Optical properties of Zn doped GaAs single crystals

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The spectral distribution of the transmittance, T, and the reflectance, R, of Zn doped GaAs single crystals have been investigated. The optical constants "n" and "k" of GaAs:Zn are estimated in the wavelength range from 200 to 2500 nm. The type of electronic transition responsible for the optical absorption is direct allowed transition, with energy gap found to be 1.38 eV. Single scattering mechanism was detected for GaAs:Zn crystals which referred to the acoustical vibrations in the wavelength range 930 – 2500 nm. The free carrier concentration was calculated theoretical and found to be 0.737×10^{17} cm^{-3}. The dispersion parameters of GaAs:Zn single crystals were calculated in the normal dispersion region.

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1. Introduction

Gallium arsenide, GaAs, is widely used in the semiconductor industry due to its wider direct band gap energy and higher electron mobility compared to crystalline silicon [1]. These properties make this material very useful for infrared light emitting and laser diode manufacturing.

Optical characteristics of p-type GaAs is complicated due to the penetration of the Fermi level into the valence bands, providing contribution from heavy holes (hhs) as well as light holes (lhs) to the free-carrier plasma [2].

Impurity diffusion in semiconductors has technological importance in the fabrication of junction devices, semi-insulating compounds and high temperature growth of material [3]. GaAs can be doped with Zinc, in order to obtain a semi-insulating Gallium Arsenide (GaAs:Zn) substrate. Zn dopant in GaAs has a high diffusion coefficient and is easy to diffuse by annealing [4]. On the other hand, zinc diffusion is used as a processing technique for construction of electronic and opto-electronic devices [5]. Knowledge and control of Zn doping is necessary for development of device performance.

The present work investigates the optical properties of Zn doped GaAs single crystals via transmittance and reflectance measurements in the wavelength range from 200 to 2500 nm. The optical constants (n,k) of GaAs:Zn single crystals are determined. Also, the dispersion energy, E_d, the oscillation energy, E_{os}, and the free carrier absorption are calculated.

2. Experimental

Zn doped GaAs single crystals (Zn:GaAs) were supplied from spectra chemical industries. The samples have wafer shape and p-type conduction with carrier concentration from 1×10^{17} to 5×10^{17} cm^{-3} at room temperature as given by sample information. The sample have dimensions of 9 × 8.5 × 0.45 mm and has mirror-like plane parallel surfaces; hence, there was no need for mechanical polishing. The surfaces were cleaned from chemical impurities and contaminations with chromic acid before measurements.

For studying the optical properties of GaAs:Zn crystal; the transmission T (λ), at normal incidence, as well as the reflectance R (λ), at an incident angle of 5°, were measured in the spectral range 200-2500 nm using a double beam spectrophotometer (JASCO, V-570 UV-VIS-NIR), at room temperature.

3. Results and discussion

3.1-Spectral distribution of T(λ) and R(λ)

The spectral distribution of T (λ) and R (λ) of GaAs:Zn single crystals at room temperature, (for a sample of thickness 0.45 mm as a representative example) is shown in Fig. 1. As seen from the figure, at $\lambda > 1000$ nm, the transmittance of GaAs:Zn decreases gradually with the decrease of the photon energy of the incident light. This behaviour may be referred to the free carrier's absorption. While the spectral distribution of the reflectance of GaAs:Zn is characterized by a sharp structures at $\lambda < 1000$ nm, which associated with high energy transitions from the valence band to the conduction band, at energies 5.54, 3.74, 2.21 and 1.54 eV. At $\lambda >$ 1000 nm, the reflectance decreases by increasing the wavelength.

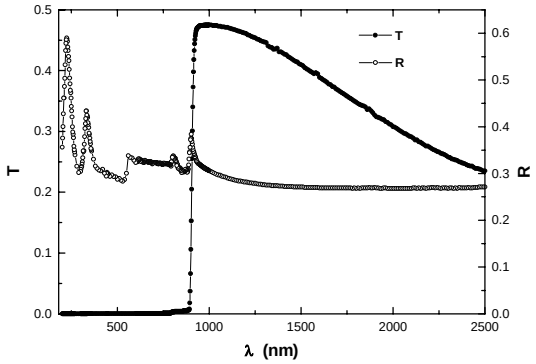

Fig. 1. The spectral distribution of transmittance, T, and reflectance, R, of GaAs:Zn single crystal.

