PAPER

Investigating optical properties of Cr:GaN system for various Cr concentrations (A DFT + U study)

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Keywords: gallium nitride, Cr doping, DFT

Abstract

We study electronic and optical properties of zincblende GaN doped with various Cr concentrations (3.12%, 6.25%, 9.37%). We conduct the calculations by employing DFT + U in Wien2K code while supercell size (1 × 2 × 2) is kept fixed for all cases. Electronic properties are changed with effect of dopant where 3d levels of dopant and 2p level of N produce p-d hybridization and this hybridization is highly affected by increasing impurity contents. Absorption spectra are blue shifted upon increase in dopant contents and absorption peaks are more pronounced in UV region. Refractive index and dielectric constant shows decrease as Cr concentration increases. Results reported in study indicate that Cr:GaN material may be considered a potential candidate for fabrication of optoelectronic, photonic and spintronic devices.

1. Introduction

Gallium nitride (GaN) is among III-V semiconductors having high chemical stability, energy efficiency, low cost and have shown considerable attraction for scientists owing to its outstanding optoelectronic and electronic applications in various technological fields including ultraviolet optoelectronic transistors, piezoelectric sensors [1], high resolution micro display [2], solid state lighting [3], photonic crystals [4], optogenetics [5], high electron mobility transistors (HEMTs) [6], automotive lighting [7], biological sensors [8] and spin lasers [9]. Among zincblende (ZB) and Wurtzite (WZ) phases, ZB phase of GaN is mostly suggested for research because of remarkable electronic properties which are highly required for fabrication of nanodevices [10, 11]. For doping, ZB structures presumed to be highly amenable than WZ GaN [12, 13] and this is the reason for our concern and motivation to choose ZB GaN structure for current density functional theory (DFT) study. We took interest in studying Cr doping into GaN as we expect that several interesting properties may emerge which may lead to novel optoelectronic applications. Over the decades, researchers have reported several experimental [14–23] and theoretical studies [24–32] on Cr:GaN system but to date no one has yet attempted to present study particularly focusing on optical properties using Wien2K. This reason motivated us to conduct a theoretical study on investigating optical properties of Cr:GaN.

Our research paper is organized as; section 2 gives computational method description and calculations details within framework of Wien2K code and section 3 comprises of explanation of results and discussions about DOS and optical properties. Finally, all the results are summarized in conclusion. We explore several intriguing and appealing facts about optical properties of Cr:GaN system which extends future scope of this material in fabricating optoelectronic, energy, spintronic and photonic devices.

2. Computational method

In current calculations, we study the effect of Cr doping on optical properties of ZB GaN and for this purpose, we have used Wien2K code. We have changed dopant concentrations (3.12%, 6.25%, 9.37%) into host GaN and...
supercell size \((1 \times 2 \times 2)\) is kept fixed for each case. Supercell contains 32 atoms and we have realized concentrations by substituting \(1 (Ga_{15}Cr_{1}N_{16})\), \(2 (Ga_{14}Cr_{2}N_{16})\) and \(3 (Ga_{13}Cr_{3}N_{16})\) Ga atoms with Cr atoms into GaN lattice. It yield the concentrations \(1/32 \sim 3.12\%\), \(2/32 \sim 6.25\%\) and \(3/32 \sim 9.37\%\). Full potential linearized augmented plane wave (FP-LAPW) based density functional theory (DFT) is used for electronic structure calculations and self-interaction error (SIE) is minimized using DFT + U \((U = 0.22\text{ Ry})[33]\). Adding Hubbard term into the GGA is useful technique and appears as a correction to SIE. We made substitution of Ga atoms with Cr atoms in each of concentrations. The states \((3d^{10} 4s^2 4p^1), (2s^2 2p^3), (3p^6 3d^4 4s^2)\) are assumed to be core states of Ga, N and Cr atoms in Cr:GaN system while remaining states are supposed frozen. Angular momentum expansion value for the wave function is \(l = 10\) while constant and spherically symmetric potential is supposed to be inside muffin-tin (MT) sphere. 0.1 eV Gaussian smearing is used and Brillion zone (BZ) integration is carried using modified tetrahedron method in irreducible wedge [34]. Energy convergence of \(10^{-4}\) Ry was obtained using 1000 \(k\)-points sampling and relaxation of the atomic positions is achieved by self-consistency criterion which involves charge convergence and force convergence of \(10^{-2}\) C, 1 mRy/au respectively. However, since we get almost same convergence with \(1 \times 2 \times 2\) and \(2 \times 2 \times 2\) supercells so we preferred \(1 \times 2 \times 2\) supercell for adding impurity with various concentrations in order to save computational time. Upon doping in each concentration, symmetry is broken and is updated when system is relaxed. Our results found to have great deal of agreement with existing literature findings. Moreover in calculations, we have chosen \(R_{\text{K\_max}}\) to be 8. In our calculations, we ignore incorporation of relativistic effects.

