Density Functional Investigation for Electronic Properties of Zinc Blende GaN and AlN

S.K. ARORA[1*], D.S. AHLAWAT[1], D. SINGH[2]

[1]Department of Physics, Chaudhary Devi lal University, Sirsa, India
[2]Department of Physics, M.M. University, Mullana, India
***Corresponding Author E-Mail:** sndp.arora@rediffmail.com

Received: 26.03.2018 *Accepted: 23.04.2018* *Published Online 15.06.2018*
https://doi.org/10.30731/ijcps.7.3.2018.43-50

Abstract

All electron full potential density functional calculations are performed to study the band structure and electronic properties of zinc blende GaN and AlN. Results obtained using the local density approximation (LDA) and the generalized gradient approximation (GGA) have been compared. Electronic properties like lattice parameter, bulk modulus and it's derivative, band energy, band gap, DOS, Fermi energy etc. are reported. In addition modified Becke-Johnson exchange potential have been used to improve the band gap. The calculated results have been compared with earlier reported results which are found to be in good agreement.

Keywords: Electronic band structure, density of states, LDA, DOS.

Introduction

The wide band gap semiconductors have attracted increasing interest for research in recent years. These materials have great potential for high temperature, electronic and optical applications due to high melting point, high thermal conductivity and a large bulk modulus. Due to large band gap these materials can be used for short wavelength light-emitting diodes (LED's), laser diodes and optical detectors. There are a number of II-VI and III-V compound semiconductors having wide band gaps. Owing to large formation energy for defects, much attention is paid to III-V nitrides as the properties of electronic devices based on high band gap II-VI semiconductors tend to degrade with time. The III-V nitrides crystallize in wurtzite structure under ambient conditions which shows a phase transition to six fold rock salt phase at high pressure. This is due to the transfer of hexagonal symmetry by sapphire substrate on which nitride films have been grown. However, the cubic GaN films have also been grown successfully on substrate like GaAs (001) where cubic phase was stabilized by the symmetry of the substrate [1]. The bulk zinc-blende GaN grown on GaAs(001) has been reported first by Mizuta et al.[2]. Among group-III nitrides GaN and AlN being the promising candidates for short wavelength light emitting diodes (LED's), laser diodes and optical detectors that are the core materials for investigation in the present calculations.

To provide a basis for understanding the materials and device properties , theoretical studies can be most valuable. A growing number of first principle calculations based on density functional theory employing the local density approximation (LDA) either in all electron formalism[3,4] or using the

pseudopotential plane wave approach has been performed. This is well known fact from reported work that the LDA underestimate the band gaps in semiconductors [5,6].

In density functional theory calculations the use of the generalized gradient approximation (GGA) for exchange correlation functional is nowadays receiving wide attention as a possible improvement over the LDA. In the present work, we perform the all electron full potential density functional calculations for ZB GaN and ZB AlN employing both the local density approximation (LDA) and generalized gradient approximation (GGA) for exchange correlation functional. On the basis of these considerations, this paper reports the structural and electronic properties of zinc blende type GaN and AlN wide band gap semiconducting materials.

Computational Method

The present calculations have been performed using FP-LAPW method in the frame work of the density functional theory (DFT), as implemented in WIEN2k code [7]. The exchange correlation potential within the GGA is calculated using the scheme of Perdew et al.[8]. Moreover, the mBJ potential has been applied in order to improve accuracy for the band gaps. In these calculations the unit cell was divided in two regions. The spherical harmonic expansion have been used inside the non overlapping spheres of muffin tin radii (R_{mt}) and the plane wave basis set for interstitial region of the unit cell. For total energy convergence, the basis functions were expanded using R_{mt} K_{max}=6.0, where R_{mt} is the smallest muffin tin radius. The values of sphere radii, the nearest neighboring distance and number of plane waves used in our calculations are listed in the table1.

Table 1: Number of plane waves (PW), nearest neighboring distance (NN),and muffin tin radius (R_{mt}) used for both zinc-blende GaN and AlN.

	PW	NN(au)	R_{mt}(au)	
	LDA		Ga	N
ZB GaN	132	3.65	1.95	1.68
			Al	N
ZB AlN	125	3.56	1.81	1.72
	GGA		Ga	N
ZB GaN	132	3.72	1.99	1.71
			Al	N
ZB AlN	125	3.61	1.84	1.75

Results and Discussion

Structural Properties

For obtaining the band structure, we first optimize the lattice parameters by fitting the total energies at different volumes to the Murnaghan equation of state[9]. The curves representing the variation in total energy as a function of volume have been shown in the figures 1-4.

