for total energy band gap in the B4 and B1 phases of GaN semiconductor are given in the Table 5.

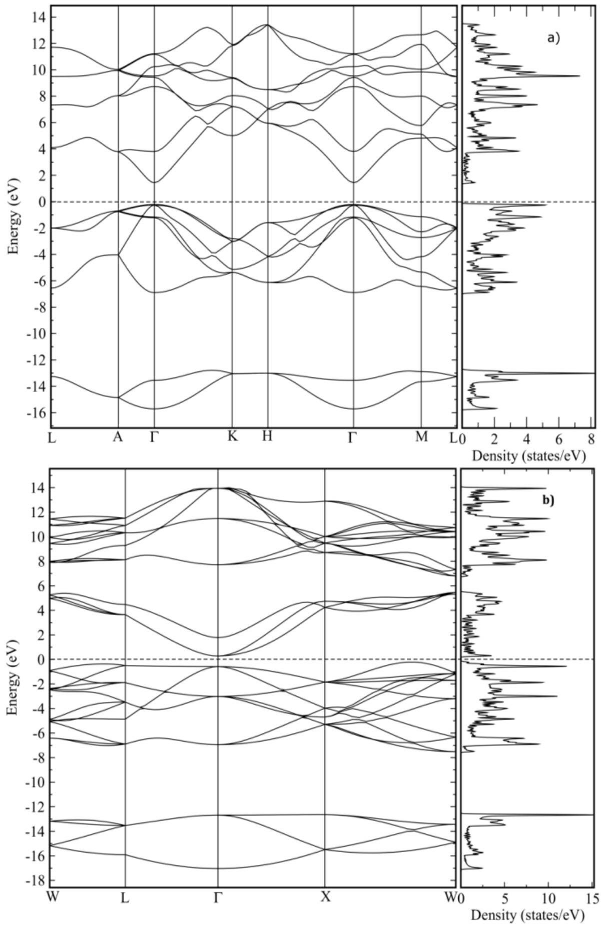

Figure 2. The calculated total energy bands and corresponding total density of state (DOS) in **a)** the wurtzite (B4) and **b)** rocksalt (B1) phases at the zero pressure of GaN. The line on the zero point represents Fermi level.

As has been pointed out by Vurgaftman et al. [55]. It is well known since the early 1970's that the energy band gap in the wurtize B4 phase of GaN semiconductor is about 3.5 eV. Notwithstanding, a precise determination from luminescence experiments is not straightforward, since what is usually measured at cryogenic temperatures are the energies for various pronounced exciton transitions. The classification of these closely spaced resonances is very difficult. For example, at very low temperatures, the lowest-order A,B and C exciton types related to the three valence bands can be resolved, as well as higher-order A(2s, 2p) exciton transitions. All of these material characteristic features contribute to the rather large experimental uncertainty in the bare direct band gap at low temperature [55].

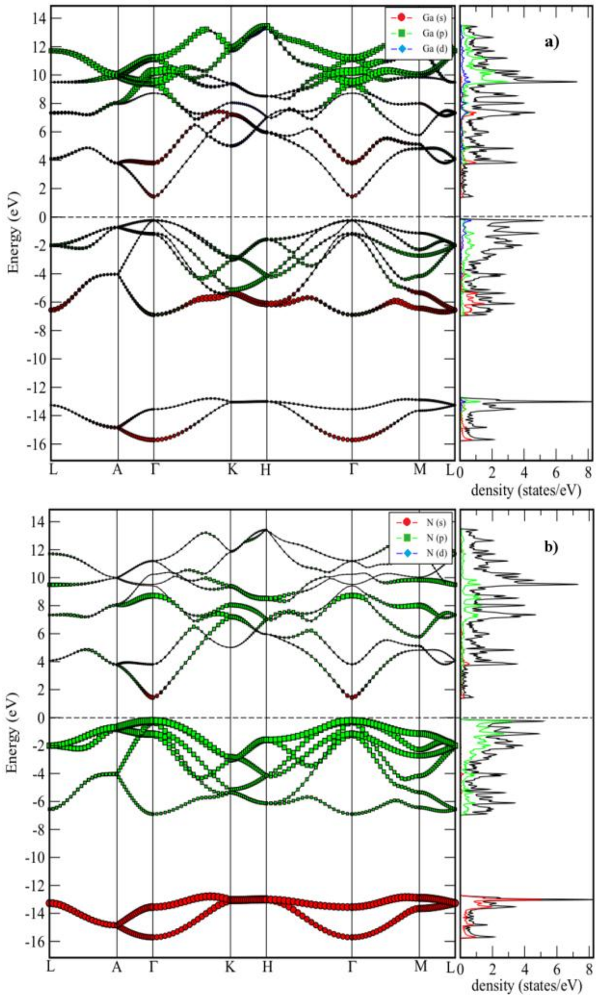

Figure 3. The calculated total energy bands and corresponding total **a)** Ga and **b)** N atoms partial DOS (pDOS) of GaN in the wurtzite (B4) phase. The line on the zero point represents Fermi level.

There are some difficulties in the theoretical calculations, similar to the difficulty of correctly determining the direct or indirect band gaps in experimental studies as noted above. One of the most important of these difficulties is choosing the pseudopotentials for the computational calculations.

Pseudopotentials are used to reduce computation time by replacing the full electron system in the coulombic potential by a system only taking explicitly into account the "valence" electrons (i.e., the electrons participating into bonding) but in a pseudopotential. This approach not only reduces the electron number but also the energy cutoff necessary (this is critical in plane-wave based computations). On the other hand, commonly the PAW potentials are more accurate than the ultra-soft pseudopotentials. The radial cutoffs are smaller than the radii used for the US pseudopotentials, and the PAW potentials reconstruct the exact valence wavefunction with all nodes in the core region [21].

