InxGa1−xN refractive index calculations

Article *in* Microelectronics Journal · February 2007

DOI: 10.1016/j.mejo.2006.11.001

CITATIONS
49

READS
9,247

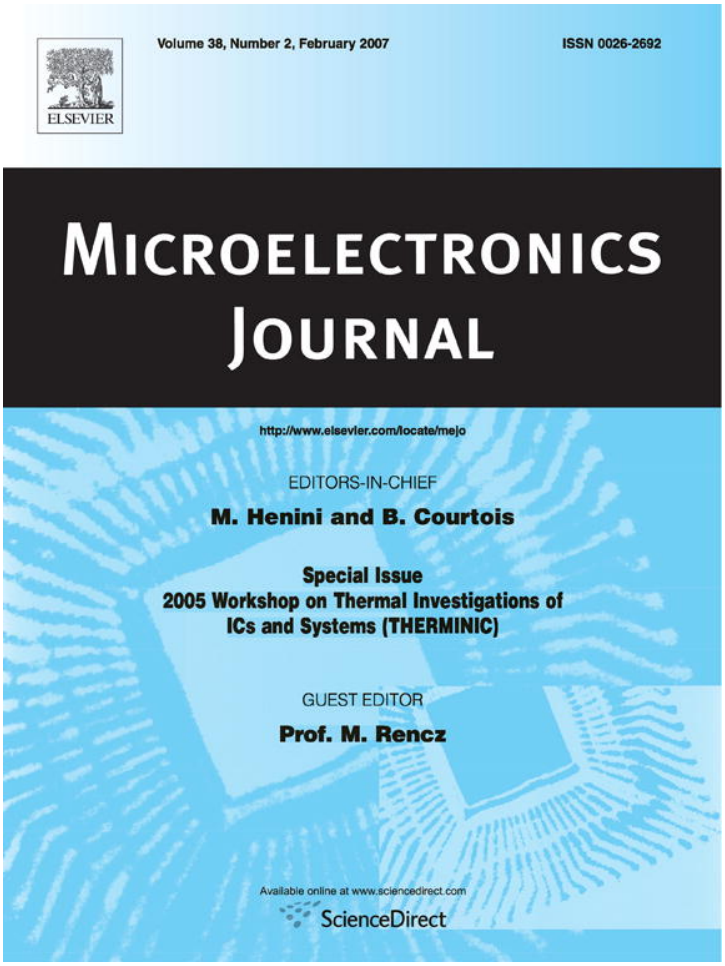
6 authors, including:

Macho Anani
University of Sidi-Bel-Abbes
58 PUBLICATIONS **289** CITATIONS
SEE PROFILE

Abid Hamza
University of Sidi-Bel-Abbes
147 PUBLICATIONS **1,541** CITATIONS
SEE PROFILE

Chama Zouaoui
University of Sidi-Bel-Abbes
41 PUBLICATIONS **245** CITATIONS
SEE PROFILE

Christian Mathieu
Université d'Artois
80 PUBLICATIONS **1,696** CITATIONS
SEE PROFILE



ELSEVIER

Microelectronics Journal 38 (2007) 262–266

Microelectronics Journal

www.elsevier.com/locate/mejo

$In_xGa_{1-x}N$ refractive index calculations

M. Anani[a,b,*], H. Abid[a], Z. Chama[b], C. Mathieu[b], A. Sayede[b], B. Khelifa[b]

[a]*Laboratoire de Modélisation des Composants et de Conception des Circuits, Département d'électronique, Faculté des Sciences de l'Ingénieur, Université Djillali Liabes de Sidi Bel Abbès, BP 89, 22000 Sidi Bel Abbès, Algeria*

[b]*Centre de calcul et de modélisation de Lens, Faculté Jean Perrin, Université d'Artois, 62300 Lens, France*

Received 5 September 2006; accepted 10 November 2006
Available online 10 January 2007

Abstract

The growth of $In_xGa_{1-x}N$ Wurtzite structure is a well established fact. It permits to design optoelectronic devices such as laser diodes or LEDs, from the near ultraviolet to the infrared light spectrum. This sweeps indeed, the whole of the visible spectrum and, hence, appears to be very useful to the recent development of liquid crystal display screens, or designing photodiodes and perhaps solar cells (after studying their energetical efficiencies). Nevertheless, refractive indices of $In_xGa_{1-x}N$ structure have not been studied.