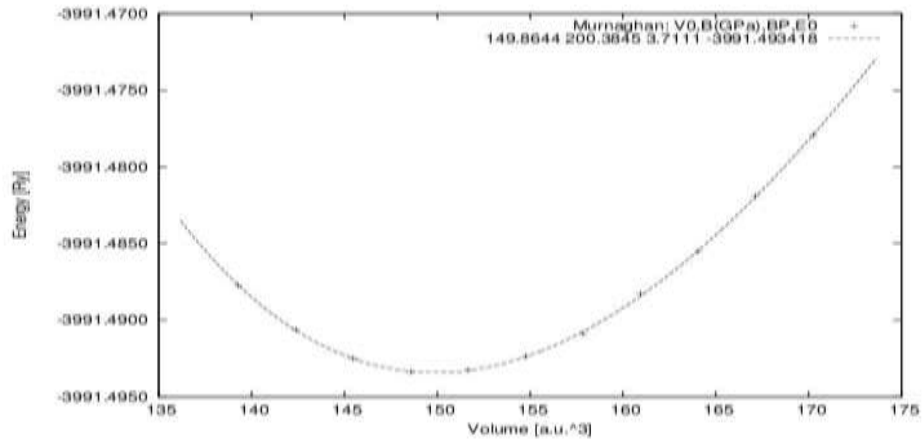

Fig. 1: Total energy vs volume for ZB GaN using LDA

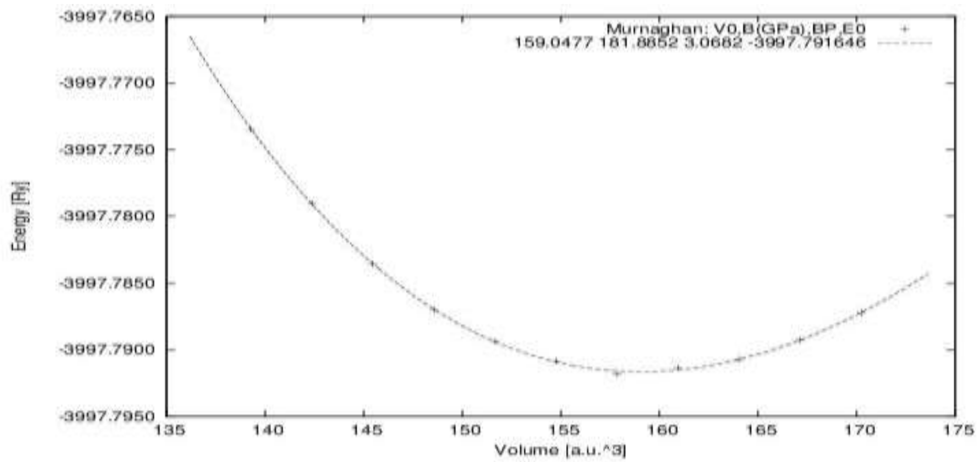

Fig. 2: Total energy vs volume for ZB GaN using GGA

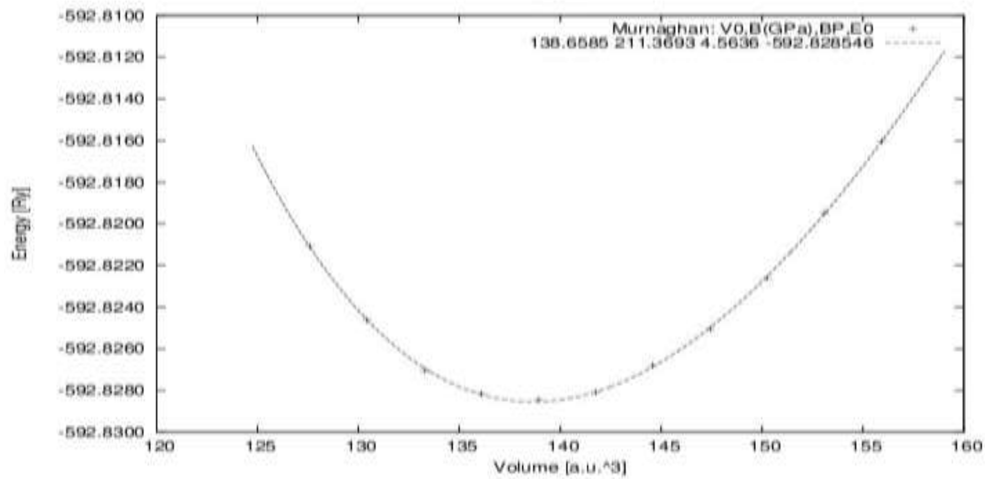

Fig. 3: Total energy vs volume for ZB AlN using LDA

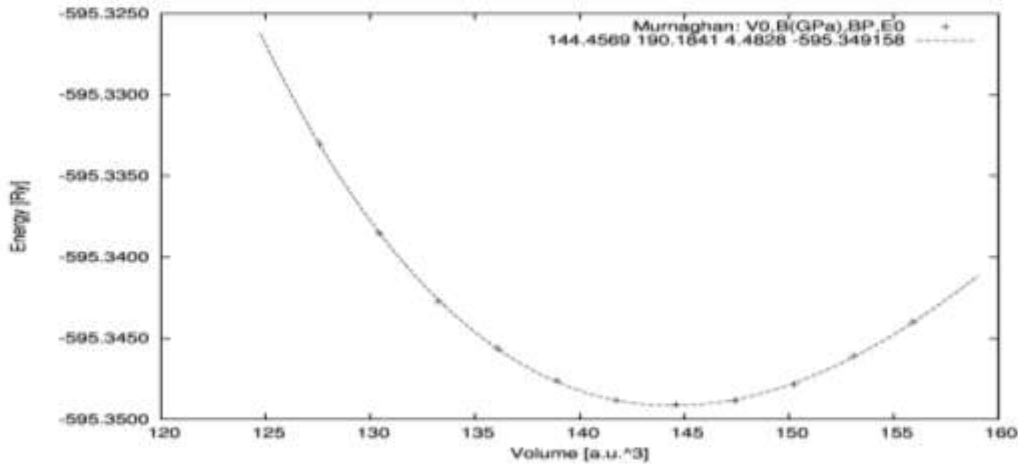

Fig. 4: Total energy vs volume for ZB AlN using GGA

The calculated equilibrium lattice parameters, bulk modulus and it's pressure derivatives are given in tables 2 and 3 for GaN and AlN respectively. We find that lattice constant in the GGA is larger by 2% for ZB GaN and by 1.4% for ZBAlN as compared to LDA results. Further the LDA yields a slightly lesser value of lattice constant than experimentally reported by 0.8% for GaN and 0.3% for AlN, while the GGA yields 1.14% larger values for GaN and 1.1% in case of AlN.

Table 2: Lattice constant a, bulk modulus B and it's derivative (B') and band gap (Eg^{Γ})of zinc blende GaN

