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First Principles Study of Europium doped Gallium Nitride in Wurzite Structure

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Abstract

In the present work, we have successfully deposited Sb antimony doped tin dioxide (SnO_2) thin films with Several advantages over well known LCD's including increased brightness and viewing angle. We are currently investigating Eu doped GaN as a potential red phosphor for TEFL display applications. Eu doped GaN films were grown by solid source molecular beam epitaxy on Si (111) substates. The material was optically characterized through temperature dependent emission spectroscopy using a He-Cd laser at 325 nm for above band gap excitation. A strong red emission was obtained at 622 nm, which corresponds to an Eu^{3+} inner 4f-shell transition from the $5D^{0}$ to $7F^{2}$ state. Therefore, the observed thermal quenching of red Eu emission is assigned to a strongly temperature dependent pumping process.

Keywords: *EuGaN,Dopping, BandGap,Spin,mBJ,DFT, Wien2K.*

1. Introduction

Transparent The electronic and optical properties, III-V compound Nitride semiconductors, namely, GaN, AlN, InN, have gained importance as wide-band gap semiconductors with critical and wide range of technological applications in microwave communication, lasers, detectors, and light emitting diodes (LEDs) due to their band gap tunable in the blue green region of the visible spectrum and ultraviolet (UV) range [16, 1, 14, 17, 13, 12, 15, 7] Gallium nitride (GaN) is a wide and direct hand-gap semiconductor 3.39 eV at room temperature, with high electron drift saturation speed, low dielectric constant, good electrical conductivity, high breakdown voltage and good laugh-temperature chemical stability and other characteristics, it's stable phase under ambient conditions with the hexagonal structure, this is anyway an excellent host for impurities a defect density of 10^{10} cm^{2} can be reached, which is extremely high if compared to other semiconductors like Si (10^{2} cm^{2}) or GaAs(10^{4} cm^{2}). The thermal expansion of Wz-GaN has been studied in the temperature range of 300-900 K by Maruska and Tietjen [11]. They reported a linear change with temperature for lattice constant, with a mean coefficient of thermal expansion of $\Delta a/a = 5.59\text{x}10^{6}\ \text{K}^{-1}$ across the entire temperature range. As grown GaN is typically n-type material with a high free carrier concentration by doping with Silicium (Si), which makes the production of p-type GaN difficult by doping with Magnesium (Mg). Optical properties are the most investigated properties of GaN because shows its great potential, especially as a light emitter, Wz-GaN is situated in the UV region, it's an ideal candidate as a host for optical dopant because of its thermal stability and especially because of its large and direct band-gap. Empirically known that if the RE ions are incorporated in an ionic solid they prefer to occupy the cation site where the selection rules are relaxed and the 4f → 4f transition probability is different from zero. In the case of W2-GaN, the big majority RE occupy a Ga^{+3} cation site further increasing the 4f → 4f transition probability. For this reason, RE doped

systems excited-state lifetimes between 1 μs and 1 ms are observable, the host material does have a very strong influence on

the radiative transition probability, i.e. the photoemission intensity. During the past decade, rare earth doped semiconductors have generated considerable attention for their application in new optoelectronic devices [6, 8, 21]. The favorable thermal, chemical, and electronic properties of Wz-GaN semiconductor suggest device feasibility using lanthanide doped. This is one of the advantages of GaN as host for the rare-earth. The possibility of introducing Europium element (Eu) into the GaN material has enabled the realization of GaN Eu blue light emitting devices including LEDs in the past decade. Characterization of the optical and electrical properties of HIV semiconductors implanted with rare earth ions has led to the development of new optoelectronic devices. When these materials are excited, intense sharp-line emission is observed due to intra 4f shell transitions of the rare-earth ion. These emission spectra cover the wavelength range from the ultraviolet to the infrared, providing important frequencies that are useful in device applications including integrated optical circuit technology. Several groups have investigated in GaN doped with rare earth ions [24, 3, 9, 20, 2]. Europium (Eu) Erbium (Er) and Thulium (Tm) are considered to be most useful among rare earth ions because they emit light in the red, green and blue region of the visible spectrum. Theoretically, Sanna et al. [18] used the local density approximation exchange-correlation energy (LDA) method to study the rare earth Eu, Er and Tm doping For the related defects of heterogeneous GaN, it's found that rare earth atoms occupy Ga sites and are easily combined with intrinsic defects o form a couples. Svane et al[22]. used SIC-LSDA to calculate the electronic structure of rare-earth instead of doped GaAs sod GaN defects. However, theoretically, there are few studies on the electronic structure and optical properties of Eu doped GaN. In this paper, the elastic structure and optical properties of Eu doped Wz-GaN is calculated using a first principles method based on density functional theory. Though calculations, it's found that Eu doped with GaN the forbidden hand, and introduce a local impunity level in the forbidden hand and sear the top of the valence band respectively, after doping Eu, the imaginary part of the dielectric function and the absorption coefficient is introduced New peaks appear in the low-energy region of the spectrum. The significance of Wz-materials for optical devices has been recognized by the 2014 Nobel Prize in Physics for efficient blue LEDs.

