Band Structure of BN, AlN and GaN

[1]* K. Benkabou
[1]Laboratory of Applied Materials, University of Sidi Bel Abbès ALGERIA.

Abstract

Optoelectronic properties of the BN, AlN and GaN are studied using tight binding method. The band structure and band gap are calculated using sp3 s* tight binding formalism. Ionicity and refractive index are also reported.

Keywords: Boron semiconductors, nitride semiconductors electronic properties, optical properties

1. Introduction

Niitrides has diversified the properties of semiconductor materials, enabling the production of commercially important light emitting devices covering many regions of the visible spectrum [1-3].

Ongoing efforts to expand the range of available materials for III–V semiconductor applications include advancing epitaxial growth techniques and engineering energy band gaps. A potential candidate for band-gap modification in the nitrides is boron [4–5] in particular, the nitride binary compounds GaN and AlN alloyed with boron are potential materials for optoelectronic devices [6,7]. Another way of increasing the flexibility of nitride alloy compounds could be achieved using boron. Boron nitride films are very useful for many applications due to their unique properties such as high thermal conductivity, hardness, excellent chemical stability and optical transparency over a wide spectral range[8-10].

In this paper we are interested by BN, AlN, GaN compounds. Our study is a theoretical investigation of the band structure, ionicity and refractive index of these compounds in zinc blende phase. The paper is organized as follows: An overview of theoretical approach is presented in Section 2, results and their discussion are presented in Section 3. Finally, a conclusion is given in Section 4.

2. Computational method

In this work, the calculations of electronic properties are based on the empirical tight binding method (ETBM) introduced by Vogl et al. and which was used to calculate the band structure of several semi-conductors compounds and alloys [11]. The concept of this method is to calculate the electronic band structure with as small as 13 parameters. These parameters are taken to

*Corresponding author: Benkabou khadidjà Address: Laboratory of Applied Materials, University of Sidi Bel Abbès ALGERIA. E-mail address: kbenkabou@yahoo.fr, Phone: +21348546162 Fax: +21348540038

reproduce the energies at several high symmetry points. The size of the Hamiltonian matrix is 10×10. Each row contains five orbital per atom and two atoms for an fcc structure.

The refractive index and energy gap of semiconductors represent two fundamentals physical aspects that characterize their optical and electronic properties. The applications of semiconductors as electronic, optical and optoelectronic devices are very much determined by the nature and magnitude of these two elementary material properties.

3. Results and discussions

The principle goal of this paper is the study of band structure of BN, AlN and GaN compounds. The energy gap is an important parameter in device conception since it determines the threshold for absorption of photons in semiconductors. The tight binding parameters of binary compounds BN, AlN and GaN used to calculate the band structure are taken from reference [12]. The energies obtained by using these parameters for BN, AIN and GaN are listed in Table (1) for the high symmetry points Γ and X in the Brillouin zone. All energies are with reference to the top of the valence band.

Table 1: Energies gaps of BN, AlN and GaN compounds at high symmetry points.

	This work			experimental - other works		
compound	BN	AlN	GaN	BN	AlN	GaN
$E_{\Gamma\Gamma}$ (eV)	11.40	5.99	3.1	11.4 [10]	6.0 [14]	3.1 [14]
$E_{\Gamma X}$ (eV)	6.34	4.90	4.70	6.4 [13]	5.1[14]	4.7 [14]

The band structures of BN, AIN and GaN are shown in Figures (1-3) respectively. The results show that GaN is a direct-gap semiconductor with the minimum of the conduction band at Γ point. BN and AIN have an indirect gap with the minimum of conduction band at X point. The calculated energy gaps of GaN, BN and AIN are 3.10, 6.34 and 5.99 eV, respectively, which are reasonably in good agreement with experimental and theoretical results as listed in Table (1).

Another feature observed from the energy spectra is the Heteropolar gap between the first and the second valence electron bands at X point, this gap is related to the difference between the cation and anion potentials. The Heteropolar gap has been proposed as a measure of crystal ionicity [15,16].