LDA calculations					
	a(Å)	**B(GPa)**	**B'**	**Eg^{Γ}(eV)**	**Eg^{Γ}(eV)(mBj)**
Present calculations	4.4619	200	3.71	1.91	3.189
Ref. 10	4.464	192.5	3.94		
Ref. 11	4.489				
Ref.12	4.46	187		1.89	
Ref. 13					3.13
GGA Calculations					
Present calculations	4.5512	181	3.068	1.53	2.815
Ref.14	4.590	156	4.25	1.28	
Ref.15	4.570				
Ref. 13					2.74
Expt.(Ref. 16,17,18,19)	4.50,4.531	190		3.45,3.21	

Table 3: Lattice constant (a), bulk modulus (B) and its derivative (B') and band gap (Eg) of zinc blende AlN.

LDA calculations					
	a(Å)	**B(GPa)**	**B'**	**Eg (eV)**	**Eg (eV)(mBJ)**
Present calculations	4.3478	211.4	4.56	3.25	5.024
Ref. 20	4.339	204	4.06	4.50	
Ref. 14	4.310	206	3.86	4.75	
Ref. 12	4.342	207		4.35	
GGA Calculations					
Present calculations	4.4076	190.18	4.48	3.34	4.97
Ref. 14	4.394	191	3.81	4.13	
Ref. 15	4.40				1.
Expt.(Ref. 17,10)	4.37,4.36	197			

