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OPTICAL PROPERTIES OF GALLIUM PHOSPHIDE (GaP)

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ABSTRACT

Optical properties of Gallium Phosphide (GaP) have been investigated by means of Kramers Kronig method. Optical properties such as refractive index, extinction coefficient, dielectric constant, transmittance, absorption coefficient, reflectance, reflection coefficient and optical conductivity are presented in the energy range 1.03 – 6.01eV. The calculated optical properties of GaP indicate promising device applications such as the design of optoelectronic devices, electronic and photonic devices.

Key words: Complex Index of Refraction, Complex Dielectric Constant, Transmittance, Absorption Coefficient, Reflection Coefficient, Reflectance, Optical Conductivity, Semiconductor

INTRODUCTION

Wide–band–gap semiconductors have attracted a great deal of attention due to their strong potentials in light emitting diodes (LEDs) operating in the blue-to-ultraviolet region. Gallium Phosphide GaP is a popular semiconductor material and considered to be a wide-band-gap semiconductor, making it a good candidate for room-temperature device applications. GaP has potential for ultraviolet, blue and blue-green detection applications from 250nm to 500nm (Beck *et al*, 2002; Liu *et al*, 2002; Zhang *et al*, 2008).

GaP is among group III-V compounds which has been extensively developed for applications to optical devices, LEDs, and photo cells. It has been found to be important for light emission devices in visible range (Hatami *et al*, 2006) and is one of the most promising materials for development of solar cells (Epstein and Grove, 1965). GaP and related compounds are important semiconductor materials that are used in a variety of optoelectronic devices (Kish *et al*, 1994, Hofler *et al*, 1998). In this work, optical properties of Gallium Phosphide (GaP) have been investigated in the photon energy range 1.03–6.01eV.

METHOD OF CALCULATION

Kramers-Kronig analysis of measured data obtained by Schubert (Schubert, 2004) was used to obtain the optical properties of the material in the study. The Reflection Coefficient which measures the fractional amplitude of the reflected electromagnetic field is given by (Fox, 2001)

$$r(\omega)=\frac{n(\omega)-1+ik(\omega)}{n(\omega)+1+ik(\omega)} \tag{1}$$

where n is the refractive index and k is the extinction coefficient.

Kramers-Kronig relations is a mathematical model that describe the existence of a fundamental connection between the real and imaginary part of the complex optical functions descriptive of the light-matter interaction phenomena, such as the dielectric function or the index of refraction. The real and imaginary parts, which describe dispersive and absorptive phenomena, respectively, are not wholly independent, but are connected by a special form of the Hilbert transform, which are termed Kramers-Kronig relations. Kramers-Kronig analysis allows one to calculate the energy dependence of both real and imaginary parts of a specimen's light optical permittivity, together with other optical properties such as the absorption coefficient and reflectivity. Because of Kramers-Kronig relation, the energy dependence of the real part of the refractive index is related to the material absorption, described by the imaginary part of the refractive index (also called the extinction coefficient).

The Reflectance (R) is given by (Yu and Cardona, 1996)

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

$$E_1=n^2-k^2 \quad (3)$$

$$E_2=2nk \quad (4)$$

The absorption coefficient (α) can be calculated using the equation (Pankove**,** 1971, Swanepoel, 1983)

$$\alpha=\frac{4\pi k}{\lambda} \quad (5)$$

where k is the extinction coefficient and λ is the wavelength.

The transmittance is obtained from the relation

$$R + T + A = 1 \quad (6)$$

where R, T and A represent the reflectance, transmittance and absorbance respectively. The sum of these macroscopic quantities must equal unity since the incident radiant flux at one wavelength is distributed totally between reflected, transmitted and absorbed intensity. The absorbance (A) is given by

$$A=\log\left(\frac{1}{R}\right) \quad (7)$$

The optical response of a material can be studied in terms of the optical conductivity (σ) which is given by the relation (Sharma and Katyal, 2007)

$$\sigma=\frac{\alpha nc}{4\pi} \quad (8)$$

where c is the velocity of light, α is the absorption coefficient and n is the refractive index. It can be seen clearly that the optical conductivity directly depends on the absorption coefficient and the refractive index of the material.