The refractive index of such structures is increasing from the GaN refractive index to the InN one, with therefore, a bowing of the curve due to the lattice mismatch between these two constituting binary alloys.

The index is, in a certain range of the "$n(x)$" characteristic, less than the GaN one. This seems to be particularly interesting in the integrated optics domain or optical waveguides realization, because the growth of GaN is easier than the growth of $In_xGa_{1-x}N$.

Keywords: III-N semiconductors; Bowing; Refractive index

1. Introduction

There has been, recently, a considerable interest in column III elements (like B, Al, Ga and In) combined to form a Nitride semiconductor materials with "N" as the V column element, and this for their so suitable optoelectronic properties. This evolution is due to the very good optoelectronic properties of the GaN, AlN and the InN.

The main characteristic is that in the Wurtzite (Hexagonal) configuration, these semiconductors have direct bandgaps, and this fact permits to multiply their optical properties, such as radiations and direct transitions, compared to the other III–V semiconductors. Excepting Boron Nitride (BN), the III-N semiconductors have large direct bandgaps energies going from 0.8 eV for the InN passing by 3.5 eV for the GaN to 6.3 eV for the AlN. They look to have wide direct bandgaps throughout the alloy composition range, strong atomic bonding and very large energies of formation. They are, thus potentially useful to make light-emitting diodes, injection lasers, high power and high temperature devices [1–3]. These energies correspond to emission wavelengths of infrared 1.55 μm to ultraviolet 0.197 μm. This range of the light spectrum makes them well suitable for short visible wavelengths area to the UV optoelectronic, largely greater than the conventional III–V semiconductors covered field. Higashiwaka et al. [4] succeeded in growing a single-crystal InN film with high crystalline quality on a sapphire substrate by plasma-assisted molecular beam epitaxy (PAMBE). Also, high quality MBE $In_xGa_{1-x}N$ and $In_xAl_{1-x}N$ films were grown on sapphire substrates with GaN or AlN buffers [5]. Both –n and –p types layers can be crystallized and the commercial blue diode based on InGaN/GaN is available [6].

2. $In_xGa_{1-x}N$ bandgap calculations

Defaults are resulting in a formation of stacking faults and dislocations in the growing crystal. This creates what is called a mismatch. Basal plane sapphire (0 0 0 1) is largely

*Corresponding author. Laboratoire de Modélisation des Composants et de Conception des Circuits, Département d'électronique, Faculté des Sciences de l'Ingénieur, Université Djillali Liabes de Sidi Bel Abbès, BP 89, 22000 Sidi Bel Abbès, Algeria. Tel.: +213 72 45 78 03; fax: +213 48 56 05 94.
E-mail address: anani66@yahoo.fr (M. Anani).

0026-2692/$ - see front matter © 2006 Elsevier Ltd. All rights reserved.
doi:10.1016/j.mejo.2006.11.001

used due to its natural high purity, availability and great success with GaN heteroepitaxy. GaN is commonly grown on sapphire (Al_2O_3), although its so high 16% mismatch to GaN, and the fact that lattice mismatch of even 10^{-3}% are sufficient to generate misfit dislocations, which degrade the luminescence efficiency of the material [7]. This so large lattice mismatch disturbs the first few layers of GaN grown on sapphire. Therefore, SiC substrates are too expensive despite of their so little 3% mismatch on GaN [1]. The mismatch can be overcome by using AlN or GaN thin buffer layers and there are many useful GaN devices made by these methods [1,2]. At ambient conditions, the thermodynamically stable structure is Wurtzite for bulk AlN, GaN and InN [8].

The value of InN lies primarily in its ability to form a ternary alloy with GaN, where the composition of such an alloy determines its bandgap and lattice parameters [9]. InN, also, appears to be an important nitride compound for optoelectronic device applications, since it can be used as a low resistivity layer for ohmic contact formation to other nitride compounds with wider bandgap, or as active layer in red or orange laser diodes (LEDs) [10].