3. Results and discussions

3.1. Electronic properties

Density of states (DOS) describes electron occupancy within a specific energy range. The partial density of states (PDOS) and total density of states (TDOS) have been shown in figures 1 and 2 where Fermi level is represented by dotted line and separating valence and conduction band. States have been plotted in energy range \(-9\text{ eV to 8.5 eV}\). Figure 1(a) depicts PDOS of pure GaN and it is evident that density of states in valence band \((-6.8\text{ eV to } -0.1\text{ eV})\) originates mainly due to Ga \(p\)-, \(d\)-states and N \(p\)-states with small contribution of Ga and N atoms.
s-states. Conduction band of pure GaN is mainly contributed by s- and p-states of Ga atoms while p-states of N atoms. On the other hand, states distribution changes when GaN system is doped with various Cr concentrations (3.12%, 6.25%, 9.37%). For lower Cr concentration (3.12%), Cr 3d states are mostly localized near Fermi level and results decrease in energy band \([-8.6 \text{ eV} \text{ to } -1.7 \text{ eV}]\). It consists of region in valence band far from Fermi level \((-8.5 \text{ eV} \text{ to } -2.26 \text{ eV})\) and contains major contribution of Ga p- and d-, N p- and Cr d-states with least contribution of Ga, N and Cr s-states. For 6.25% and 9.37% Cr concentrations energy region comprising atomic states in valence band is located in \((-8.5 \text{ eV} \text{ to } -2.26 \text{ eV})\) and \((-8.1 \text{ eV} \text{ to } -2.0 \text{ eV})\) respectively. Higher Cr concentrations (6.25%, 9.37%) do not have states on top of valence band which makes excitations of electrons more difficult. Hybridization region \((-8.5 \text{ eV} \text{ to } -2.4 \text{ eV})\) is dominated by Cr 3d and N 2p interactions and is found well below Fermi level. GGA + U improve repulsion of impurity states and in conduction band role of Cr 3d states is viable with least contribution of Ga d-, N s- and Cr s-states [27]. Our results matches with the other works however difference may be due to use of Wien2K code using DFT + U and use of various techniques (experimental and theoretical) which researchers have reported [24, 29]. The study extends future scope of material which may be essentially needed in developing spintronic and photonic applications.

Individual atoms behavior in a specific energy range without mentioning orbital contribution is encoded in the plot of total density of states (TDOS). Energies obtained through solving Kohn–Sham equations are used to plot TDOS. In case of pure GaN, the dominance of N atoms can be clearly seen in both valence and conduction band. On other side, the TDOS plots of Cr doped GaN shows distinct changes upon increasing Cr concentrations. It is obvious that for lowest Cr concentration (3.12%), Cr states are localized near Fermi level. However, increasing Cr contents induces evident changes on influence of nitrogen atom character and it can be observed that in valence band for higher dopant concentrations, the role of N is dominant but in conduction band, dominance of dopant is noted [28].

### 3.2. Optical properties
Calculation of optical properties of GaN is important in order to predict its novel optical applications and are mostly based on quantum confinement effects. In our study, optical properties of pure GaN and Cr doped ZB GaN have been shown in figures 3 and 4. Optical absorption \(\alpha(\omega)\) is one of the important optical constant and it provides understanding of behavior of materials when light incident on them. It is found in term of dielectric constant (real \(\varepsilon_1(\omega)\)) and imaginary part \(\varepsilon_2(\omega)\) and is given as [36],

