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# Optical constants and dispersion energy parameters of gallium phosphide

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UV-Vis-NIR spectrophotometer was used to study the optical constants and dispersion energy parameters of gallium phosphide (GaP) single crystal wafer grown by liquid- encapsulated Czochralski. The optical band gap of GaP was determined using band to band transition theory and was found to be 2.32 eV. The refractive index was evaluated from reflectance spectra and its value lies in the range 1.3 to 2.1 corresponding to the photon energy 1.5 to 5 eV. The dispersion energy and oscillator energy values of the GaP were determined using single oscillator model and their values are found to be 14.26 eV and 3.61 eV, respectively. The relation between optical band gap and oscillator energy was found to be $E_o \approx 1.55 x E_g$. Further, real and imaginary dielectric constants were plotted and the peak shows the photo transition process with electromagnetic interaction inside material.

*Keywords: GaP semi-insulating, optical constants, Single oscillator model*

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## 1. Introduction

The knowledge about the optical parameters of semiconductor is very important to be used as optoelectronic devices. Among various III–V based binary, ternary and quaternary semiconductors, GaP ($E_g$ =2.25 eV at 300 K) is widely used for the fabrication of optoelectronic devices [1–2]. Furthermore, GaP is well studied material of interest for microelectronic devices of high-temperature electronics as a wide-gap semiconductor that can be obtained in the form of single crystals or as epitaxial layers [3]. From the fundamental and a technological viewpoint, the determination of optical parameters of the semiconductor materials are very important for their optical applications. Furthermore, knowing the changes in refractive index are important for controlling optical properties of semiconductors, because optical properties are directly related to their structural and electronic properties.

The purpose of this study is to investigate the optical properties and determine optical constants of the semi-insulating GaP by optical characterization method.

## 2. Experimental details

n-type semi-insulating gallium phosphide single crystal wafer grown by liquid- encapsulated Czochralski (LEC) was purchased from Sigma Aldrich company. The crystal structure, conductivity type, carrier concentration of the GaP are cubic (a = 5.4505Å), Undoped (N-type semiconductor), 2-6 × $10^{16}$ $cm^{-3}$, respectively. The diffuse reflectance, transmittance, and absorbance spectra of the GaP were measured in the 200–800 nm wavelength range using an integrating sphere for the SHIMADZU UV-VIS-NIR 3600 spectrophotometer. Barium sulfonate $BaSO_4$ was used as reference to provide a nominal 100% reflectance measurement.

## 3. Results and discussion

Fig. 1 shows the transmittance spectra of semi-insulating Gallium phosphide (n-type GaP) grown by LEC method growth by liquid- encapsulated Czochralsk. The transmittance spectra show an absorption edge near 550 nm.

The optical bandgap of GaP was obtained by taking the derivation of transmittance.

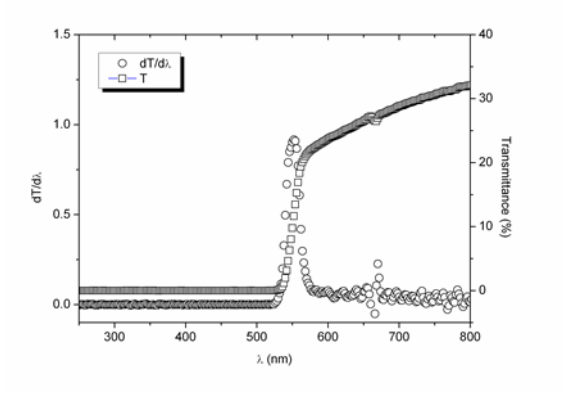


***Fig.1:*** *Transmittance and derivate spectra of n-type semi-insulating gallium phosphide*

The maximum peak position corresponds to optical band edge. The optical band gap was found to be 2.25 eV. The band structure of the n-GaP semiconductor obeys either direct or indirect transitions. Dixit et al. [4] could not separate out indirect band gap transition from direct transition. In present investigation an attempt has been made to separate out indirect bandgap absorption from direct bandgap. The optical gap of the GaP can be determined using band-to-band transitions theory [5]

$$\alpha h\nu = A(h\nu - E_g)^m \qquad (1)$$

where A is an energy-independent constant and $E_g$ is the optical band gap. This equation can be also written as [5-6],

$$\frac{d[\ln(\alpha h\nu)]}{d[h\nu]} = \frac{m}{h\nu - E_g} \qquad (2)$$

The type of optical transition can be determined finding the value of m. The d{ln*(αhν)*}/d*(hν)* versus *hν* was plotted in order to obtain m value, and the figure shows a peak and the