2. Details of calculations

We have investigated electronic, optical and transport properties of Eu doped Wz-GaN using ab-initio all-electron FP-LAPW method based on density functional theory (DFT), as implemented in WIEN2K software package [22]. To calculate the exchange correlation potential, we applied the LSDA, we have used Habbard (U) effective potential $\boldsymbol{Ueff = 8.71\ \mathrm{eV}}$ for 4f electrons of Eu as already reported by Harmon et al [4], and modified Becke-Jenson approximation (mBJ) [5] with So. We obtained the most accurate results using FP-LAPW with mBj. Wz-GaN structure contains 16 atoms, 8 atoms of Ga and 8 atoms of N. one atom of Ga was substituted by one Eu atom, to obtain the $Eu_{0.125}$ $Ga_{0.875}$ N corresponding to a doping concentration 12.5% of Eu. The wave function are expanded into planes waves in the interstitial region with a cut-off $\boldsymbol{K_{max} = 8/RMT}$ where RMT has the smallest of all MT sphere radii and K_{max} is the plane wave cut-off. We used 1000 K-point in the irreducible Brillouin Zone for our calculation. The dielectric function a fundamental property required to investigate the optical nature of material. This function describes the linear response of the system to electromagnetic radiation and related to electron-photon interactions Bolt Trap code [23] is using to calculate the thermoelectric (TE) properties from ab-initio data using semi-classical Boltzmann transport theory within the constant relaxation time and rigid band approximations.

3. Results and discussion

3.1. Electronic properties

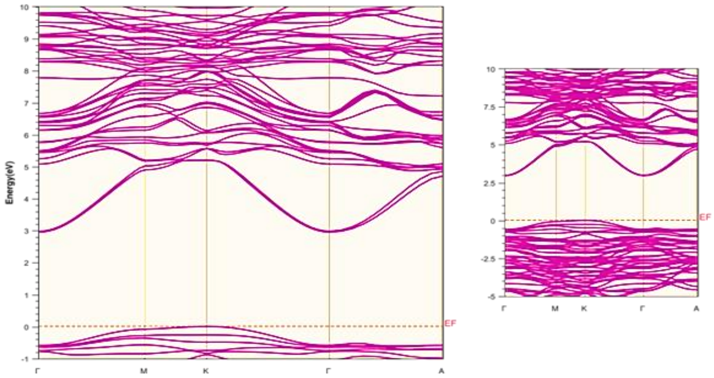


Figure 1. Band structure spin up of **$Eu_{0.125}$ $Ga_{0.875}$ N** with LSDA+mBJ+U+So approach.

We have calculated band structure and density of states by FP-LAPW using mBJ, LSDA with U_{eff} and So. The difference appears lies in the band-gap, the minimum of conduction band (CB) and the maximum of valence band (VB) is located M-point and Γ-point respectively of the Brillouin zone which means that we have an indirect band-gap.

Table 1. Band gap for **$Eu_{0.125}$ $Ga_{0.875}$ N** materials with different aproach.

Materials	Approximations	Eg spin up (eV)
$Eu_{0.125}$ $Ga_{0.875}$ N	LSDA	2.25
	mBJ	3.42
	mBJ+U	3.65
	mBJ+U+So	3.48

These values with different approaches are depicted in table 1. We note that both spin-up and spin-dn have the same band-gap at 3.43 eV with So. We have also calculated spin-polorised density of states by these approximations, show in fig 2. For these approach the total and partial density of states show semiconducting The total Dos shown fig 2 proves it's semiconductor at value of ≈ 3.4 eV. The valence band is domin by the 4f state of Eu with a weak contribution from Ga-4p and N-2p states, on the other hand in partial density of states the conduction bands is composed by the major contribution for minority-spin of Eu-4f states with a weak contribution for both spins of N-2p and Ga-4p states.