Increasing the "x" composition factor in $In_xGa_{1-x}N$ makes difficult to control the active layers due to the potential of phase separation [11]. Indium incorporation is strongly dependent upon the growth rate, temperature, pressure, carrier gas and V/III ratio. O'Donnell [12] have grown epilayers of InGaN using the metallorganic vapor phase epitaxy (MOVPE) at relatively low temperature (less than 800 °C), in order to maximize the incorporation of Indium.

Evaluating the gap of an $A_xB_{1-x}C$ alloy, and opposing to the lattice constant tendency, which is a pondered mean, the energetic gaps are considerably dependent on the average of their constituting gaps:

$$\overline{\mathrm{E}}\mathrm{g}(x) = xE_{\mathrm{AC}} + (1-x)E_{\mathrm{BC}}. \tag{1}$$

Several experimental measures of the Eg(x) energy gap can be interpolated in the below quadratic form:

$$\mathrm{Eg}(x) = \overline{\mathrm{E}}\mathrm{g}(x) + bx(1-x), \tag{2}$$

where "b" is the optical bowing parameter.

Eqs. (1) and (2) show that Eg(x) reach an extreme at the concentration:

$$x_{\mathrm{m}} = \frac{1}{2}\left(1 + \frac{\Delta E}{b}\right), \tag{3}$$

where $\Delta E = E_{\mathrm{BC}} - E_{\mathrm{AC}}$ corresponding to an energetic value of

$$\mathrm{Eg}(x_{\mathrm{m}}) = \frac{E_{\mathrm{AC}} + E_{\mathrm{BC}}}{2} - \frac{\Delta E^2}{4b} - \frac{b}{4}. \tag{4}$$

By experiment, there is a fact that the gap almost bows below the straight-line average ($b>0$) in pseudo-binary alloys, and our structure does not derogate to this law.

The bowing is due to the virtual crystal average of the pseudopotential and can be either positive or negative but very small, and also from fluctuations about the virtual crystal average which occurs in $A_xB_{1-x}C$ alloy and is always expected to be positive at least in wide-gap alloys, because the fluctuating potential couples different eigenstates of the virtual crystal band structures [2].

Thus, the bowing seems to be large in $In_xGa_{1-x}N$ alloy and some workers found a very large bowing, but they note that it depends strongly with the bond relaxation assumption taken. Using the basal hexagonal (Wurtzite) structure for our compound, Van Schilfgaarde et al. [2] have approximated the gap x-dependence with a parabola, and then, the bowing parameter was defined as

$$\mathrm{Eg}_{\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}} = \mathrm{Eg}_{\mathrm{GaN}} - x(\mathrm{Eg}_{\mathrm{GaN}} - \mathrm{Eg}_{\mathrm{InN}}) - bx(1-x). \tag{5}$$

Table 1 contains the bowing parameters encountered in the literature.

In polycrystalline configuration the $In_xGa_{1-x}N$ gap is evaluated relatively to the following formula [19]:

$$\mathrm{Eg}_{\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}} = x\mathrm{Eg}_{\mathrm{InN}} + (1-x)\mathrm{Eg}_{\mathrm{GaN}} - bx(1-x). \tag{6}$$

Bechstedt et al. [20] thought that the bowing is not constant but itself composition-dependent. They found that $b(x) = (1-x)(11.4–19.4x)$ eV, and thus the bowing depends greatly on the considered value of "x".

The InN gap was earlier evaluated to be equal to 1.89 eV [21,22], in the polycrystalline structure and the theoretical approach, but a mean value of 1.90 eV for the Wurtzite structure was frequently encountered. Therefore, the recent experiments show that the InN bandgap varies from 0.75 to 0.9 eV. This has been confirmed by transmission PL and PLE studies [20]. For Perrsson et al. [23] it is about 1.03 eV and for Grossner et al. [24] close to 0.8 eV, Yu Davydov et al. [15] a value of 0.79 eV and Bechstedt et al. [20] have found a value of 0.81 eV. This latter is the mean value of this bandgap and was taken in the calculations. The mean value of the GaN Wurtzite bandgap is 3.50 eV [2], according to the majority of the recent works.