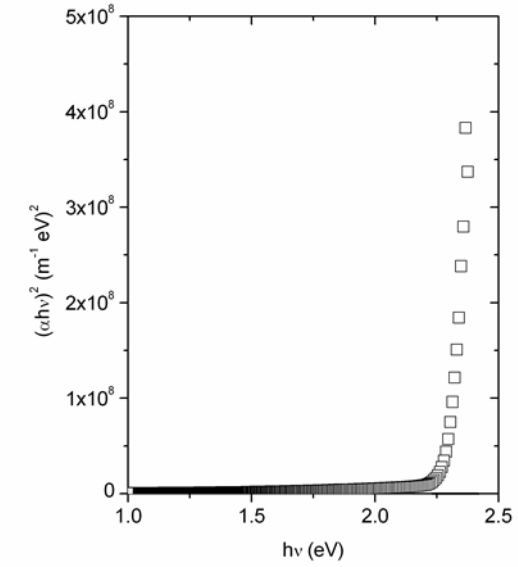


***Fig.2:*** *Plot of $(\alpha h\nu)^2$ v.s hν of n-type semi-insulating gallium.*

maximum value of the peak gives us optical band gap value, $E_g$ approximately. The curve of *ln(αhν) vs. ln(hν-$E_g$)* was plotted using the obtained $E_g$ value to determine m value and it was found to be about 1/2 from the slope of plotted curve. Thus, the relation for the obtained optical transition type is given by,

$$\alpha h\nu = A(h\nu - E_g)^{1/2} \qquad (3)$$

where $E_g$ is the optical band gap. A is an energy-independent constant given by,

$$A = \left[\left(\frac{e^2}{nch^2 m_e^*}\right)\right]\left(2\mu^*\right)^{3/2} \qquad (4)$$

here $m^*$ is the reduced electron and hole effective mass, e is the electronic charge, c is the velocity of light, h is the Planck constant and n is the refractive index. The plot of $(\alpha h\nu)^2$ v.s *hν* is shown in Fig. 2 and this plot shows a straight line. $E_g$ value was calculated from the intercept of this straight line and was found to be $E_g$=2.32 eV. The optical band gap of the n-type semi-insulating GaP is higher than semiconductor GaP ($E_g$=2.25) [7-11].

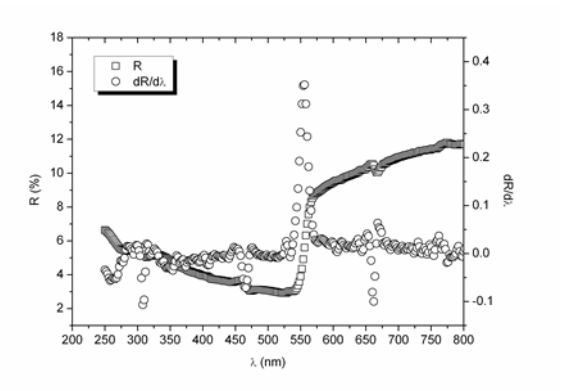


***Fig.3:*** *Reflectance and derivate spectra of n-type semi-insulating gallium phosphide*

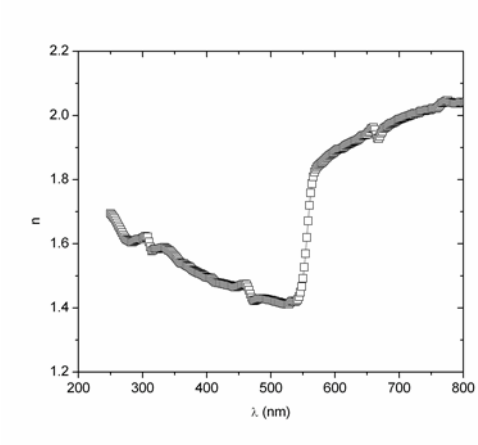


***Fig. 4:*** *The refractive index dispersion curve of n-type semi-insulating gallium phosphide.*

*3.2. Refractive index dispersion and optical constants of n-type semi-insulating GaP*

Fig. 3 shows a plot of reflectance (R) and derivate dR/dλ as a function of wavelength. spectra of n-GaP. Fig.3 reveals that, the reflectance decreases with the increase in wavelength up to 550 nm and then increases. The maximum peak position in dR/dλ vs λ plots corresponds to the optical band edge. In present investigation we make use the reflectance spectra to determine the refractive index of GaP using the following relation:

$$n(\lambda) = \frac{(1+R(\lambda)) + \sqrt{4R(\lambda) - (1-R(\lambda))^2 k(\lambda)^2}}{1-R(\lambda)} \qquad (5)$$

where k is the extinction coefficient (k=α λ /4π). The dependence of refractive index on the wavelength is shown in Fig. 4. The refractive index in the visible region is found to be 1.6.

