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RESEARCH ARTICLE

Theoretical Study of Optoelectronic Properties for Gallium nitride Under High pressure

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Abstract

The effect of the hydrostatic pressure and temperature on the direct energy gap in wurtzite and zinc-blende GaN semiconductor has been studied using different EOSs (Birch-Murnaghan, Bardeen, Libby and Libby, and Born-Mie). The variation of the energy gaps with pressure up to 12 GPa and with temperature up to 300 K has been done. The calculated fundamental energy gap at different pressures show a good agreement in comparison with the available experimental and theoretical data of literature. The effect of pressure on the refractive index of zinc-blende GaN has been studied. The refractive index decreases linearly with increasing pressure showing a negative pressure coefficient.

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INTRODUCTION

Over the last years, study of materials under high pressure has become extremely important subject displaying explosive growth, because both theoretical and experimental developments have facilitated such work (Degheidy and Elkenany, 2011).The origin of the semiconductivity of GaN is briefly explained by using a linear combination of atomic orbitals (LCAO) model. An isolated gallium atom has three electrons in the outer shell which are presented by spectroscopic notation ($3d^{10}$) $4s^2$ $4p^1$, while nitrogen atom has the structure $2s^2$ $2p^3$. In order to form bond between nitrogen and gallium, one s electron from $4s^2$ is promoted to 4p to obtain the configuration 2s $2p^3$ and ($3d^{10}$) 4s $4p^3$ which simulate the semiconductor material electronic configuration. In the above, it is assumed that an s electron has been promoted into a p orbital in each case and the resulting sp^3 electron configuration is hybridized into the four linear combination of atomic orbitals. They are defined by:

$$1/2\,(s + p_x + p_y + p_z)$$
$$1/2\,(s + p_x - p_y - p_z)$$
$$1/2\,(s - p_x + p_y - p_z)$$
$$1/2\,(s - p_x - p_y + p_z) \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

where p_x etc represent the orbital of the stated symmetry.

The normalized combination of ϕ_{Ga} and ϕ_N forming what are roughly the new orbitals come about by hybridization between orbitals on different centers.

GaN is one of the III-V nitride wide-band gap semiconductors, it is particular interest because of the importance in science and technology for optoelectronic applications and the many outstanding physical and chemical properties in the short-wavelength range as well as for high temperature, high power and high-frequency electronic devices (Sun *et al.,* 2005), thus, wide band gap semiconductor materials extend the field of semiconductor applications of the limit where classical semiconductors such as Si and GaAs fail (Kanoun, 2004).

GaN is a wide-gap semiconductor that usually crystallizes in the wurtzite lattice (also known as hexagonal or α-GaN). However, under certain conditions, zinc-blende GaN (sometimes referred to as cubic or β-GaN) can also be grown on zinc blende substrates under certain conditions, Fig. 1 shows these two structures. Under very high pressure, GaN experience a phase transition to the rock salt lattice structure (Vurgaftman and Meyer, 2003). GaN form covalent binding being tetravalent with a sp^3 hybridization. In the case of zinc blende there are two sublattices, one for cations and another one for anions, while in the case of the wurtzite structure there are four sublattices which

can also be considered as two hexagonal compact sublattices. In both case, one cation of one sublattice is surrounded by four anions of the another sublattice, and anion is surrounded by four cations forming such tetrahedrons (Morkoc, 2008).

This work present a theoretical high pressure study for energy gap of GaN in wurtzite and zinc-blende structures. Further to evaluate variation of refractive index under high pressure using different equations of state.

Energy Gap and Band Structure in GaN:

The energy gap in an important parameter in device conception, since it determines the threshold for absorption of photons in semiconductors. The band structure of GaN has a direct lowest band gap as shown in Fig.(2) for wurtzite and zinc-blende GaN, the conduction band has a single minimum at Γ point in the Brillouin zone (BZ). The valence band top is split at Γ by the combine action of the crystal field and spin-orbit interaction (Monemar, 1999). GaN is categorized as direct gap semiconductors, because the momentum of electrons and holes is the same in both the conduction band and the valence band, such as electron con directly emit a photon.