The Heteropolar gap has been calculated from the band structure data, it is equal to 4.7603, 6.976521, and 6.098664 eV for BN, GaN and AlN, respectively, suggesting, therefore, that GaN is more ionic than AIN and BN. The model of ionicity in reference [16] is described by:

*Corresponding author: Benkabou khadidjà Address: Laboratory of Applied Materials, University of Sidi Bel Abbès ALGERIA. E-mail address: kbenkabou@yahoo.fr, Phone: +21348546162 Fax: +21348540038

$$f_i = \left[\left(\frac{E_h}{(E_h - 1}\right)^{-1} - 0.75\right] - \left[\left(\frac{1}{E_h}\right) - 0.66\right] \qquad (3)$$

Here, E_h is the Heteropolar gap.

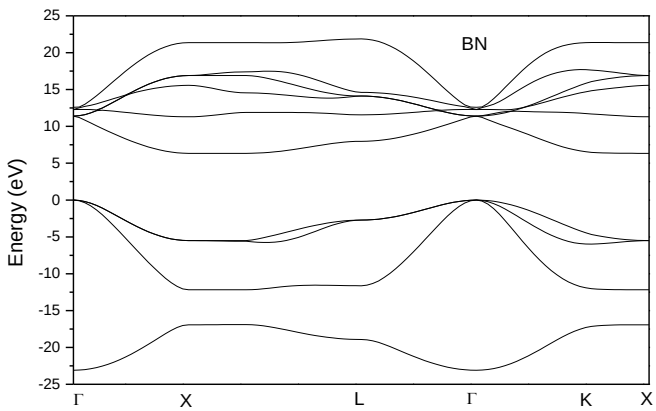

Figure 1: Band structure of BN

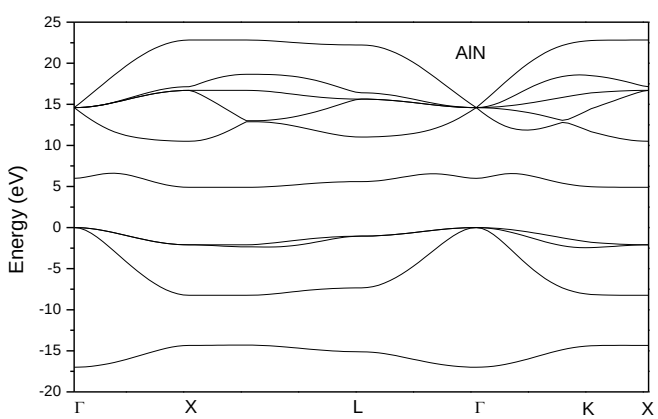

Figure 2 : Band structure of AlN

*Corresponding author: Benkabou khadidjà Address: Laboratory of Applied Materials, University of Sidi Bel Abbès ALGERIA. E-mail address: kbenkabou@yahoo.fr, Phone: +21348546162 Fax: +21348540038

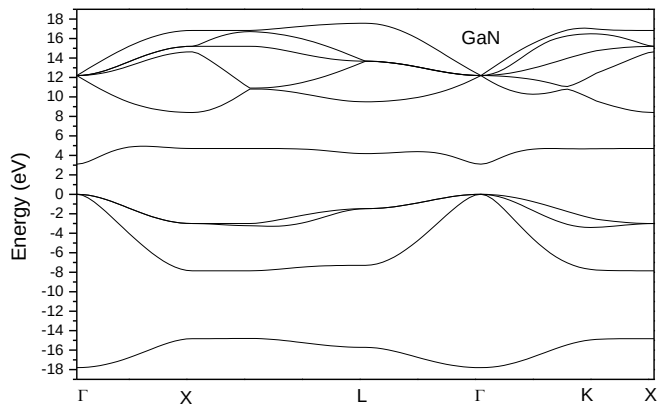

Figure 3 : Band structure of GaN

Using this model, we have calculated the ionicity of binary compounds BN, GaN, AlN. The calculated ionicity values of BN, GaN and AlN compared with those of Phillips [17] and Garcia and Cohen [18], are given in Table (3). The results in Table (3) show that our calculated ionicity exhibit the same chemical trends as those found by Phillips and Garcia and Cohen : ionic character should increase when going from BN to GaN through AIN. However, our calculated values agree more with Garcia values than with Phillips values for BN compound while the calculated values of ionicity for GaN and AlN are situated between those of Garcia and Phillips.

Table 2 : The ionicity values of BN, AlN and GaN compounds.