3.2- Optical parameters

By knowing the transmission T (λ) and the reflection R (λ) at the same wavelength (λ), the absorption coefficient,α, of GaAs:Zn single crystals can be calculated by the following relation [6]:

$$\alpha = (1/d)\ \ln\ \{(1-R)^2/2T + [((1-R)^4/4T^2)+R^2]^{1/2}\} \quad (1)$$

where d is the sample thickness in cm. The dependence of the absorption coefficient, α, on the energy of the incident photons is shown in Fig. 2. As observed from the figure, the features of the behaviour of α versus hν can be attributed to free carrier absorption which decreases with the increase of the photon energy in the energy range from 0.49 to 1.34 eV, then followed by an increase due to interband transition of electron from the valence to the conduction band.

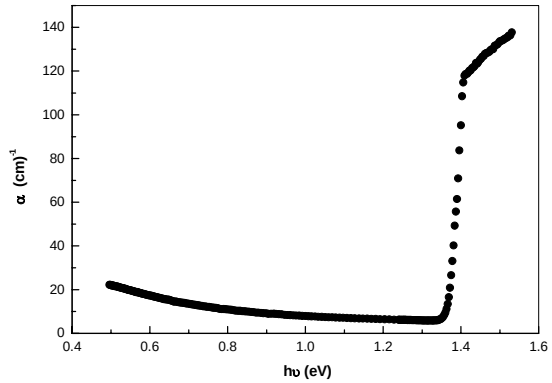

Fig. 2. The spectral distribution of absorption coefficient, α, of GaAs:Zn single crystal.

The variation in the absorption coefficient is related to the photon energy (hν) for inter-band transition by the following relation [7]:

$$(\alpha h\nu) = A\ (h\nu - E_g)^r \quad (2)$$

where À is a constant, h is the planck′s constant, E_g is the energy band gap and r is a parameter takes the values : 1/2 , 2 , 3/2 and 3 which related to allowed direct , allowed indirect, forbidden direct and forbidden indirect optical transitions, respectively. Therefore, the dependence of $(\alpha h\nu)^{1/r}$ on energy (hν) of GaAs:Zn single crystal was checked. The best plot was obtained for r = 1/2, as shown in Fig. 3, which represents an allowed direct transition. Extrapolating the linear part of the figure towards lower photon energies, the point of interception with the hν axis exists at $(\alpha h\nu)^2 = 0$ giving the corresponding direct energy band gap. The obtained value is 1.38 eV. This value of E_g is smaller than that obtained for pure GaAs crystal (E_g = 1.42 eV) [1], this may be attributed to the doping of Zn atoms in GaAs single crystal, where the doping of Zn atoms increases the ionic bonds as commonly observed for all the III-V compounds [8].

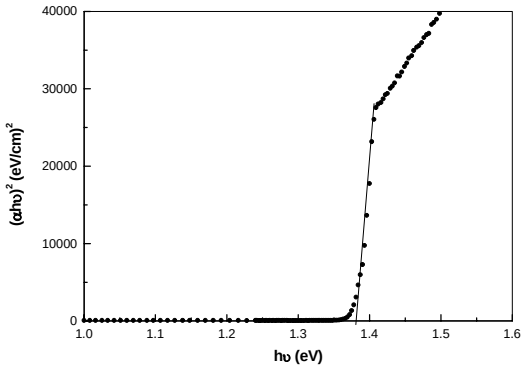

Fig. 3. Plot of $(\alpha h\nu)^2$ against $(h\nu)$ for GaAs:Zn single crystal.

Absorption due free carriers is commonly written as $\alpha \propto \lambda^P$, where the index *P* depends primarily on the scattering mechanism and the free carrier concentration. In the case of lattice scattering one must consider scattering by acoustic and optical vibrations as well as impurity ions. For scattering by acoustic vibrations $P \approx 1.5$, for optical vibrations $P \approx 2.5$, and for impurity ions $P \approx 3.5$. The observed free carrier absorption coefficient will then have all the three contributions [9]:

$$\alpha = A_{\text{acoustic}}\ \lambda^{1.5} + B_{\text{optical}}\ \lambda^{2.5} + C_{\text{impurity}}\ \lambda^{3.5} \quad (3)$$

To know the scattering mechanism that may exist in GaAs:Zn crystal, log α is plotted as a function of log λ, as shown in Fig. 4. This relation yields single distinct linear part, exists in the wavelength range 930-2500 nm, where α

was found to be proportional to $\lambda^{1.4}$. Accordingly the dominant scattering mechanism is occurred by acoustical vibrations.

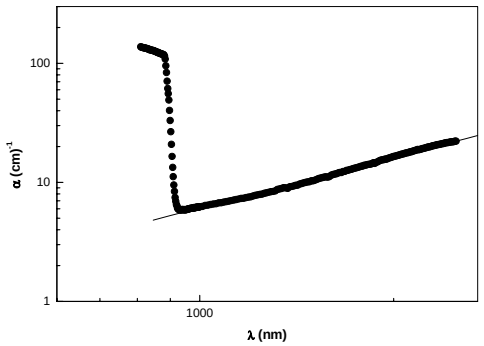

Fig. 4. Plot of ln α versus ln λ.