Theoretical Details and Results

Effect of High Pressure on the Energy Gap at Room Temperature.

Two approaches have been used in studying the effect of pressure and temperature on the band gap of wurtzite and zinc-blende GaN. One of them by evaluating E_g under high pressure by using the following equation (Dridi *et al.,* 2002):

$$E_g(p) = E_g(0) + \alpha p + \beta p^2 \quad \ldots (2)$$

Where $E_g(0)$ is energy gap at p=0 and T=0, α is the first order pressure derivative (dE_g/dp) and β is second order pressure derivative (d^2E_g/dp^2), and energy gap dependence on temperature is obtained from Varshni's empirical formula (Varshni, 1967).

$$E_g(T) = E_g(0) - \frac{AT^2}{T+B} \quad \ldots (3)$$

Where A and B temperature coefficients, combining equations (1) and (2), one obtain:

$$E_g(p,T) = E_g(0) + \alpha p + \beta p^2 - \frac{AT^2}{T+B} \quad \ldots (4)$$

Which represent the pressure and temperature effect on energy gap of semiconductors (Arezky et al, 2009). Using Eq.(4) with the values of $E_g(0)$, A, B, α, and β tabulated in Table (1). Fig. 3, shows variation of energy gap under high pressure at T=300 K for wurtzite and zinc-blende GaN, where energy gap increases with increasing pressure in constituent with normal behavior of E_g variation under pressure for semiconductors.

The other approach is to evaluate the variation of E_g with pressure, through estimating variation of lattice constant a(p) under high pressure by using Murnaghan equation of state (Murnaghan, 1937),

$$a(p) = a(0)(1 + \frac{B_o'}{B_o} p)^{\frac{-1}{3B_o'}} \quad \ldots (5)$$

Where

$a(0)_{ZB-GaN}$ = 4.52 Å (Levinshtien *et al*., 2001)

($B_o = 184 GPa$ and $B_o' = 4.6$) are the bulk modulus and its first order pressure derivative at zero pressure (Christensen and Gorczyca, 1994).

and then substituting Δa in the following equation displayed by (Bouarissa, 2002):

$$E_g = a^* + b^*\left(\frac{\Delta a}{a_o}\right) + c^*(\frac{\Delta a}{a_o})^2 \quad \ldots (6)$$

where a*, b* and c* are fitting parameters and their values for zinc-blende GaN are a*=3.2 eV, b*=-23.83 eV, c*=195.62 eV (Bouarissa, 2002), and Δa= a(p)-a(0).

Eq.(5) can be rewritten in the form

$$a(p) = a(0)(\frac{V_p}{V_o})^{\frac{1}{3}} \quad \ldots (7)$$

Since Eq.(7) represent the general form of the variation of lattice constant with pressure, we found that it is suitable to evaluate the variation of lattice constant under high pressure.

On combining eq. 7, and eq. 6 with different EOSs (Birch-Murnaghan, Bardeen, Libby and Libby and Born-Mie), which are expressed bellow:

- Birch-Murnaghan EOS (Birch 1952)

$$P_{BM} = \frac{3B_o}{2}\left(\eta^{-\frac{7}{3}} - \eta^{-\frac{5}{3}}\right)\left[1 + \frac{3}{4}(B_o' - 4)\left(\eta^{-\frac{2}{3}} - 1\right)\right] \quad \ldots (8)$$

- Bardeen EOS (Bardeen, 1938)

$$P_B = 3B_o\left(\eta^{-\frac{5}{3}} - \eta^{-\frac{4}{3}}\right)\left[1 + \frac{3}{2}(B_o' - 3)\left(\eta^{-\frac{1}{3}} - 1\right)\right] \qquad \ldots\ldots\ldots\ldots\ldots(9)$$

