Archive of SID

OPTICAL PROPERTIES OF INDIUM DOPED GaN

N. Arabhajji, T. Movlarooy*
Department of physics, Shahrood University of Technology, Shahrood, 361999516, Iran

Abstract- The optical properties of in doped GaN with different doping concentration, in zinc blende structure were calculated using density function theory with the plane-wave ultrasoft pseu-dopotential method. The influence of in doping on the optical properties of GaN were analyzed. The results show that the interactions among atoms are reduced, band gap decreases, and absorption spectra have red shift along with in doping concentration.

1. Introduction

Among the III-V semiconductors, the nitrides have attracted both scientific and technological interest in recent years due to their fascinating mechanical properties, such as hardness, high melting point, high thermal conductivity, and large bulk modules. These properties, as well as the wide band gaps, are closely related to their strong (ionic and covalent) bonding and smaller lattice constants. These materials can, therefore, be used for short-wavelength light-emitting diodes (LEDs), laser diodes, and optical detectors, as well as for high-temperature, high-power and high-frequency devices. The III-group nitrides can grow in cubic and hexagonal phases. Theoretical investigations of the lattice dynamics of these nitrides have been made by using a variety of methods, such as the valence-force model[1], the adiabatic bond-charge model[2], the rigid-ion model[3], and *ab initio* calculations with the frozen phonon approach[4,5], supercell approach[6], and linear-response approach[7,8], while *ab initio* calculations are computationally more extensive recently. In this work, we present an *ab initio* computation about optical properties of Indium doped GaN in the zinc-blende structure.

2. Theoretical method

We used the first-principle pseudopotential method based on the density function theory (DFT). The pseudopotentials for all atoms were generated according to the scheme of Troullier and Martins [9]. The Troullier and Martins procedure yielded soft-core pseudopotentials that greatly reduced the number of plane waves needed to achieve convergence in the calculated properties. DFT was implemented with a local density approximation (LDA). We first carried out full structural relaxation; next, response-function calculations were carried out in order to obtain first derivations of the occupied wave functions with respect to perturbations of the atomic displacements, uniform electric field and strain; then these first derivations were used to compute the elementary second derivative response-function tensors. In order to show clearly the energy-band structure we chose three high symmetry directions, and to perform accurate Brillouin zone integrations for bulk $In_xGa_{1-x}N$, we used a 4×4×4 *k*-point mesh.

3 Results and discussion

The photoelectric properties of optoelectronic materials in GaN are characterized mainly by the dielectric function, absorption coefficient and reflection coefficient. According to the definition of direct transition probability and Kramers–Kronig dispersion relation, the imaginary and real parts of the dielectric function, absorption coefficient, and reflection coefficient can be deduced. Consider the theoretical formula below [10–12]:

$$\varepsilon_2(\omega) = \frac{\pi}{\varepsilon_0}\left(\frac{e}{m\omega}\right)^2 \cdot \sum_{V,C}\left\{\int_{BZ}\frac{2dK}{(2\pi)^2}|a\cdot M_{V,C}|^2\delta[E_C(K)-E_V(K)-\hbar\omega]\right\} \quad (1)$$

$$\varepsilon_1(\omega) = 1 + \frac{2e}{\varepsilon_0 m^2}\cdot\sum_{V,C}\int_{BZ}\frac{2dK}{(2\pi)^2}\frac{|a\cdot M_{V,C}(K)|^2}{[E_C(K)-E_V(K)]/\hbar}\cdot\frac{1}{[E_C(K)-E_V(K)]^2/\hbar^2-\omega^2} \quad (2)$$