![Figure 2. TDOS of (a) Pure GaN, (b) 3.12%, (c) 6.25% and (d) 9.37% Cr concentrations.](image-url)
Optical absorption of pure GaN and GaN doped with various Cr concentrations (3.12%, 6.25%, 9.37%) have been demonstrated in figure 3(a). All the calculations have been executed by employing DFT + U in Wien2K code. Absorption for all cases has been recorded in energy range 0–8 eV and increasing absorption trends have been noted. In case of pure GaN, absorption rises in steps, attains maximum value at 7.8 eV (∼159 nm) [36, 37]. Absorption peak of pure GaN appearing at low energy ∼3.91 eV (317 nm) matches with reported works [36, 38, 39]. On other side, absorption trends for various Cr concentrations are different than trend of pure GaN which shows strength and effect of doping. Cr:GaN system exhibits high absorption in the ultraviolet region but shows decrease in visible and near infrared region (NIR). Absorption edges occurring at lower energies are shifted to higher energies with increase in Cr concentration and appears due to quantum confinement effects [36]. Trends of absorption spectra vary along with increasing Cr concentrations and may emerge due to electrons excitations from valence to conduction band. Absorption humps broadening may occur due to effect of doping and because of impurities interband transitions. Absorption spectra changes due to

\[ \alpha(\omega) = \sqrt{\frac{1}{2} \left[ \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega) \right]^2}. \]

Figure 3. Optical (a) absorption, (b) refractive index, (c) dielectric constant and (d) conductivity of pure and Cr doped GaN.

Figure 4. (a) Extinction coefficient and (b) Reflectivity of pure and Cr doped GaN.
intermediate energy levels appearing with effect of doping and because of varying Cr concentrations. Absorption maxima for various Cr concentrations doped into host GaN lattice appear at energy values; 7.43 eV ~ 3.12%, 7.61 eV ~ 6.25% and 7.71 eV ~ 9.37%. In comparison to pure GaN, absorption spectra are blue shifted as when dopant concentration is increased. Emergence of blueshift along with increase in Cr contents relative to pure GaN drives to nanostructure formation [36].

Refractive index \(n\) enumerate behavior of the material when light penetrate inside it as material. Light when enter inside material then its velocity changes and in response the \(n\) of the material changes accordingly.

Figure 3(b) is a manifestation of plot of refractive indices of pure GaN and various Cr concentrations doped into GaN. These traits are obtained by DFT + U calculations executed in Wien2K code. We demonstrated possible change in \(n\) for all concentration cases and compared them with pure GaN. Graphs are scaled in energy range 0–8 eV, taken along abscissa while variations in values of refractive indices are shown along y-axis. \(n_{\text{max}}\) (~3.0) for pure GaN occurred at energy value 5.39 eV (~230 nm). For pure GaN, \(n\) increases in steps and after attaining maximum value it starts decreasing which is due to effect of increase in reflectivity. \(n\) trends for all cases are almost similar (increasing and decreasing) but the values are different which is due to effect of doping. Moreover, maximum values of \(n\) for all concentration cases are; 4.5 ~ 3.12%, 4.2 ~ 6.25% and 3.9 ~ 9.37%.

Variation in values of \(n\) is due to successful internal reflections and may be reasoned to photon trapping by grain boundaries. Decrease in value of \(n\) may be ascribed to presence of various impurities and defects. Experimentally achieved value of \(n\) for pure GaN is 2.38 at 632.8 nm (~1.95 eV) [37, 40]. However, static refractive indices values as obtained in our DFT + U study are; 2.3 ~ pure GaN, 4.5 ~ 3.12%, 4.2 ~ 6.25% and 3.4 ~ 9.37%. It is evident that our DFT + U values of \(n\) significantly decrease upon increase in Cr concentrations into host ZB GaN. Prominent variations in \(n\) are observed in UV region while in visible region \(n\) trends shows constant rise and in near IR region, behavior of \(n\) is decreasing. In our case, \(n\) values are greater than one and may be associated to slowing down of photons by successive interactions with electrons. Decrease in \(n\) may be connected to a medium with less density and so they show lower refractive indices. In our study, lowering of \(n\) values may be related to PDOS plots (figure 1) where density of states varies along with increase in Cr contents.