RESULTS AND DISCUSSION

The refractive index spectrum of GaP in the energy range 1.03eV to 6.01eV is as shown in Figure 1. There is an increase in the refractive index in the energy range 1.20eV to

3.65eV, with a peak value of 5.50 at 3.65eV as shown in Figure 1.

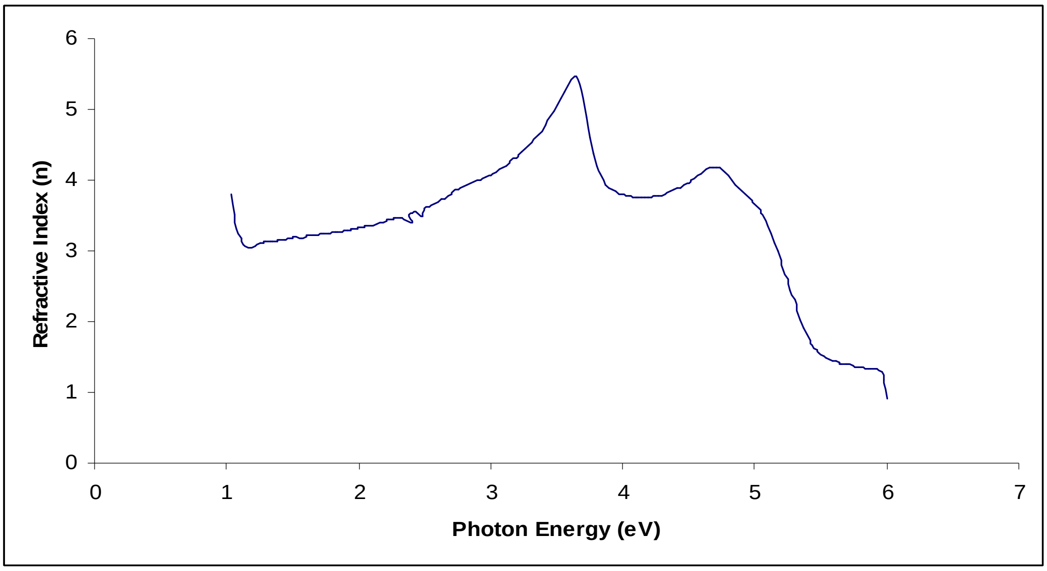

Figure 1: Refractive Index of Gallium Phosphide (GaP)

The refractive index decreases afterwards in the energy range 3.65–6.01eV. This decrease in refractive index indicates that GaP shows normal dispersion behaviour. Our result for refractive index is higher than that reported by Nelson and Turner (3.44) (Nelson and Turner, 1968) and Matsumoto and Kumabe (3.62 and 4.5) (Matsumoto and Kumabe, 1979) this difference is suspected to have come from the experimental procedures taken in the other works. Two peaks are observed at 3.65eV and 4.80eV, they are mainly due to Γ transition (Zhang et al 2011).