- Libby and Libby EOS (Libby and Libby, 1972)

$$P_{LL} = 3B_o\left(\eta^{-\frac{5}{3}} - \eta^{-\frac{4}{3}}\right) \qquad \ldots\ldots\ldots\ldots\ldots(10)$$

- Born-Mie EOS (Anderson, 1995)

$$P_{B-Mi} = \frac{3B_o}{3B_o' - 8}\left(\eta^{-(B_o' - \frac{4}{3})} - \eta^{-\frac{4}{3}}\right) \qquad \ldots\ldots\ldots\ldots\ldots(11)$$

Fig. 4 show a comparison for present results of energy gap variation with pressure, for zinc-blende GaN, using the above EOSs (eqs. 8-11), further to Murnaghan EOS (eq. 5) used by (Bouarissa, 2002).

We see from the Fig.(5), that energy gap variation with pressure using different EOSs are a good agreement with the literature except of that result by Born-Mie EOS. Excellent agreement seen by Birch-Murnaghan and Bardeen EOSs.

Calculations of E_g variation with pressure and temperature.

Eq.(2) is an expression for the variation of the energy gap with temperature for semiconductors at atmospheric pressure. Fig.(5) shows the variation of energy gap with temperature for wurtzite and zinc-blende GaN.

The variation of E_g with T at different pressure, using Eq.3, for wurtzite GaN and zinc-blende GaN respectively are shown in (Fig. 6 and 7).

Fig. 6 and 7 shows the effect of the positive value of first order pressure derivative for energy gap (dE_g/dp) in wurtzite and zinc-blende GaN, i.e. although Eg decreases with increasing temperature, the increase of pressure increases E_g. The gradient of the energy gap with temperature, at certain pressure, for zinc-blende GaN (Fig. 7) is greater than that for wurtzite GaN (Fig. 6).

Calculations of Refractive index Variation with Pressure

Three models have been used to calculate the refractive index (n) for zinc-blende GaN:

1-The Moss formula (Gupta and Ravindra, 1980)

$$E_g n^4 = k \qquad \ldots\ldots\ldots\ldots(12)$$

Where k is a constant has the value 108 eV.

2-The Ravindra expression (*Ravindra et al.,* 1979)

$$n = \alpha_1 + \beta_1 E_g \qquad \ldots\ldots\ldots\ldots\ldots(13)$$

whereα_1=4.084 and β_1=-0.62 eV^{-1}

3-Herve and Vandamme relation (Herve and Vandamme, 1994)

$$n = \sqrt{1 + \left(\frac{A_1}{E_g + B_1}\right)^2} \qquad \ldots\ldots(14)$$

with A_1=13.6 eV and B_1=3.4 eV

In Fig. 10, the refractive index of GaN is plotted against the pressure according to three different models described above with relation shown in (Bouarissa, 2002) which is:

$$n = n_0 + b^{**}\left(\frac{\Delta a}{a_o}\right) + c^{**}\left(\frac{\Delta a}{a_o}\right)^2 \qquad \ldots\ldots\ldots\ldots(15)$$

Similar to E_g variation with pressure, we evaluate the variation of lattice constant using Birch-Murnaghan, Bardeen, Libby and Libby, and Born-Mie EOS, then evaluate the variation of refractive index with pressure. The results of using the above EOSs with eq.(14)at T=300 K for zinc-blende GaNare shown in Fig. 8.

As shown in Fig. 8, where present results obtained by using (Birch-Murnaghan, Bardeen, Libby and Libby) EOSs are in exact agreement with results obtained by using the three relations mentioned in Table 2. While Born-Mie EOS used in the present work give results of less agreement with literature, and disagreement increases as pressure coefficient of refractive index increases as it reveals in Fig. 8, where (Ravindra*et al.,* 1979 *).* relation, has largest pressure refractive index coefficient.