$$\alpha \equiv \frac{2\omega k}{c} = \frac{4\pi k}{\lambda_0} \quad (3)$$

$$R(\omega) = \frac{(n-1)^2+k^2}{(n+1)^2+k^2} \quad (4)$$

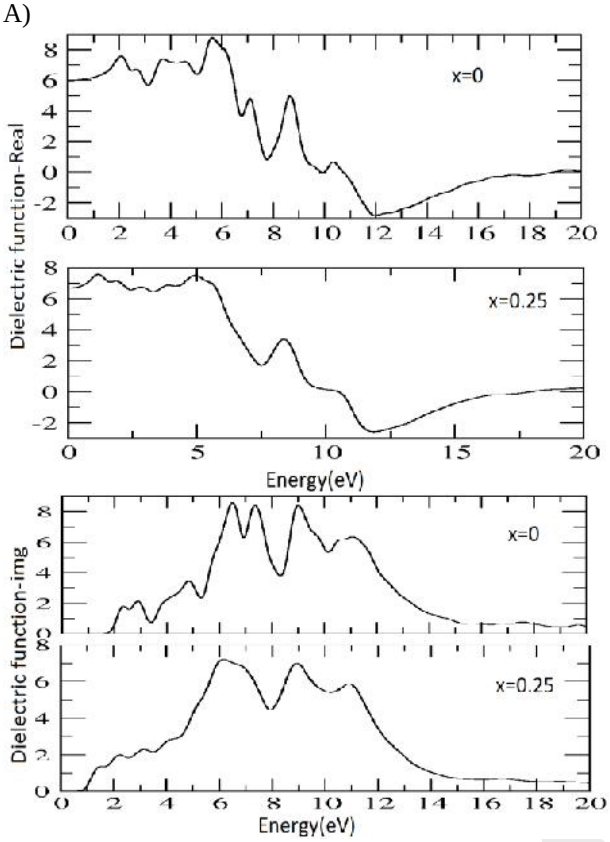
where $E_C(K)$ and $E_V(K)$ are the intrinsic energy levels of the conduction band and valence band, respectively; ω is the angular frequency; n is the refractive index; κ is the extinction coefficient;ε_0 is the vacuum dielectric constant; λ_0 is the wavelength of light in vacuum; C and V are the conduction band and valence band respec-tively; BZ is the first Brillouin zone; K is the electron wave vector; a is the unit direction vector of the vector potential A; and $M_{V,C}$ is the transition matrix element. The above formulae expound the mechanism of spectrum produced by electron transitions between crystal energy levels and provide a theoretical basis for analyzing the band structures and optical properties of crystal. Dielectric functions of $In_xGa_{1-x}N$ with x = 0 and x=0.25 are shown in Fig. 1. The peak intensity of dielectric function with x = 0 is slightly higher than that with x = 0.25, they are very close to each other. The main reason is that the polarizability strength of In–N is less than that of Ga–N because Ga radius is less than in radius.

* Corresponding author Email: tayebeh.movlarooy@yahoo.com

www.SID.ir

Archive of SID

A)



B)

Fig.1.Dielectric function.,A) The real part ,B) The imaginary part

The static dielectric functions are 6 and 6.92 with x = 0 and x = 0.25, respectively. There are seven peaks in imaginary part of dielectric functions of pure GaN corresponding to the photon energies. The imaginary part of dielectric functions of In0.25Ga0.75N has red shift compared with that of pure GaN.

Doping causes red shift of reflection peak, enhances reflection in visible light and infrared parts, but they all still below 0.2.

The absorption spectra are similar in variation trend before and after in doping. The absorption edge energies are 2 eV and 1.2 eV before and after in doping, respectively (Fig. 3), corresponding to the transitions between the top of valence band to the bottom of conduction band. Red shift of absorption edge occurs after In doping in agreement with the experimental results [13-17], corresponding to the shift of conduction band to lower energy and the band gap becoming smaller after In doping. The red shift expands the light response range of InGaN. The red shift of absorption edge is the key of photocatalys is of InGaN in visible light application. After In doping, the positions of absorption peak have red shift, and the values of absorption peak decrease, indicating that the interaction of in and N being weaker than that of Ga and N, utilization to lightbeing reduced.