Examining Fig. 1, taken from Ref. [20], the mean value of the bowing obtained by polynomial interpolation is

Table 1
Bandgap bowing parameters "b" in eV, by several authors

Structure	$Al_xGa_{1-x}N$	$In_xAl_{1-x}N$	$In_xGa_{1-x}N$
Wurtzite [13]	0.34	3.6	1.7
Wurtzite, present work			2.17
Wurtzite [12]			5.9
Wurtzite [14]			4.64
Wurtzite [15]			−3.06
Zinc-blende [13]	0.62	3.5	1.3
Zinc-blende [16]	−0.40		
Zinc-blende [2]			2.6
Zinc-blende [17]	0.98		
Experiment [18]	−0.6 ± 0.2		1.0

equal to 2.17 eV, and this allows us to plot the bandgap x-related. The results are shown in Fig. 2.

According to the above mentioned formula (5), we have calculated the x-gap dependence of our compound and make a comparison in Fig. 2. These characteristics are not linear and we can see that the bowing increases from the experimental structure to our structure. The Wurtzite crystal, which is the most thermodynamically stable form, has a so relative average bowing.

The experimental bowing, equal to 1.0 eV allows us to make a comparison. The obtained characteristic has a hyperbola quadratic form, and decreases gradually and not linearly. The bandgap is always underestimated, close to Strite and Morkoc [13] model and averaged to the Bechstedt et al. one. This occurs because the obtained bowing is greater than the experimental one, and thus the curve must be much concave and much incurved in the whole of the range. The slope of the characteristic is constant according to the experiment when the Bechstedt et al. one presents a zero in the mid-range and is different in the first half than the second half of the curve. There was an interruption and this is due to the fact that the measures were not taken on the same sample, because $In_xGa_{1-x}N$ is difficult to grow in the second half of the stoichiometric range.

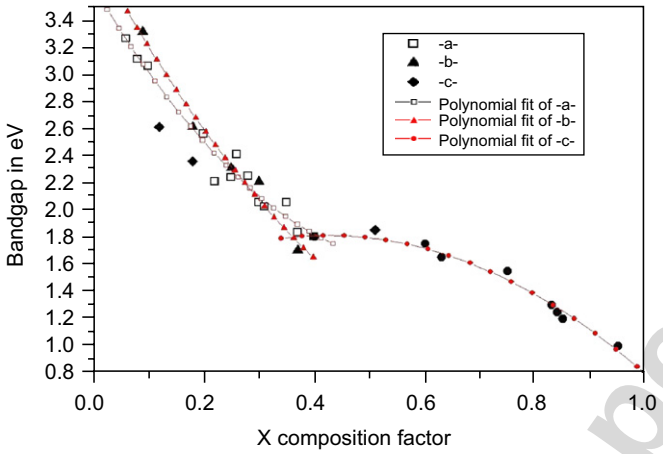


Fig. 1. $In_xGa_{1-x}N$ structure bandgap variations related to the molar fraction "x". (a), (b) Donnell [12] and (c) Kim et al. [14].

3. $In_xGa_{1-x}N$ refractive index

The importance of the refractive index is due to its direct reverse proportional relation with the gap of a material, and has a hyperbola profile. The refractive index expresses also, the ratio between the light celerity in vacuum and its celerity in the considered material.

The wavelength is also reversely proportional to the bandgap of a material in the relation $Eg = 1.24/\lambda$, which is straight. Thus the relation between the refractive index and the wavelength must be directly proportional, and have the parabolic form. By interpolation one can deduce the relation $n(\lambda)$, by taking some semiconductors known refractive indices and their corresponding wavelengths. The results are confined in Fig. 3.

Morkoç et al. [21] have given several values for the GaN refractive index, affirming that Ejder has measured the refractive index of GaN using transmission and absorption measurements. This gives 2.67 for 3.38 eV and 2.33 for 1.0 eV. Let us note that there is a good agreement concerning the 2.15 average value of the AlN refractive index [4].