Conclusions

The energy gap and refractive index of semiconductor represent two fundamentals physical aspects that characterize their optical and electric properties. The applications of semiconductors as electronic, optical and optoelectronic devices are well determined by the nature and magnitude of these two elementary material properties, present work has performed evaluation of the pressure and temperature dependent on the energy gap for GaN in the wurtzite and zinc-blende structures using different equation of states, the variation of the direct band gap as a

function of hydrostatic pressure up to 12 GPa shows a linear behavior and are in a good agreement with the available experimental and calculated data. The variation of the refractive index as a function of pressure for ZB-GaN is linear and shows a negative pressure coefficient for all used models. However, the effect of pressure on refractive index seems to be stronger when using the (*Ravindra et al.,* 1979*)* relation.

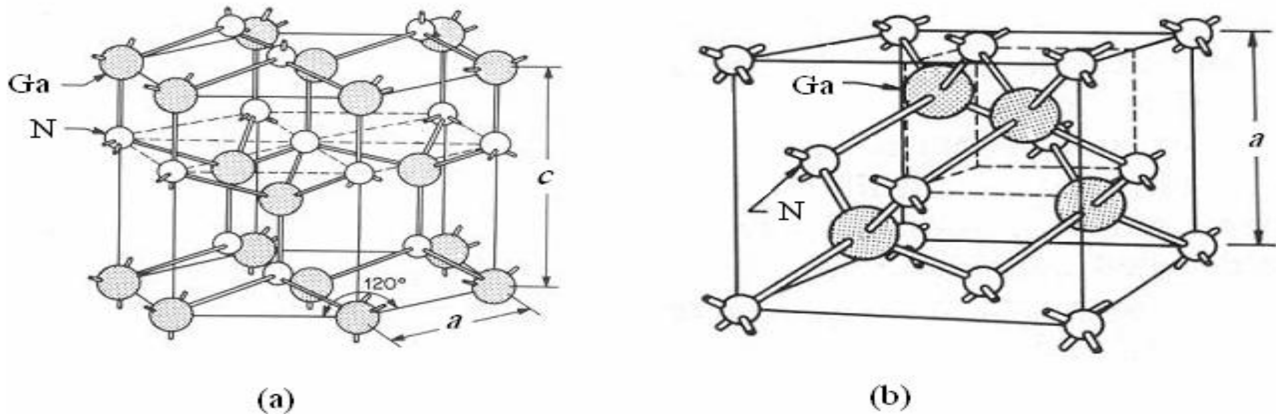

Fig.(1): Structure of GaN in (a) wurtzite (b) zinc-blende (Miskufova, 2011)

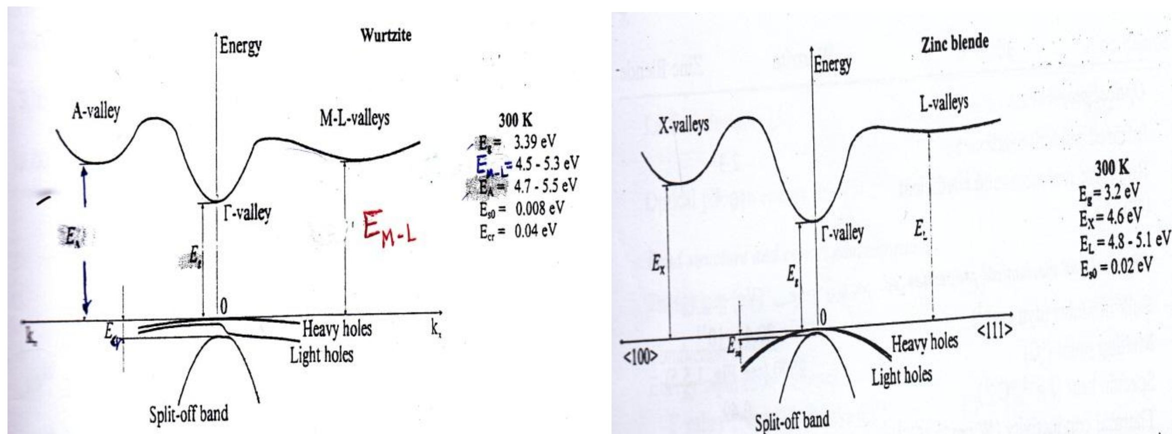

Fig.(2): Band structure of GaN (Levinshtein *et al.,* 2001)