Table 5. The calculated direct and indirect energy band gap $E_g(eV)$ of GaN in the wurtzite B4 and rocksalt B1 structures along different transition, compared with available previous theoretical calculations and experimental studies.

Structure	Methods	Energy band gap $E_g(eV)$	Type of band gap	Ref.
B4 Wurtzite	Our Cal.	1.702	Direct	
	Exp.			
	Other Cal.	1.886	Direct	[7]
		1.76	Direct	[35]
		2.3	Direct	[53]
		1.9	Direct	[54]
		3.47-3.50	Direct	[55]
		1.992	Direct	[56]
B1 Rocksalt	Our Cal.	0.777	Indirect	
	Exp.			
	Other Cal.	1.036	Indirect	[7]
		0.94	Indirect	[58]
		1.9	Indirect	[59]

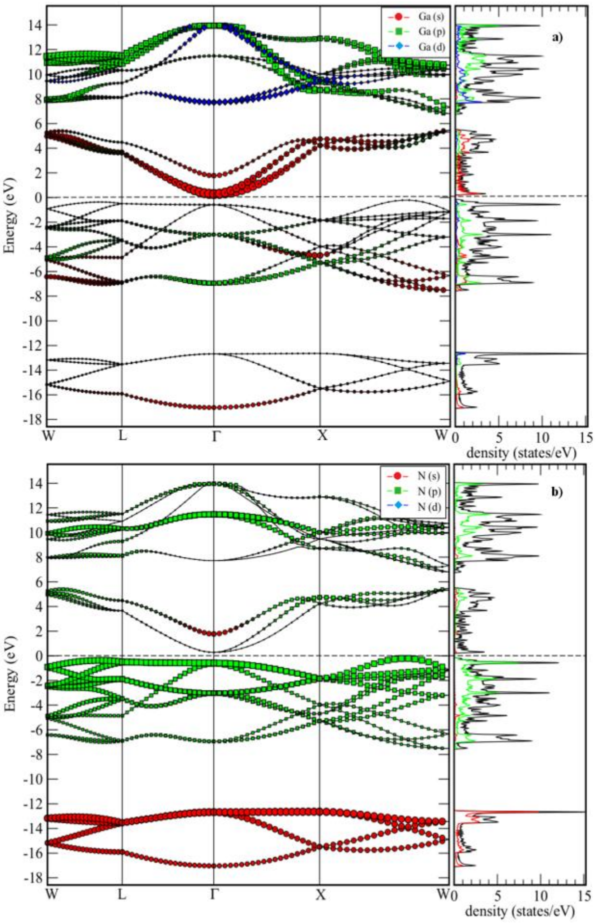

Figure 4. The calculated total energy bands and corresponding total **a)** Ga and **b)** N atoms partial DOS (pDOS) of GaN in the rocksalt (B1) phase. The line on the zero point represents Fermi level.

Our calculated not only direct band gap value for wurtzite B4 phase but also indirect band gap value for rocksalt phase are in good agreement with the earlier ab-*initio* predictions [7, 35, 54] and [58], respectively. However, our calculated indirect band gap direction $(L-\Gamma)$ in rocksalt B1 phase is not in good agreement with previous ab-initio calculations such as based on periodic Hartree-Fock (HF) approximation on the CRYSTAL92 program for GaN by Pandey et al. [42] and computed by the first-principles full-potential augmented plane wave approach FP-LAPW method within the generalized gradient approximation (GGA) by Arbouche et al. [7].

In the light of above information relate to choosing potential, when we compared our calculation with previous first-principle calculation by Arbouche [7] according to choice of potential, we used to PAW method for interactions of the ions-electrons with each other's [21] and the valence electron configurations are Ga-$4s^24p^1$ and N-$2s^22p^3$ atoms in this study. Other calculation performed to FP-LAPW method within the valence electron configurations are [Ar] $3d^{10}$ $4s^2$ $4p^1$ for Ga and [He] $2s^2$ $2p^3$ for N atoms by used Arbouche et al. We think that the reason our calculated the indirect band gap direction to be different from the calculated by Arbouche in the rocksalt B1 phase, because the potential selection and the contributions from the valence electrons are different.

4. Discussion and Conclusion

We carried out the ab-*initio* total energy calculations in the B4 and B1 structures of Gallium nitride based on DFT in the approach of the GGA in an effort to investigate the structural, mechanical and electronic properties of GaN material. We obtained the structural parameters such as lattice constants, bulk modulus and its pressure derivative were comparable with the available experiment and other theoretical studies. Additionally, when previous and recent theoretical and experimental studies were reviewed, it was observed that usually these studies focused on the structural parameters of potential phases, mechanisms of the phase transition and electronic properties for B1 and B4 phases. To our knowledge, no elastic constants calculation of B1 phase has been observed experimentally or theoretically in GaN so far. Therefore, to our knowledge the elastic constants in the rocksalt B1 phase of GaN were computed for the first time in our study. We calculated the equilibrium phase transition pressure using the common tangent construction via numerical accuracy either on the total energy curve fitting. The equilibrium transition pressure ($\boldsymbol{P_t}$) was predicted as 33.66 GPa from wurtize to rocksalt phase. The fact remains that while the indirect band gap in the rocksalt B1 structure of GaN was reported from the valance band maximum at the $\boldsymbol{L}-$point to the conduction band minimum along the $\boldsymbol{X}$ direction [7], We observed the indirect energy band gap from the valance band maximum at the $\boldsymbol{L}-$point to the conduction band minimum along the $\boldsymbol{\Gamma}$ direction for B1 phase.

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