Consulting Table 2, InN has a mean refractive index of 2.953 at 1.55 μm wavelength, while the $n(\lambda)$ relation gives a value of 3.01. This same relation gives also a value of 2.36

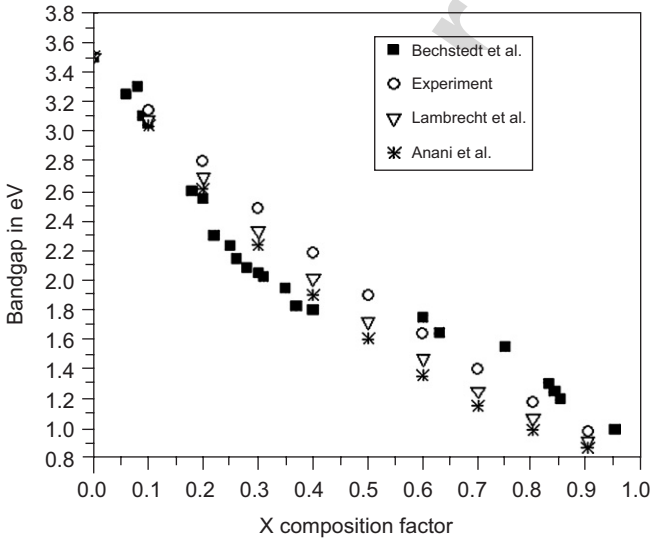


Fig. 2. Bandgap variations versus the "x" composition factor of $In_xGa_{1-x}N$ Wurtzite structure.

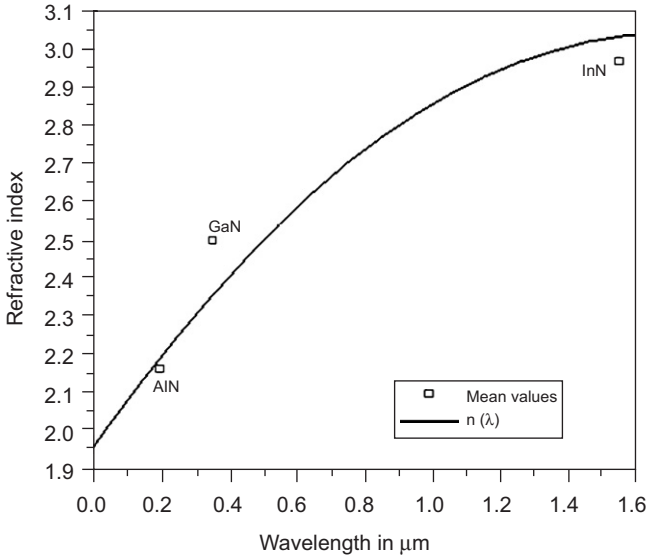


Fig. 3. Refractive index versus wavelength in the III-Nitrides group.

Table 2
Refractive index of InN

Refractive index	Wavelength (nm)	Ref.	Comment
2.88 ± 0.15	Long limit	[25]	Theoretical
2.90 ± 0.3	600–800	[26]	—
2.90	900–1200	[27]	Transmission interference
3.05 ± 0.03	—	[28]	—
2.65	620	[29]	Normal incidence reflectance of synchrotron radiation
2.93	820	[30]	$n > 10^{20}\,\mathrm{cm}^{-3}$
2.676	1503	[20]	
2.85	1771	[13]	

for GaN and 2.16 for AlN, despite their 2.484 and 2.15 mean values refractive index, respectively.

Many rules and empirical relations have been developed or found to make the more accurate approximations and to model as well physical mechanisms in the fundamental goal to design semiconductor-alloys-based optoelectronic devices such as lasers and LEDs. By this way, it has been developed models to approach the real values of refractive index versus bandgap of such compounds.

These assumptions allow us to calculate the refractive index of $In_xGa_{1-x}N$ structures. The refractive index of $In_xGa_{1-x}N$ obeys to the same law which governs the bandgap evolutions, which is the relation (5) in our case. This led to

$$n_{In_xGa_{1-x}N} = n_{InN}x + (1-x)n_{GaN} - bx(1-x). \quad (8)$$

Fig. 4 shows the evolution of the refractive index related to the $In_xGa_{1-x}N$ molar fraction x.