Electric field associated with photons is responsible for unoccupied and occupied optical transitions. Due to this reason, dielectric constant carries mandate and for every physical system its calculations are important to estimate optical behavior of material. Dielectric function may be evaluated by the formula,

\[
\varepsilon_i(\omega) = \frac{4\pi^2}{m^2\omega^2} \int_{\text{BZ}} \frac{2}{2\pi} \sum_{\text{C,V}} |M_{\text{C,V}}(k)|^2 \delta(E_i^C - E_i^V - \hbar\omega) d^3k,
\]

\[
\varepsilon_r(\omega) = 1 + \frac{2}{\pi} \rho_0 \int_0^\infty \frac{\omega'}{\omega'^2 - \omega^2} d\omega.
\]

Where \((\omega, C, V)\) stands for the notion of angular frequency, conduction band and valence band respectively. \(k, \text{BZ}, (E_i^C, E_i^V)\) stands for reciprocal lattice vector, Brillion zone, intrinsic energy level of valence and conduction band respectively. Many body wave function upon solution yields \(\varepsilon_i(\omega)\) and from imaginary part conversion through Kramers-Kronig, we may get \(\varepsilon_r\). Figure 3(c) gives a comparison among real part of dielectric constant trends of pure GaN and various Cr concentrations. Dielectric plots represents variations in energy range 0–8 eV and are obtained through DFT + U calculations using Wien2K code. They represents ability of material (Cr: GaN) to allow electromagnetic field to pass through it when the effect of various Cr concentrations are incorporated. Dielectric trends for pure GaN, 6.25%, 9.37% shows steady rise and then decrease up to certain energy value while for 3.12% Cr concentration, the trend shows sudden decrease. Dielectric maxima for each case is; 8.8 ~ pure GaN, 19.79 ~ 3.12%, 18.10 ~ 6.25%, 15.33 ~ 9.37% and after that the graph starts decreasing until become almost constant for higher energy values. A viable resemblance is obtained between graphs shown in figures 3(b) and (c) as dielectric constant mathematically is interpreted as square of \(n\). However, static dielectric constants (at zero frequency limit) for each case are; 5.3 ~ pure GaN, 19.79 ~ 3.12%, 18.04 ~ 6.25% and 12.15 ~ 9.37%. For pure GaN, our calculated value obtained by DFT + U matches with the works [41–43]. We interpreted decrease in dielectric constant value as we increase Cr concentrations into the host GaN. Dielectric variations are mostly observed in UV region but decreases in visible and near IR region. Decrease in dielectric constant may be explained by dipoles and applied electric field does not affect these dipoles [36, 44]. Moreover, polarizable bond breaking may be responsible for dielectric constant decrease and may be caused by addition of different Cr concentration into host GaN lattice.

We present graphs of conductivity of pure GaN and GaN doped with various Cr concentrations (3.12%, 6.25%, 9.37%) in figure 3(d). Conductivity is denoted by \(\sigma(\omega)\) and is mathematically realized using the formula [36],

\[
\sigma(\omega) = -\frac{i\omega}{4\pi} \varepsilon(\omega) - 1].
\]

Conductivity traits are obtained through DFT + U calculations using Wien2K code and for pure GaN, we note a steady increase after 2.3 eV which then attains \(\sigma_{\text{max}}\) at 7.1 eV and then after a decrease, shows another
hump at 7.72 eV [36, 37]. Conductivity traits of all Cr concentrations are different from each other because of interaction of Cr atoms with the N atoms as noticed in PDOS plots (figure 1). However, $\sigma_{\text{max}}$ for 3.12%, 6.25%, 9.37% Cr concentrations is achieved at 7.3 eV, 7.4 eV and 7.45 eV respectively. It is to note that well defined conductivity peaks are appearing in UV region and may arise because of interband transitions. Conductivity humps emerging in low energy region are due to quantum confinement effects [36]. Decrease in conductivity in certain regions may be the result of absorption decrease in those regions whereas peaks are the result of electromagnetical waves deep penetration inside material and causes increase in conductivity accordingly.