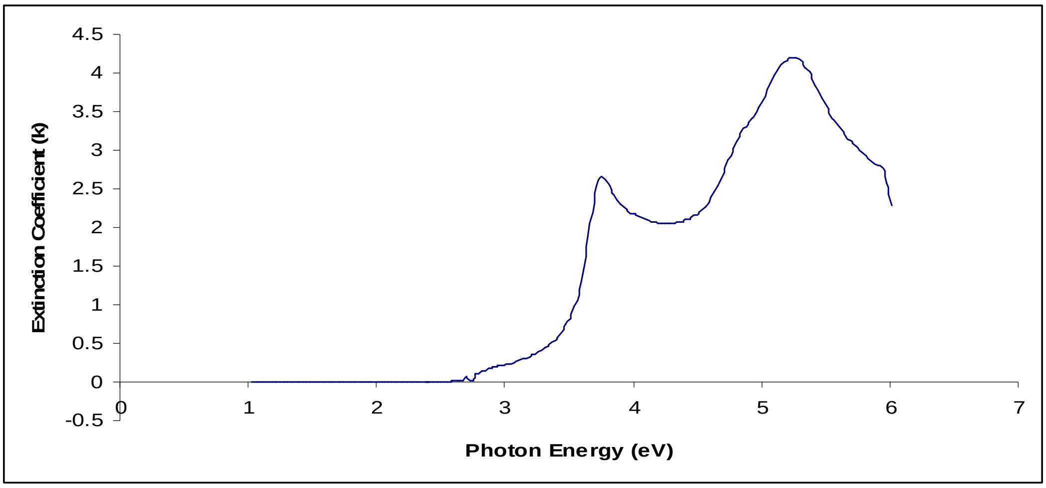

Figure 2: Extinction Coefficient of Gallium Phosphide (GaP)

The extinction coefficient spectrum in the energy range 1.03eV-6.01eV is as shown in Figure 2. There is an increase in extinction coefficient in the energy range 2.7 – 5.7eV as shown in figure 2. It has a peak value of 4.2 at 5.27eV and then decreases to a value of 2.3 at 6.01eV. The increase in extinction coefficient with increase in photon energy in the energy range 2.7 – 5.7eV shows that the fraction of light lost due to scattering and absorbance increases in this energy range and the decrease in the extinction coefficient in the photon energy range 5.7 – 6.01eV shows that the fraction of light lost due to scattering and absorbance decreases in this energy region. The extinction coefficient is zero in the photon energy range 1.03 – 2.7eV which means that GaP is transparent in this energy region. The peak value of extinction coefficient indicates a good absorption in the energy range. Two peaks are observed at 3.8 and 5.27eV, they are mainly due to Γ transition (Zhang et al; 2011).

Figure 3 shows the dielectric constant of GaP. There is an increase in the real part of the dielectric constant of GaP in the energy range 1.1 – 3.61eV as shown in Figure 3. It peaks at a value of 27.4 at 3.61eV. The increase in dielectric constant with increase in photon energy in the photon energy range 1.1 – 3.61eV shows that the loss factor increases with increase in photon energy in this energy range. The real part of the dielectric constant then decreases with increase in photon energy in the photon energy range 3.61 – 6.01eV with a minimum value of -12.5 at 5.34eV. This shows that the loss factor decreases with increase in photon energy in this energy range.