The characteristics concerning $In_xAl_{1-x}N$ and $Ga_xAl_{1-x}N$ were plotted using the bowing values of Table 1. The considered structures are in the Wurtzite (hexagonal) configuration and the functions are quadratic. The $In_xGa_{1-x}N$ curve reaches a minimum at $x = 0.41$, and is decreasing in the $x = [0, 0.41]$ interval and then increases quickly to reach the InN refractive index value. The big value of the bowing parameter is responsible of this form, because it introduces the quadratic term of the relation. The refractive index in this range is less than the refractive index of the GaN. This can be particularly useful in designing optical waveguides where there is a condition of light guiding and confinement in the optical structure. This condition says that the refractive index of the guiding material must be greater than the substrate supporting this guide, and thus, because it is easier to grow GaN than $In_xGa_{1-x}N$ one has just to grow the GaN layer on the $In_xGa_{1-x}N$ one, in this range. This form of the characteristic is due to the lattice mismatch between the growths of InN in the GaN structure. This mismatch disturbs the first few layers of $In_xGa_{1-x}N$, where x is not so important, and alters then the natural increasing tendency of the structure bandgap. But when the structure begins to become really more InN than GaN the natural increasing tendency of the refractive index is the dominant phenomenon.

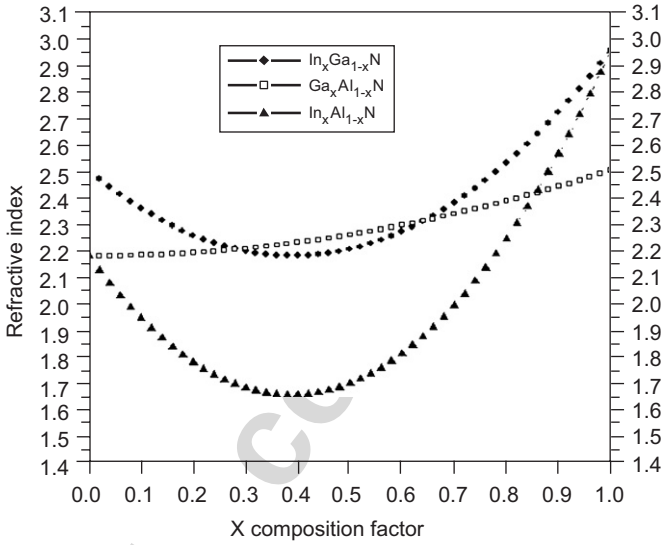


Fig. 4. Refractive index of Wurtzite $In_xGa_{1-x}N$, $Ga_xAl_{1-x}N$ and $In_xAl_{1-x}N$ alloys versus the molar fraction "x".

4. Conclusion

Despite of the lack of data concerning refractive index of III-N ternary alloys semiconductor structures, this theoretical study have been made to give more informations concerning their optical characteristics.

The main feature remains the refractive index. Firstly, the investigations were directed to the ability of InN to be grown on GaN to make $In_xGa_{1-x}N$ alloy. Since a lot of workers have succeeded to grow $In_xGa_{1-x}N$, especially with a low value of x, it has been developed a relation to compute the refractive index of such devices.

The decreasing tendency of the refractive index of the $In_xGa_{1-x}N$ structure in the first quarter of the molar fraction is probably due to the lattice mismatch which seems to disturb the first few layers of $In_xGa_{1-x}N$, where x is not important. But, when the alloy begins to contain more and more Indium, the natural tendency of decreasing gap takes again its real place and the increase of the refractive index becomes normal and consequently greater.

The obtained results show as well the reverse $n(\mathrm{Eg})$ correspondence and the direct $n(\lambda)$ relation in their quadratic form. This nonlinear shape appears further during the crystal growth and is due essentially to the bowing parameter.

References

[1] R.D. Dupuis, J. Cryst. Growth 178 (1997) 56–73.
[2] M. Van Schilfgaarde, A. Sher, A.-B. Chen, J. Cryst. Growth 178 (1997) 8–31.
[3] R.F. Davis, M.J. Paisley, Z. Sitar, D.J. Kester, K.S. Ailey, K. Linthicum, L.B. Rowland, S. Tanaka, R.S. Kern, J. Cryst. Growth 178 (1997) 87–101.
[4] M. Higashiwaka, T. Inushima, T. Matsui, Phys. Stat. Sol. (b) 240 (2) (2003) 417–420.