The refractive index dispersion plays an important role in the optical communication and designing of optical devices. So it is important to determine dispersion parameters. The dispersion parameters can be determined using the relation given below [13]:

$$n^2 = 1 + \frac{E_d E_o}{E_o^2 - (h\nu)^2} \qquad (6)$$

where *n* is the refractive index, *h* is Planck's constant, *v* is the frequency, *hv* is the photon energy, $E_o$ is the single oscillator energy for electronic transitions and $E_d$ is the dispersion energy, which is a measure of the strength of interband optical transitions. These parameters can be easily obtained by plotting of $1/n^2$-1 *vs* $(hv)^2$ (Fig. 5). The $E_o$ and $E_d$ values were determined from the slope $(E_dE_o)^{-1}$ and intercept $(E_o/E_d)$ on the vertical axis which were found to be 14.26 eV and 3.61 eV, respectively. The relation between optical band gap and oscillator energy is $E_o$=D$E_g$, here D is a constant. For the GaP, this relation was found to be $E_o \approx 1.55 x E_g$.

The obtained D value is in agreement with the value which is valid for the lowest direct band gap (D=1.5). This confirms that the direct optical transitions are formed in the GaP.

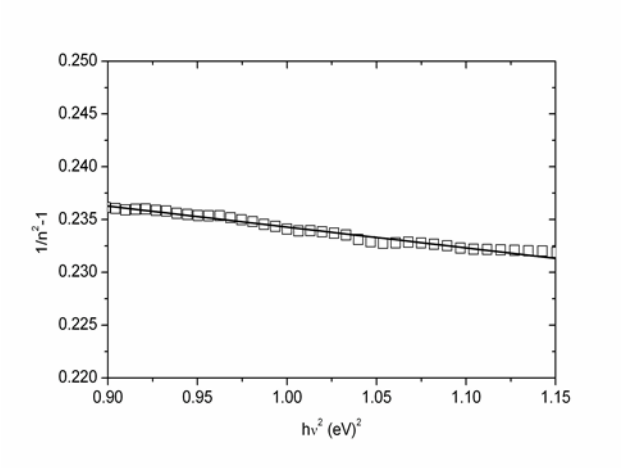


***Fig.5:*** *Plot of $1/n^2$-1 vs $(h\nu)^2$ of n-type semi-insulating gallium phosphide.*

Also, the refractive index dependence on wavelength is expressed by the following dispersion relation [5,13],

$$n^2 - 1 = \frac{S_o \lambda_o^2}{1 - (\lambda_o / \lambda)^2} \qquad (8)$$

where $\lambda$ is the wavelength of incident light. $S_o$ is the average oscillator strength and $\lambda_o$ is an average oscillator wavelength. Eq. 8 also can be transformed

$$\frac{n_\infty^2 - 1}{n^2 - 1} = 1 - \left(\frac{\lambda_o}{\lambda}\right)^2 \qquad (9)$$

The parameters, $n_\infty$, $\lambda_o$ and $S_o$ values were determined from the slope and intercept of $(n^2\text{-}1)^{-1}$ vs $\lambda^{-2}$ curves plotted and 2.22, 344.04 nm and $1.33 \times 10^{13}$ ($m^{-2}$), respectively. $M_{-1}$ and $M_{-3}$ moments of the optical spectrum can be obtained from the following relations [14]:

$$E_o^2 = \frac{M_{-1}}{M_{-3}} \qquad E_d^2 = \frac{M_{-1}^3}{M_{-3}} \qquad (10)$$

The $M_{-1}$ and $M_{-3}$ values were calculated using these relations and were found to be 3.95 and 0.30 ($eV^{-2}$).

The second method we use is single oscillator Forouhi-Bloomer model [15]. In this method, the refractive index and extinction coefficient constants can be expressed by the following relations,

$$n = n_\infty + \frac{B_o E + C_o}{E^2 - BE + C} \qquad (11)$$

and

$$k = \frac{A(E - E_g)^2}{E^2 - BE + C} \qquad (12)$$

where $B_o$, $C_o$, A, B, C are constants, E is the photon energy and $E_g$ is the optical band gap.