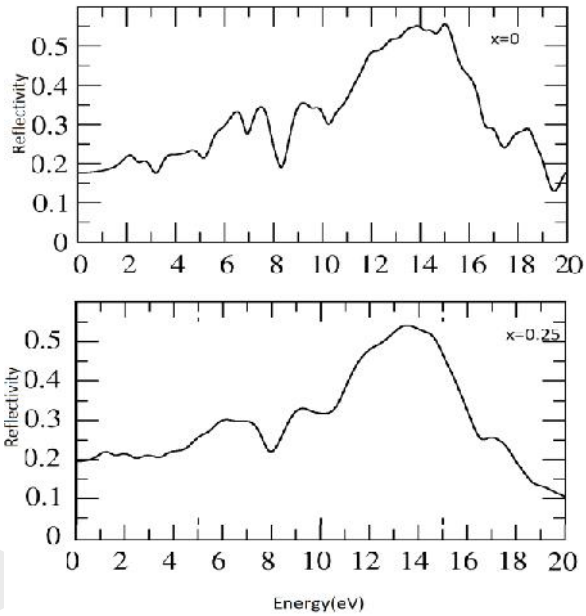


Fig.2. Reflectivity

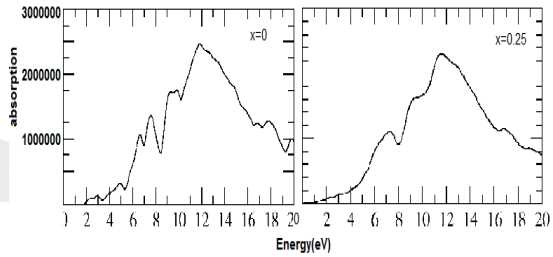


Fig.3.absorption spectra

4 Conclusions

Optical properties of InGaN compound are studied using the first principles. The results show that doping caused the conduction band move to low energy, valence band shrink, band gap be reduced and absorption spectrum have red shift.

5. References

[1] H. Siegle, G. Kaczmarczyk, L. Filippidis, et al, Phys Rev B. (1997).
[2] H.M. Tütüncü, G.P. Srivastava, Phys Rev B. (2000).
[3] V.Y. Davydov, Y. E Kitave, I.N Goncharuk, et al, Phys Rev B. (1998).
[4] D.R. Hamann, X.F. Wu, K.M. Rade, et al, PhysRev B. (2005).
[5] K. Shimada, T. Sota, K. Suzuki, J Appl Phys. 84 (1998).
[6] K. Parlinski, F. Bechstedt. Phys Rev B. (1999).
[7] A. Siegel, K. Parlinski, U.D. Wdowik. Phys Rev B. (2006).
[8] R. Miotto, A.C. Ferraz, G.P. Srivastava, Solid State Commun. (2000).
[9] N. Troullier, J.L. Martins, Phys Rev B. (1991).
[10] Y.J. Du, B.K. Chang, H.G. Wang, J.J. Zhang, M.S. Wang, Chin. Opt. Lett. 10 (2012) 051601.
[11] X.C. Shen, Science Press, Beijing. (2002).
[12] Q. Chen, Q. Xie, W.J. Yan, Sci. China G. 38 (2008) 825–833.
[13] D.Y. Zhang, X.H. Zheng, X.F. Li, Y.Y. Wu, H. Wang, J.F. Wang, H. Yang, Chin. Phys. B. 21 (2012) 087802.

www.SID.ir

Archive of SID

[14] Y.J. Du, B.K. Chang, J.J. Zhang, X.H. Wang, B. Li, M.S. Wang, Adv. Mater. Rapid Commun. 5 (2011) 1050–1055.
[15] Y.R. Wu, Y.Y. Lin, H.H. Huang, S. Jasprit, J. Appl. Phys.105 (2009) 013117.
[16] P.G. Moses, M. Miao, Q. Yan, C.G. J. Chem. Phys.134 (2011) 084703.
[17] V.Y. Davydov, A.A. Klochikhin, V.V. Emtsev, D.A. Kurdyukov, S.V. Ivanov, V.A.Vekshin, F. Bechstedt, J. Furthmüller, J. Aderhold, J. Graul, A.V. Mudryi, H.Harima, A. Hashimoto, A. Yamamoto, E.E. Haller, Phys. Status Solidi (b) 234 (2002) 787–795.

www.SID.ir