[5] J. Wu, W. Walukiewicz, K.M. Yu, J.W. Ager III, E.E. Haller, H. Lu, W.J. Schaff, Phys. Stat. Sol. (b) 240 (2) (2003) 412–416.
[6] S. Porowski, I. Grzegory, J. Cryst. Growth 178 (1997) 174–188.
[7] G. Mendoza-Diaz, K. Stevens, A. Schwartzman, R. Beresford, J. Cryst. Growth 178 (1997) 45–55.
[8] J.H. Edgar, Properties of group III-Nitrides, Datareviews series no. 11, IEE Inspec., London, February 1994, pp. 3–6.
[9] B.A. Ferguson, C.B. Mullins, J. Cryst. Growth 178 (1997) 134–146.
[10] S.M. Bedair, F.G. McIntosh, J.C. Roberts, E.L. Piner, K.S. Boutros, N.A. El Masry, J. Cryst. Growth 178 (1997) 32–44.
[11] S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsushita, H. Kiyoku, Y. Sugimoto, Appl. Phys. Lett. 69 (1996) 1477.
[12] K.P. O'Donnell, Mater. Res. Soc. Symp. 595 (2000) W11.26.1.
[13] S. Strite, H. Morkoç, J. Vac. Sci. Technol. B 10 (1992) 1237.
[14] M. Kim, J.-K. Cho, I.-H. Lee, S.-J. Park, Phys. Stat. Sol. (a) 176 (1999) 269.
[15] V.Yu. Davydov, A.A. Klochkhin, V.V. Emtsev, S.V. Ivanov, V.V. Vekshin, F. Bechstedt, J. Furthmüller, H. Harima, A.V. Mudryi, A. Hashimoto, Y. Yamamoto, J. Aderhold, J. Graul, E.E. Haller, Phys. Stat. Sol. (b) 230 (2002) R4.
[16] A.F. Wright, J.S. Nelson, Phys. Rev. B 50 (1994) 2159; A.F. Wright, J.S. Nelson, Phys. Rev. B 51 (1995) 7866.
[17] H. Schulz, K.H. Thiemann, Solid State Commun. 23 (1977) 815.
[18] K. Osamura, S. Naka, Y. Murakami, J. Appl. Phys. 46 (1975) 3432.
[19] D. Jenkins, Properties of group III-Nitrides. Datareviews series no. 11, IEE Inspec., London, June 1994, pp. 159–162.
[20] F. Bechstedt, J. Furthmüller, M. Ferhat, L.K. Teles, L.M.R. Scolfaro, J.R. Leite, V.Yu. Davydov, O. Ambacher, R. Goldhahn, Phys. Stat. Sol. (a) 195 (3) (2003) 628–633.
[21] H. Morkoç, S. Strite, G.B. Gao, M.E. Lin, B. Sverdlov, M. Burns, J. Appl. Phys. 76 (1994) 1363.
[22] J.B. MacChesney, P.M. Bridenbaugh, P.B. O'Connor, Mater. Res. Bull. (USA) 5 (1970) 789–790.
[23] T.L. Tansley, C.P. Foley, J. Appl. Phys. (USA) 59 (9) (1986) 3241–3244.
[24] C. Perrsson, R. Ahuja, A. Ferreira da Silva, B. Johnson, J. Phys.: Condens. Mater. 13 (2002) 8945.
[25] U. Grossner, J. Furthmüller, F. Bechstedt, Phys. Rev. B 58 (1998) R1722.
[26] S.N. Grinyeav, V.Ya. Malakhov, V.A. Chaldyshev, Sov. Phys. J. (USA) 29 (1986) 311–314.
[27] C.P. Foley, Mater. Res. Bull. (USA) 5 (1970) 789–790.
[28] J. Misek, Mater. Res. Bull. (USA) 5 (1970) 789–790.
[29] H. Hovel, Mater. Res. Bull. (USA) 5 (1970) 789–790.
[30] M. Ilegems, Mater. Res. Bull. (USA) 5 (1970) 789–790.