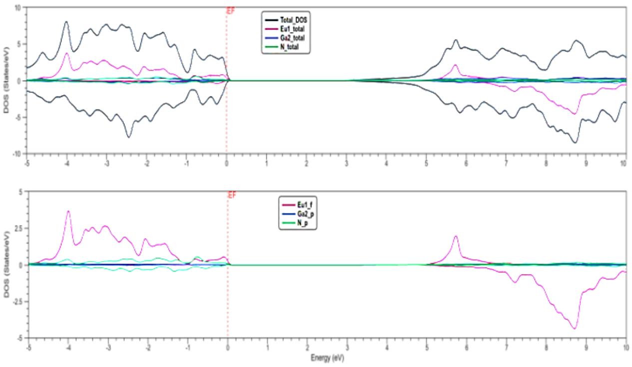


Figure 2. Total and Partial density of states of $\mathrm{Eu}_{0.125}Ga_{0.875}N$ with LSDA+mBJ+U+so approach.

Fig.2 By observing the curves of the total and partial density of states in the two compounds of each atom before and after doping we infer that the GaN's compound is activated by the Eu. How thier densities is increased. By the figure we found that the contribution of atomic levels (=5d = 3d) in the cases of the two sides of Spin (Spindown and SpinUp) in the electronic construction of the compound, with a single Band Valence BV, when the energy field from - 4 to the level of Fermi E_F.

3.2. Optical properties

The dielectric function describes the linear response of a material to electromagnetic radiation wavelength or photon energy which relates to the interaction of photons with electrons, can be expressed as:

$$\epsilon(\omega) = \epsilon_1(\omega) \pm i\epsilon_2(\omega) \qquad (1)$$

Where the real part ϵ_1 can be written as:

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\omega\prime\, \epsilon_2(\omega\prime)}{\omega\prime^2 - \omega^2}\, d\omega' \qquad (2)$$

And imaginary part $\boldsymbol{\epsilon_2}$ can be written as:

$$\boldsymbol{\epsilon_2(\omega) = \frac{2\omega}{\pi} P \int_0^\infty \frac{\epsilon_1(\omega\prime)}{\omega\prime^2 - \omega^2}\, d\omega'}$$

(3)

relate to the polarization and absorption, respectively. Where is the integration variable, P represents the Chauchy principal value of the integral similarly one can relate the real and imaginary parts of the polarizability. Based on the $\boldsymbol{\epsilon(\omega)}$, the absorption coefficient $\boldsymbol{\alpha(\omega)}$, the real part of the refractive index n$(\boldsymbol{\omega})$, the imaginary part of the refractive index K($\boldsymbol{\omega}$) and optical conductivity can be calculated with formulas reported Below, Other optical properties can be derived from the complex dielectric function [19].

$$\boldsymbol{n(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{K(\omega\prime)}{\omega\prime - \omega} d\omega'}$$

(4)

And

$$\boldsymbol{K(\omega) = \frac{2}{\pi} P \int_0^{\infty} \frac{K(\omega\prime)}{\omega\prime - \omega} d\omega'}$$

(5)

The absorption coefficient $\boldsymbol{\alpha\big((\omega)\big)}$ can be given by:

$$\boldsymbol{\alpha\big((\omega)\big) = \frac{4\pi}{\lambda} K\big((\omega)\big)}$$

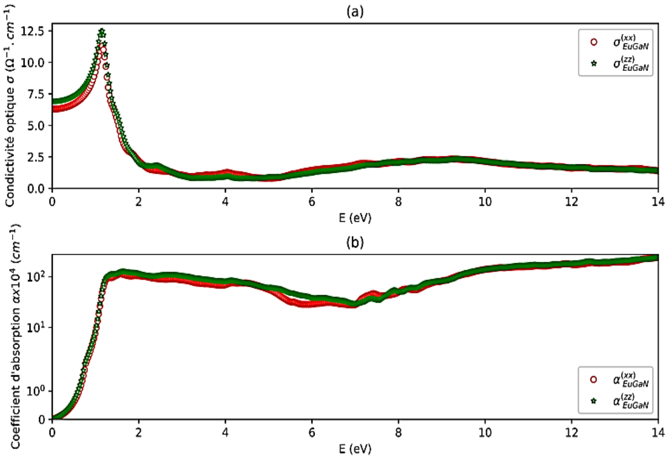
(6)

Where $\boldsymbol{\lambda}$ is the wavelength of light in vacuum. The real part of the optical conductivity is calculated according to the following relation:

$$\boldsymbol{\sigma(\omega) = \frac{\omega}{4\pi} \epsilon(\omega)}$$

(7)

This optical parameter calculated of $Eu_{0.125}$ $Ga_{0.875}$ N using Wien2k package with mBJ+U approach including spin orbit coupling effect.