Table 1: Values of Eg(0), pressure coefficient α and β, temperature coefficient A and B for wurtzite and zinc-blende GaN.

Material	$E_g(0)$ eV	$\alpha x10^{-2}$eV/GPa	$\beta x10^{-3}$eV/GPa^2	$Ax10^{-4}$eV/K	B K
WZ-GaN	3.47[a]	4.2[a]	-1.8[a]	7.7[a]	600[a]
ZB-GaN	3.28[a]	3.1[b]	-0.21[b]	7.7[a]	600[a]

a- Levinshtein *et al.,* 2001 b- Riane *et al.,*2010

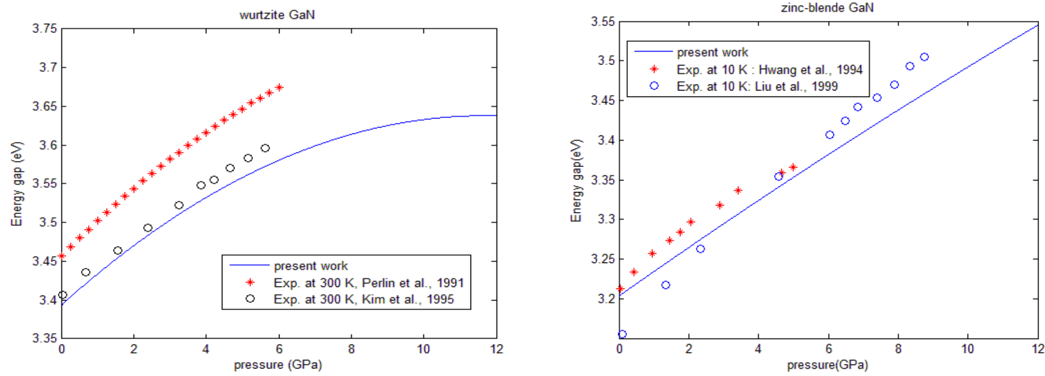

Fig.(3): The variation of the energy gap with high pressure for GaN using eq. (4) in comparison with experimental data of literature

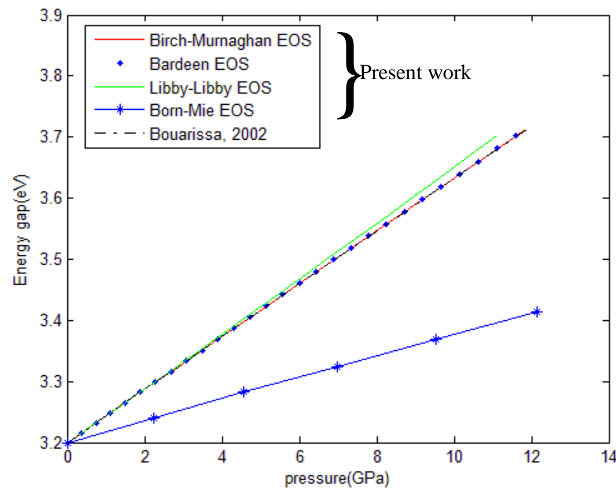

Fig.(4): variation of the band gap energy with pressure, for zinc-blende GaN, using different EOSs further to results of (Bouarissa, 2002).