Electronic Properties

Using the optimized structural parameters, the electronic properties including band structure, total density of states and atomic site projected density of states were calculated for both AlN and GaN using mBj-LDA and mBj-GGA approximations. The band structures of GaN and AlN as calculated using LDA and GGA are shown in figures 5-8.The energy bands in electron dispersion curves along the high symmetry directions of the brillouin zone have been drawn relative to the Fermi level (shown by dotted line).The comparison of band structure calculated with LDA and with mBJ LDA potential shows that this potential displaced the conduction bands towards higher energies with respect to the valence bands, thereby increasing the energy band gap and bring closer to its experimental values. In case of GaN the band gap is obtained about 0.38 eV smaller for GGA as compared to the LDA while it is 0.09 eV greater for AlN. Although the band structures obtained using GGA are found almost similar to that from LDA.

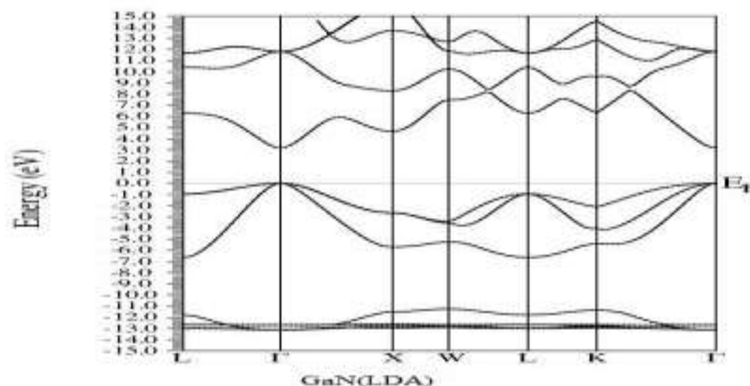

Fig. 5: Band structure for ZB GaN using LDA-mBj.

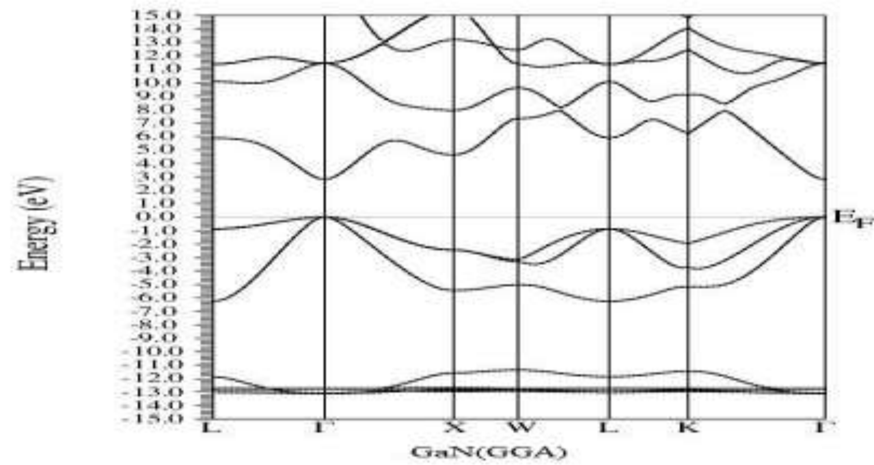

Fig. 6: Band structure for ZB GaN using GGA-mBj.

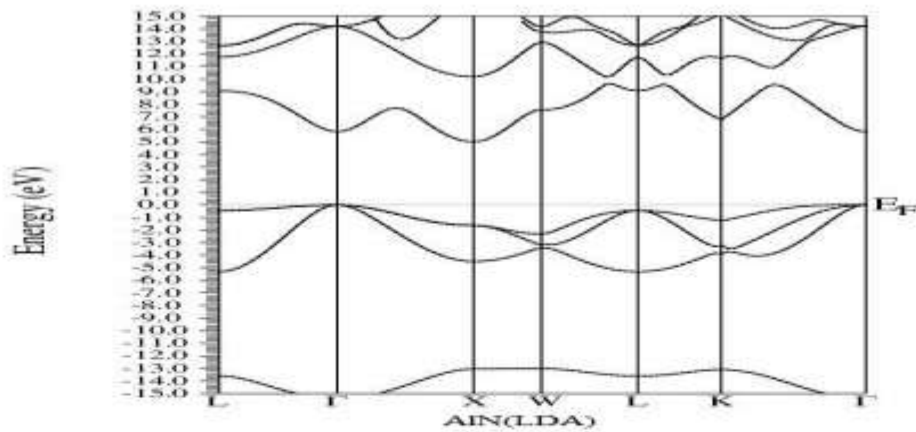

Fig. 7: Band structure for ZB AlN using LDA.