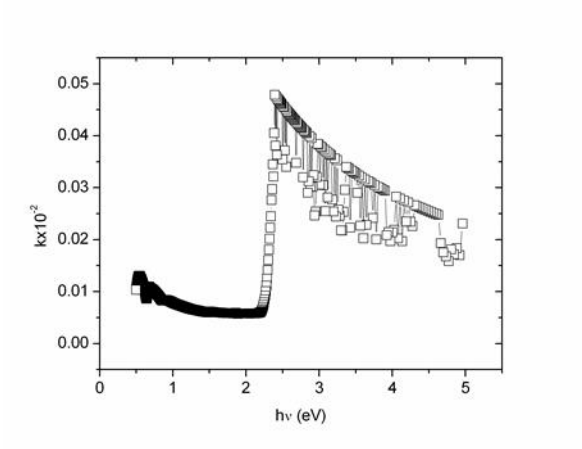


***Fig.5****: The extinction coefficient curve of n-type semi-insulating gallium.*

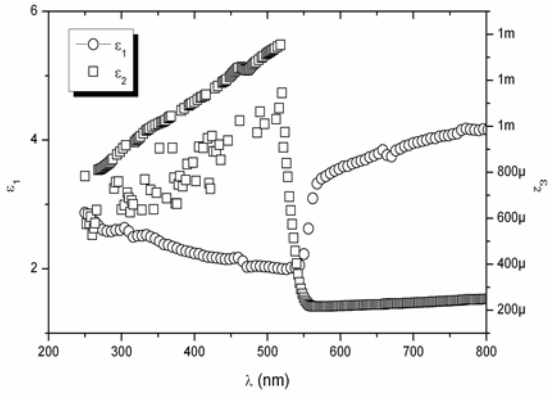


***Fig.6:*** *Variation of the real and imaginary parts of the complex dielectric constant with wavelength of n-type semi-insulating gallium..*

The plot of extinction coefficient for the GaP is shown in Fig. 6 and as seen in Fig.6, the extinction coefficient spectra of the GaP wafer indicate a minimum point corresponding to optical band gap. The optical band gap was determined from Fig.6 and was found to be 2.30 eV. The obtained optical band gap is in agreement with the optical band gap obtained from Eq.3. The fundamental electron excitation spectra of GaP was described by the means of frequency dependent of the complex dielectric constant which is expressed as,

$$\varepsilon^* = \varepsilon_1 + i\varepsilon_2 \qquad (13)$$

where $\epsilon_1$ is the real part and $\epsilon_2$ is the imaginary of the dielectric constant. $\epsilon_1$ and $\epsilon_2$ values were determined by the following relations [16-17],

$$\varepsilon_1 = n^2 - k^2 \quad (14)$$

and

$$\varepsilon_2 = 2nk \quad (15)$$

**Fig. 7** shows the real and imaginary parts dependence on photon energy. $\epsilon_1$ and $\epsilon_2$ values change with the photon energy. The plot of $\epsilon_2$ gives a peak reflecting the overall band structure information. The presence of this peak is due to photoexcitation process, in which the electrons are excited from valence band to conduction band. The dissipation factor (tan $\delta$) which is a measure of loss-rate of power of a mechanical mode is expressed by the following relation,

$$\tan\delta = \frac{2nk}{n^2 - k^2} \quad (16)$$

The plot of tanδ vs. h$\nu$ for the GaP is shown in Fig.8. The tanδ value has the highest value in the band edge. The dissipation factor is attributed to the electric power losing in GaP wafer.

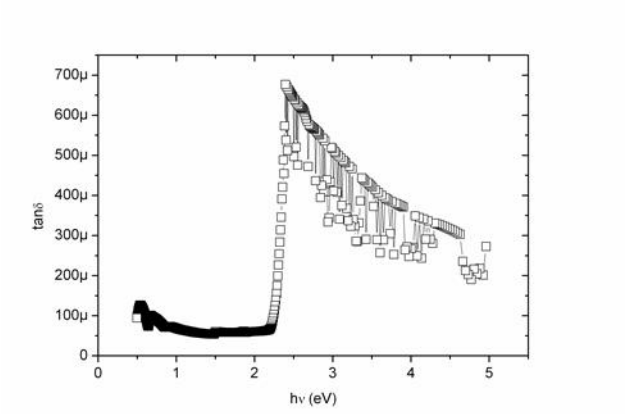


***Fig.8:*** *Plot of tanδ vs. hν for n-type semi-insulating gallium phosphide I-V characteristics of silicon and GO deposited silicon solar cells.*

## Conclusions

The optical properties of semi-insulating GaP have been investigated. The optical constants and optical band gap of the GaP were determined. The refractive index has values of 1.3-2.1 at the energy range of 1.5-5 eV. Optical band gap, $E_g$, dispersion energy and oscillator energy values of the film were determined to be 2.32 eV, 14.26 eV and 3.61 eV, respectively. The relation between optical band gap and oscillator energy was found to be $E_o \approx 1.55 x E_g$.

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