Compounds	BN	AlN	GaN
f_i present work	0.489	0.582	0.623
f_i Phillips [17]	0.256	0.449	0.500
f_i Garcia [18]	0.475	0.754	0.778

The band-gaps obtained from the computed electronic band structures are further used to obtain refractive index. The refractive index in the semiconductor is a fundamental property since it is a measure of its transparency to incident spectral radiation. A correlation between energy gap and refractive index has been the subjects of many works [19].The refractive index of the binary compounds is calculated using the Moss's formula [20] which relates the wavelength independent refractive index to the band-gap by the relation:

$$n^4 = \frac{95}{E_{\Gamma\Gamma}} \qquad (4)$$

the refractive index of BN, AlN and GaN compounds are found respectively 1.96, 1.99, 2.35 eV.

*Corresponding author: Benkabou khadidjà Address: Laboratory of Applied Materials, University of Sidi Bel Abbès ALGERIA. E-mail address: kbenkabou@yahoo.fr, Phone: +21348546162 Fax: +21348540038

Conclusion

We have presented a theoretical analysis of the electronic properties O boron nitride binary compounds BN, AlN and GaN using tight binding sp3s* method. We have found From the band structure calculations that GaN is a direct gap semiconductor while BN and AlN are indirect band gap semi-conductors which is in good agreement with experimental and ab-initio results. The Heteropolar gaps and refractive index of these compounds have been also investigated

References

[1] J.W. Orton, C.T. Foxon, Rep. Prog. Phys. 61 (1998) 1.
[2] F.A. Ponce, D.P. Bour, Nature (London) 386 (1998) 1.
[3] S.C. Jain, M. Willander, J. Narayan, R. Van Overstraeten, J. Appl. Phys. 87 (2000) 965.
[4] Y. Al-Douri, B. Merabet, H. Abid, R. Khenata, Superlattices and Microstructures 51 (2012) 404.
[5] B. Ghebouli, M.A. Ghebouli, M. Fatmi, S.I. Ahmed, Computational Materials Science 48 (2010) 94.
[6] J.F. Geisz, D.J. Friedman, J.M. Olson, S.R. Kurtz, R.C. Reedy, A.B. Swartzlander, B.M. Keyes, A.G. Norman, Appl. Phys. Lett. 76 (2000) 1443.
[7] J.F. Geisz, D.J. Friedman, S.R. Kurtz, J.M. Olson, A.B. Swartzlander, R.C. Reedy, A.G. Norman, J. Cryst. Growth 225 (2001) 372.
[8] R.M. Wentzcovitch, M.L. Cohen, P.K. Lam, Phys. Rev. B 36 (1987) 6058.
[9] O.A. Golikova, Phys. Status Solidi a 51 (1997) 11.
[10] M.P. Surh, S.G. Louie, M.L. Cohen, Phys. Rev. B 43 (1991) 9126.
[11] P. Vogl, H.P. Hjalmarson, J.D. Dow, J. Phys. Chem. Solids 44 (1983) 365.
[12] H. Aourag, M. Certier, J. Phys. Chem. Solids, 59 (1998) 1145.
[13] V. A. Fomichev and M. A. Rumsh, J. Chem. Phys. 48 (1968) 555; J. Phys. Chem. Solids 29 (1968) 1015.
[14] W.J. Fan, M.F. Li, T.C. Chong, X.B. Xia, J. Appl. Phys. 79 (1996) 188.
[15] J. R. Chelikowsky, T. J. Wagener, J. H. Weaver, A. Jin, Phys. Rev. B40 (1989) 9644.
[16] Y. Al-Douri, H. Abid, A. Zaoui, H. Aourag, Physica B 301 (2001) 295.
[17] J. C. Phillips, Rev. Mod. Phys. **42** (1970) 317.
[18] C A. Garcia, M.L. Cohen, Phys. Rev. B 47 (1993) 4215.
[19] N.M. Ravindra , Preethi Ganapathy, Jinsoo Choi, Infrared Physics & Technology 50 (2007) 21.
[20] T.S. Moss, Phys. Stat. Sol. (B) 131 (1985) 415.

*Corresponding author: Benkabou khadidjà Address: Laboratory of Applied Materials, University of Sidi Bel Abbès ALGERIA. E-mail address: kbenkabou@yahoo.fr, Phone: +21348546162 Fax: +21348540038