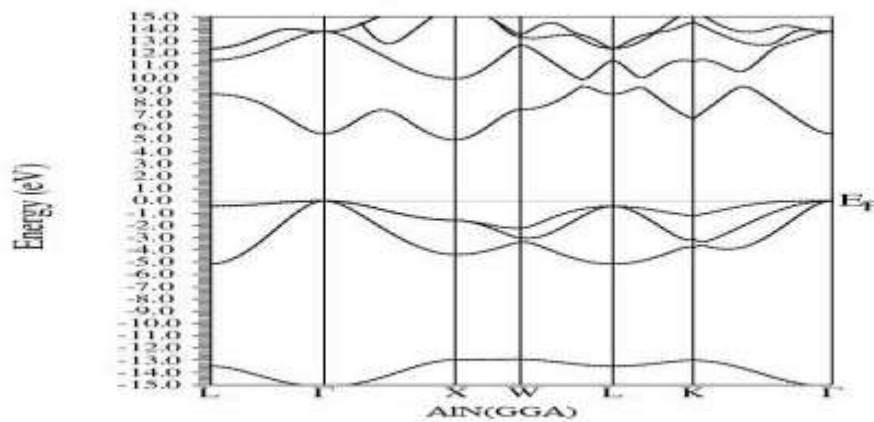

Fig. 8: Band structure for ZB AlN using GGA.

Further the density of states (DOS) for ZB GaN using LDA is shown in the figures 9 (a), (b), (c). The DOS in the lower energy region are mainly derived from Ga-3d orbital while those in the higher energy region mainly consist of N-p and Ga-s orbitals.

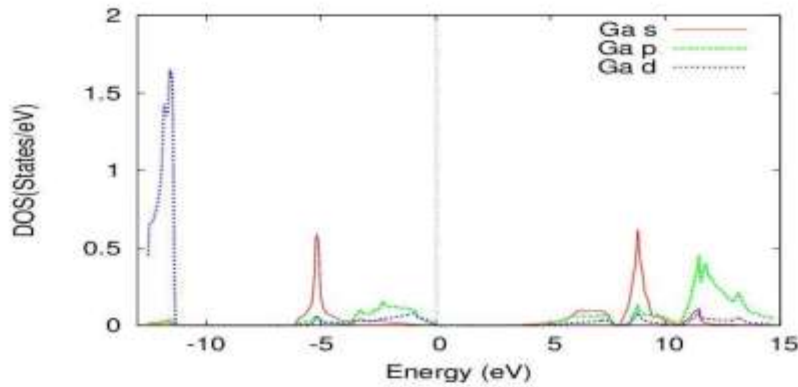

Fig. 9(a)

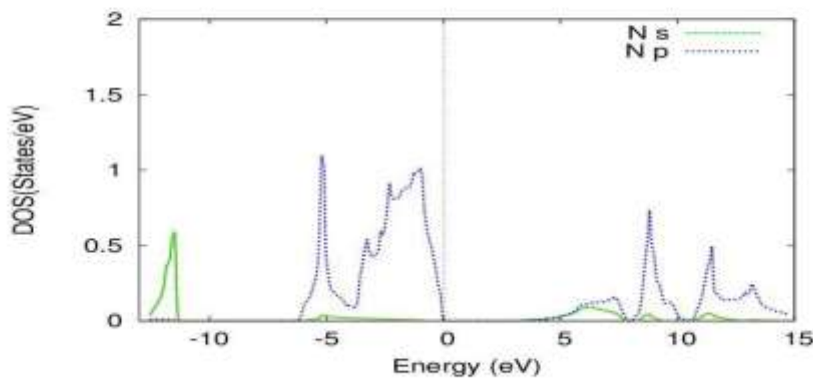

Fig. 9(b)