Extinction coefficient ($k$) is understood by light absorption in any material and may be calculated as [36],

$$k = \frac{\alpha \lambda}{4\pi}.$$  

Figure 4(a) manifest variations in $k$ of pure GaN and various Cr concentrations. $k$ variations have been recorded in energy range 0–8 eV and represent material behavior for various Cr concentrations by energy absorption on its surface. Plots presented in figure 4(a) are achieved by the solution of many-body wave function. At shorter wavelengths, absorption increases which exhibit that light appears to extinct quickly and therefore will have higher $k$ values. It is obvious from resemblance between plots presented in figures 3(a) and 4(a) as absorption ($\alpha$) and $k$ are interrelated. Similar extinction trends are noticed for three Cr concentrations where we achieve their maxima in low energy range (0–2 eV) while for pure GaN, $k$ trend is almost constant in the same energy range. Increase in $k$ along with increase in corresponding energy values is because of the result of quantum confinement effect which is connected to crystallite size variations. Extinction humps shifts to higher energies (lower wavelength) as Cr composition increases. In case of pure GaN, $k$ maxima is obtained at 7.8 eV which afterwards shows continuous decrease and becomes constant for rest of higher energy values. Extinction humps appearing in low energy region may be associated to quantum effects while their sudden rise is connected to photon energy increase. They may be related to the density of states which may found localized around Fermi level (as seen in figure 1) with effect of addition of impurity. Maximum extinction for three Cr concentrations is observed near IR and visible region while for pure GaN, it is noted in UV region. Maximum values of $k$ may be understood in term of impurities maximum attenuation and represent high cross section absorption. It may be reasoned as the absorption of light at defect side. $k$ value for pure GaN as obtained through experimental studies is 0.26 at energy value of 1.98 eV (626.1 nm) [36, 41]. $k$ values (0–0.77) obtained in our DFT + U study are higher than its experimental value. These values indicate higher absorption at higher wavelength (lower frequency) and represent material transparency to light. Hence, rise and fall in $k$ is with effect of variations in absorption at different energy values.

Variations in reflectivity of pure GaN and various Cr concentrations (3.12%, 6.25%, 9.37%) have been shown in figure 4(b). Reflectivity is denoted by $R(\omega)$ and may be evaluated by the formula [36],

$$R(\omega) = \frac{\sqrt{n(\omega)} + i\varepsilon_{2}(\omega)}{\sqrt{n(\omega)} + i\varepsilon_{2}(\omega) + 1}.$$  

Changes in reflectivity trends are plotted in energy range 0–8 eV and a careful analysis of all graphs manifest that reflectivity first increases and then decreases until reflectivity maxima is attained. In case of various Cr concentrations, major reflectivity peaks appears in low energy regions; 0–0.4 eV $\sim$ 3.12%, 0–0.9 eV $\sim$ 6.25% and 0–1.7 eV $\sim$ 9.37% which shows that reflectivity spectra are more pronounced in low energy (larger wavelength) region. For pure GaN, reflectivity increase take place in steps until get maxima at energy value of 7.8 eV ($\sim$159 nm) which significantly means that at this wavelength, pure GaN reflects all the light falling on it. Reflectivity of pure GaN have great deal of agreement with the works [36, 41]. Reflectivity maxima shifts to higher energy values (lower wavelength) upon increase in Cr concentrations but their reflectivity maxima are obtained at 0.05 eV $\sim$ 3.12%, 0.4 eV $\sim$ 6.25% and 0.7 eV $\sim$ 9.37%. Reflectivity maxima occur as a result of interband transitions from valence to conduction band and may be due to effect of collective oscillations of free electrons. In low energy regions, reflectivity is because of multiple reflections in the material and may be connected to fact that material shows transparency at lowest photonic energy values.

4. Conclusion

We calculated electronic and optical properties of Cr doped zincblende GaN by employing DFT + U in Wien2K code. Electronic properties are elaborated by examining plots of PDOS and TDOS where hybridization of Cr 3d and N 2p states is obvious with minor contribution of Ga s- and p-states. Repulsion of Cr 3d states to higher energies above valence band maxima occurs due to addition of dopant concentration and employing DFT + U. In comparison to pure GaN, blueshift in absorption spectra is observed along with increase in Cr concentrations. Refractive indices and dielectric constant found to decrease upon adding dopant contents into host GaN. Our study direct that Cr:GaN may be a good candidate for fabrication of optoelectronic, photonic and spintronic devices.
Acknowledgments

Authors would like to acknowledge department of physics, school of sciences and engineering, Lahore University of Management Sciences (LUMS) and National center for physics (NCP), Islamabad, Pakistan.

Funding

National Key (R&D) Program of China (2017YFB1002900), National Natural Science Foundation of China (NSFC) (61975014, 61575024) and the United Kingdom Government’s Newton fund.

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