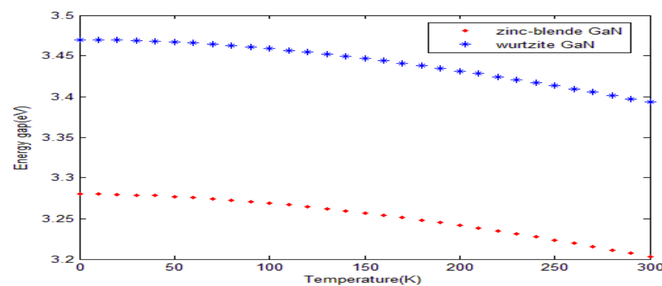

Fig.5: The variation of energy gap with temperature using Eq.(2) for wurtzite and zinc-blende GaN

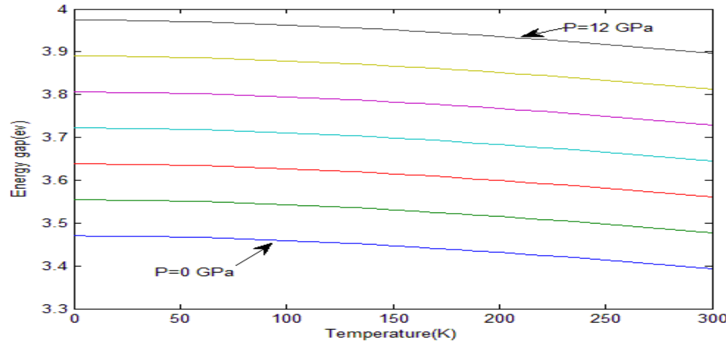

Fig. 6:variation of Eg with temperature T at different pressures using Eq. 3 for wurtzite GaN.

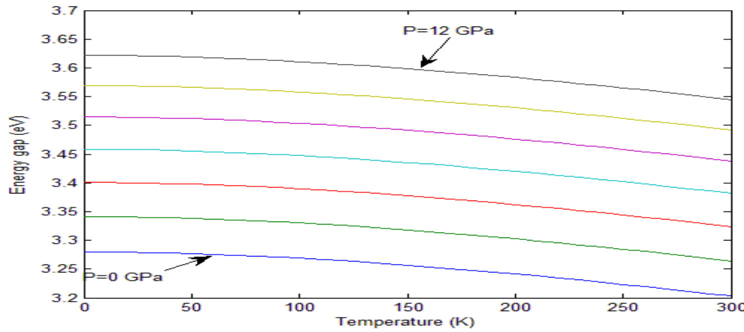

Fig. 7:variation of E_g with temperature T at different pressures using Eq. 3 for zinc-blende GaN.

Table (2):Refractive indices n at zero pressure and constants b and c** for zinc-blende GaN**

Model	n_0	b**	c**	Refs.
Moss relation	2.41	3.97	-32.6	Gupta and Ravindra, 1980
Ravindra et al relation	2.10	14.24	-159.27	Ravindra*et al.,* 1979
Herve and Vandamme relation	2.29	6.71	-19.11	Herve and Vandamme, 1994

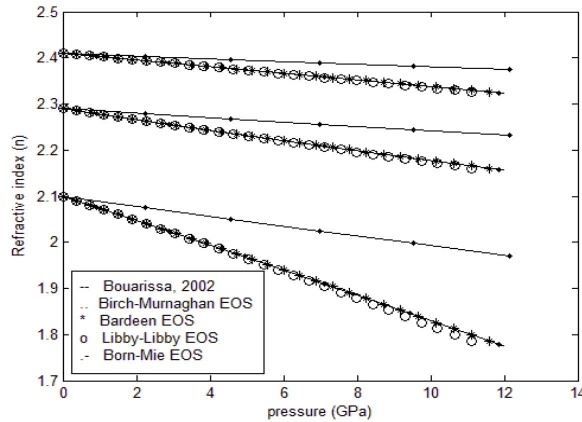

Fig. 8:Variation of the refractive index with pressure from different EOSs at T=300 K using eq.(14) for three models.

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