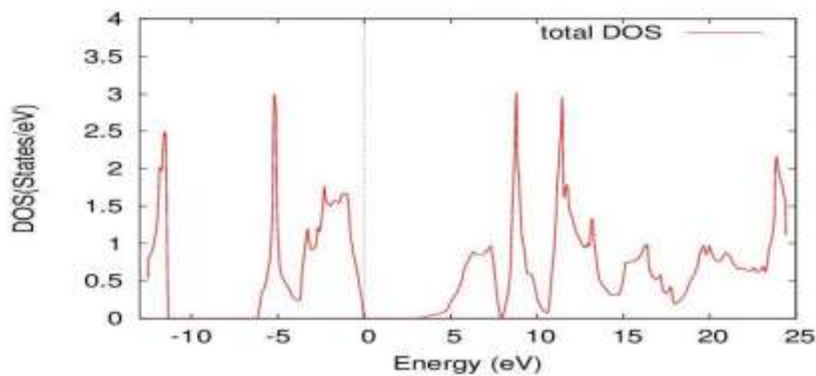

Fig. 9(c)

Fig. 9: DOS for ZB GaN using GGA-mBj.

Conclusions

We have successfully investigated the various properties like lattice constant, bulk modulus and it's pressure derivative, energy band gap, Fermi energy for GaN and AlN in zinc blende crystal phase using the all electron FP-LAPW method employing the LDA and GGA for exchange correlation functional. The comparison of GGA results with those for LDA are performed for both of these wide band gap semiconducting materials. The calculated lattice constants, bulk modulus and band gaps are found to be in good agreement with other calculations. The energy band gap calculated with modified Becke Johnson potential have been found to be larger as compared to already reported values using LDA and GGA approximations and are found to be much closer to their experimental values. The density of states for ZB type GaN by using LDA+mBJ have also been derived in the lower and higher energy region from Ga-3d orbital and Ga-s with N-p orbital respectively.

References

[1] D. P. Xu, Y. T. Wang, H. Yang, S. F. Li, D. G. Zhao, Y. Fu, S. M. Zhang, and R. H. Wu, *J.Appl. Phys.* 88, 2000, 6.
[2] M. Mizuta, S. Fujieda, Y. Matsumoto and T. Kawamara, Jpn. *J. Appl. Phys.*, 25,1986,L945 .
[3] P.K. Saini, D. S. Ahlawat and D. Singh, *J. Metallurgy and Mat. Sc.* 59, 2017, 29-37.
[4] P.K.Saini, D. Singh, D.S. Ahlawat, *Indian J. of Pure and Appl. Physics* 55, 2017, 649-654.
[5] J. P. Perdew and M. Levy, *Phys. Rev. Lett.* 51, 1983, 1884.
[6] L. J. Sham and M.Schluter, *Phys. Rev. Lett.* 51, 1983, 1888.
[7] P. Blaha and K. Schwarz, WIEN2k, *Vienna University of technology Austria* (2009).
[8] J. P. Perdew, S. Burke and M. Ernzerhof, *Phys. Rev. Lett.* 77, 1996, 3865.
[9] F. D. Murnaghan, Proc. *Natl. Acad. Sci. USA* 30, 1944, 5390.
[10] F Saad Saud, J.C. Plenet, L. Louail, D. Maouche, *Computational and Theortical Chemistry* 96 4 , 2011, 65-71.
[11] M.A. Caro, S. Schulz and E.P.O'Reilly *Phys. Rev. B* 86, 2012, 014117.
[12] A.F.Wright and J. S. Nelson, *Phy. Rev. B* 51, 1995, 7866.
[13] J.A. Camrago-Martinez and R. Baquero, *Phys. Rev. B* 86, 2012, 195106.
[14] C. Stampfl and C. G. Van de Walle, *Phy. Rev. B* 59, 1999,5521.
[15] M. Van Schilfgaarde, A. Sher and A. B. Chen., *J. Cryst. Growth* 178, 1997, 8.
[16] K. Kim, W.R. Lambrecht and B.Segall, *Phys. Rev. B* 53, 1996 16 310.
[17] *Properties of Group-III Nitrides*, edited by J. H. Edgar, EMIS Datareviews Series *IEE, London,* 1994.
[18] Vurgaftman, Meyer and Ram Mohan, *J. Appl. Phys.* 89, 2001, 11.
[19] Handbook of Nitride Semiconductors and Devices (*WILEY-VCH Verlag Gmbh & Co KGa, Weinheim ISBN:978-3-527-40837-5*), 2008.
[20] A.Satta, V. Fiorentini, A. Bosin and F. Meloni, in *Gallium Nitride and Related Materials*, edited by R. D. Dupuis et. al., *MRS Symposia Proceedings No. 395 (Material Research Society, Pittsburg, 1996)*, p. 515.