The classical formula for free carrier absorption coefficient,α , [10] can be written as:

$$\alpha.n = (N_f e^3/4\pi^2\varepsilon_o c^3 \mu m^{*2})\, \lambda^2 \qquad (4)$$

where n is the refractive index, N_f is the carrier concentration, e is the electron charge, c is the light speed, ε_o is the free-space permittivity, μ is the mobility of charge carriers and m^* is the effective mass of free carriers. Fig. 5 shows the variation of α.n with λ^2. Knowing the slope of the straight line in Fig. 5 and the values of the constants μ and m^* (μ= 460 cm^2/Vs and $m^*/m_o = 0.5$) [11], the carrier concentration value can be calculated. The value of N_f was calculated and found to be 0.737×10^{17} cm^{-3} which is comparable with the sample data.

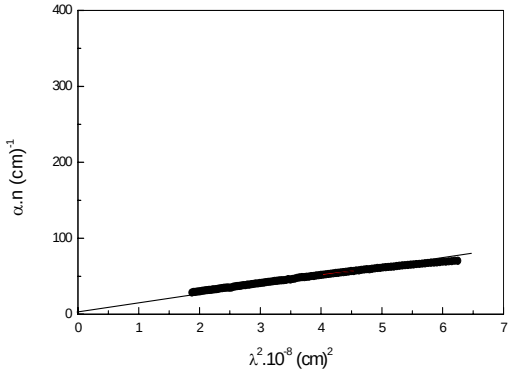

Fig. 5. The relation between (α.n) and λ^2 for GaAs:Zn single crystal.

The spectral distribution of the refractive index, n, can be determined by knowing the values of the reflectance, R, and the absorption index, k, at the same wavelength, for different wavelengths by the following equation [12]:

$$n = [\,(1+R)/(1-R)\,] + [(4R/(1-R)^2) - k^2]^{1/2} \qquad (5)$$

where $k = \alpha\lambda/4\pi$. The spectral dependence of (n) of GaAs:Zn single crystal is shown in Fig. 6. As shown from the figure, the spectrum of n is characterized by sharp structure due to valence to conduction bands transitions with energies E_g, E_0, E_1, E'_0 and E_2. Their values are tabulated in Table 1. The values of peak positions agree with the band structure of GaAs single crystal.

Table 1. Interband transition corresponding to peak positions in the absorption index spectrum for GaAs:Zn single crystal.

Parameters	*E_0 (eV)*	*E_1 (eV)*	*E'_0 (eV)*	E_2 (eV)
Transitions[13]	Γ_{15v}-Γ_{1c}	Λ_3-Λ_1	Γ_{15v}-Γ_{15c}	X_{5v}-X_{1c}
GaAs:Zn	1.54	2.21	3.74	5.54
GaAs	1.55[13]	2.99[13]	4.2[13]	5.12[13]
	1.43[14]	2.92[14]	3.14[14]	4.96[14]
	1.51[15]	3.16[15]	3.38[15]	4.83[15]

The single oscillator model can be applied in the region of normal dispersion for the spectral distribution of the refractive index at $h\nu < 1.24$ eV ($\lambda > 1000$ nm). The refractive index (n) can be expressed as a function of the wavelength (λ) by the following equation [16]:

$$n^2 = \varepsilon_L - (e^2/\pi c^2)\,(N/m^*)\,\lambda^2 \qquad (6)$$

where ε_L is the lattice dielectric constant and N/m* is the ratio of carrier concentration to its effective mass. Fig. 7 shows the dependence of n^2 as a function of λ^2 for GaAs:Zn. The value of ε_L can be determined by extrapolating the linear part in Fig. 7 towards short wavelengths. The point of interception with the ordinate at $\lambda^2 = 0$ yield the value of ε_L which is found to be 11.62. The value N/m* was calculated from the slope of the linear part of the graph (Fig.7) and found to be 3.18×10^{47} $cm^{-3}gm^{-1}$.

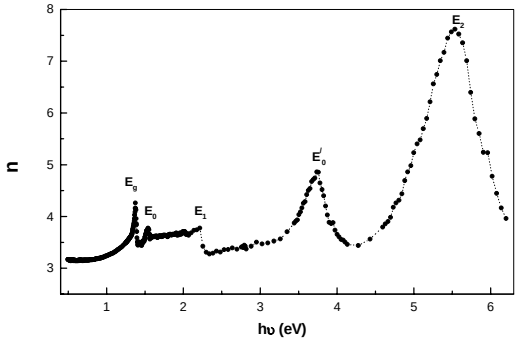

Fig. 6. The spectral behaviour of the refractive index, n, of GaAs:Zn single crystal as a function in (hν).