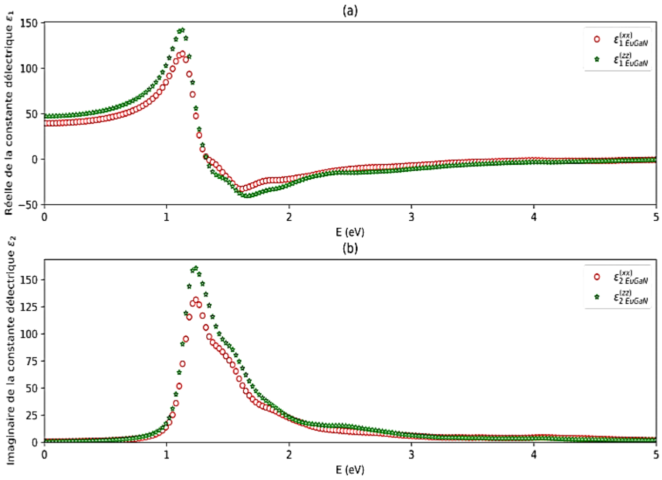


Figure 3. Optical properties: (1) optical conductivity (a) and absorption coefficient (b), (2) the imaginary part (e,) of dielectric functions (b) and (a) its real part of $Eu_{0.125}$ $Ga_{0.875}$ N materials.

Fig.3 The variation of the optical conductivity is shown in fig.3 (1,a), it begins to increase and arrives at maximum 1.6 and 1.8 to both (xx) and (zz) directions. (1,b) shows the results of absorption coefficient, we noted increasing absorption trends while changes in absorption during energy range 0-14 eV. It is worth noting that absorption begins at 1.75 eV (377 nm). The evolution of the refractive index and extinction coefficient are shown in fig.4. We note these static refractive indexes at 0.75 and 0.8, it begins to increase until reaches its maximum at 1.65 and 1.7 for both directions. So the extinction coefficient starts to increase from a threshold equal to 1.3 eV.

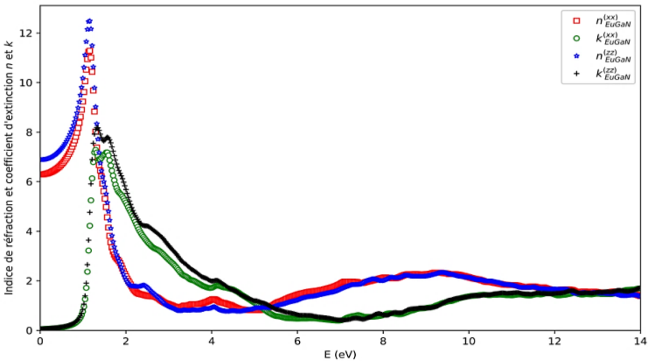


Figure 4. Index refraction and extinction coefficient of $Eu_{0.125}$ $Ga_{0.875}$ N materials.

Fig.4 We observe that the extinction coefficient curve of $Eu_{0.125}$ $Ga_{0.875}$ N increases significantly at photonic energies weaks, and be as great as possible at energies corresponding to the basic absorption edge, then it decreases rapidly and surprising in the high photon energies. These changes are exactly identical to the behavior of the refraction's curve as a sign of the direct relationship between the two optical phenomena of extinction and refraction.

4. Conclusion

$Eu_{0.125}$ $Ga_{0.875}$ N were studied with the ab-initio calculation using DFT. The obtained results of electronic properties show clearly $Eu_{0.125}$ $Ga_{0.875}$ N to be a semiconductor with an indirect band gap at 2.96 eV using mBJ+U approaches, which is in good agreement with other calculations. The real and imaginary parts of the dielectric function and the optical coefficients were determined. Seebek coefficient, electronic thermal conductivity, and electronic power factor have been determined. their values show that these materials could be potential candidates for heat energy conversion.

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