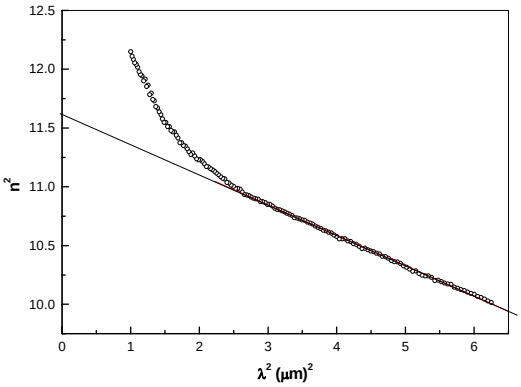

Fig. 7. The variation of n^2 against λ^2 for GaAs:Zn single crystal.

The energy dependence of the refractive index for GaAs:Zn single crystal can be expressed by using Wemple and DiDomenico relation [17] as:

$$(n^2\text{-}1)^{-1} = (E_{os} / E_d) - (1/ E_{os} E_d) (h\nu)^2 \qquad (7)$$

where E_{os} is the oscillator energy and E_d is the dispersion energy. The values of E_{os} and E_d can be determined by plotting a relation between $(n^2\text{-}1)^{-1}$ and $(h\nu)^2$ as shown in Fig. 8. From the slope and the intercept of the extrapolated straight line, the values of E_{os} and E_d were calculated and found to be 3.26 eV and 30.66, respectively.

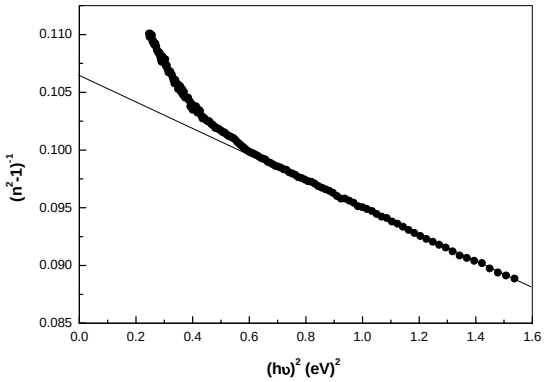

Fig. 8. The variation of $(n^2\text{-}1)^{-1}$ against $(h\nu)^2$ for GaAs:Zn single crystal.

The dielectric constant at infinite frequency, ε_∞, can also be determined from the dispersion relation (eq. 7), by extrapolation of the linear part, in Fig. 8 in the direction of ordinate axis at $(h\upsilon)^2 = 0$. The obtained dispersion parameters for GaAs:Zn single crystal are tabulated in Table 2.

Table 2. The calculated values of dispersion parameters of GaAs:Zn single crystal.

Parameters	ε_L	ε_∞	E_{os} (eV)	E_d (eV)	N/m* ($cm^{-3}gm^{-1}$)
GaAs:Zn	11.62	10.40	3.26	30.66	3.18×10^{47}

The dispersion energy is a measure of the strength of interband optical transitions and it was found to obey the simple empirical relationship [18]:

$$E_d = \beta N_c Z_a N_e \qquad (8)$$

where N_c is the co-ordination number of the cation nearest neighbour to the anion, Z_a is the formula chemical valence of the anion, N_e is the effective number of valence electrons per anion and β is a parameter between 0.26 ± 0.04 eV for ionic materials and 0.37 ± 0.05 eV for covalent materials. In the present investigation, the value of β can be determined using the calculated value of E_d (30.66 eV) and the values of $N_c = 4$, $Z_a = 3$, $N_e = 8$ [19]. The value of β was calculated and found to be 0.32 eV, which agrees with the value of 0.37 ± 0.05 eV for covalent materials.

4.Conclusions

The transmittance and reflectance of GaAs:Zn single crystals were measured in the spectral range 200-2500 nm. The optical constants "n and k" were determined. The spectral distribution of the reflectance, R, and the refractive index, n, show a sharp structure due to valence to conduction bands transitions. The investigation of optical properties of GaAs:Zn single crystal showed that GaAs:Zn single crystals exhibit direct allowed optical transition. The value of the optical band gap deceases by the zinc doping. Single scattering mechanism was detected for GaAs:Zn crystals which referred to the acoustical vibrations in the wavelength range 930-2500 nm. Theoretical calculation of free carrier concentration gave the value 0.737×10^{17} cm^{-3}. The dispersion energy, E_d, and the single oscillator energy, E_{os}, for GaAs:Zn single crystals were also calculated.

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