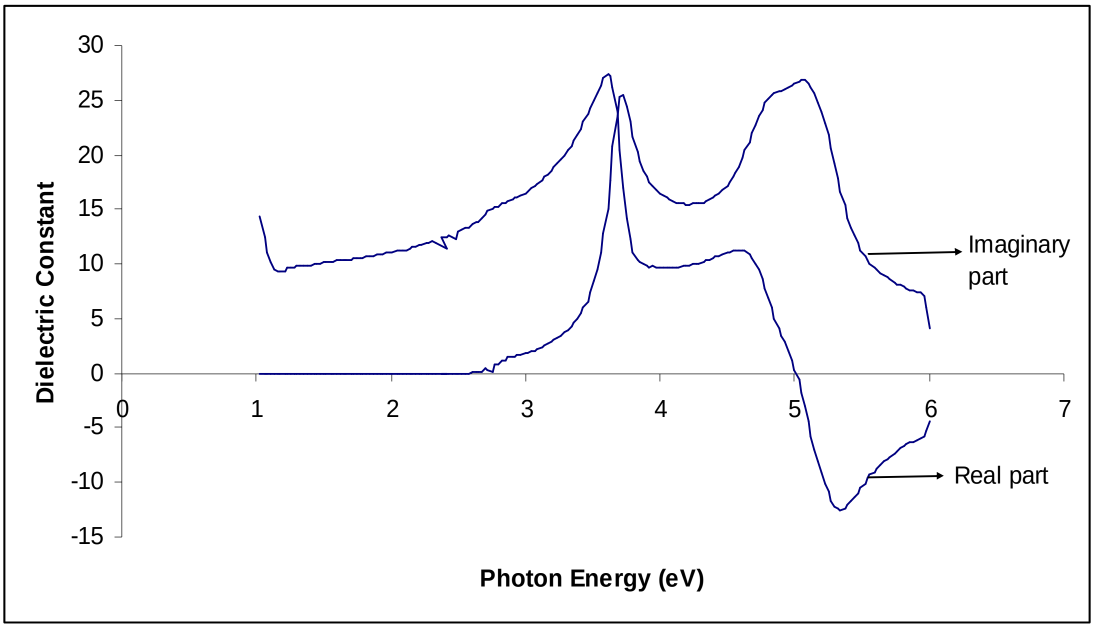

Figure 3: Dielectric Constant of Gallium Phosphide (GaP)

There is an increase in the imaginary part of the dielectric constant of GaP in the energy range 2.6 – 5.07eV as shown in figure 3. It peaks at a value of 26.9 at 5.07eV. The increase in imaginary part of the complex dielectric in the photon energy range 2.6 – 5.07eV shows that the loss factor increases with increase in photon energy in this energy range. The imaginary part of the dielectric constant then decreases in the energy range 5.07 – 6.01eV which shows that the loss factor decreases with increases in photon energy in this energy range.

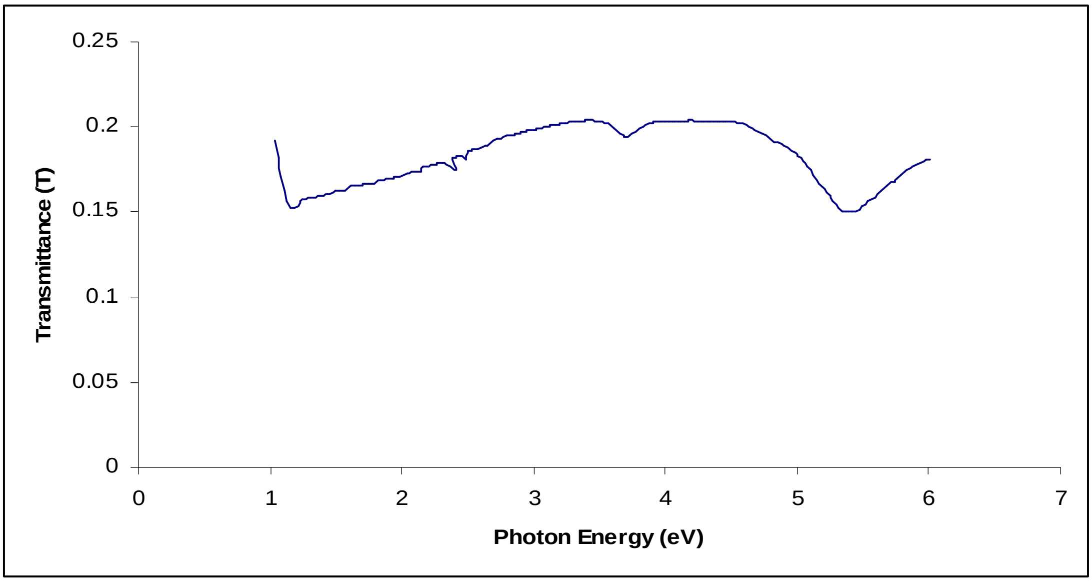

Figure 4: Transmittance of Gallium Phosphide (GaP)

Figure 4 shows the transmittance of GaP. The transmittance of GaP peaks at a value of 0.20 (20%) at 4.63eV indicating a low transparent material. With a maximum of 0.20 for transmittance it means that GaP is not a good transmitter of electromagnetic wave in this energy region because for a good transmitter the transmittance is 60% and above.

The absorption coefficient, α of GaP is as shown in Figure 5. It peaks at a value of 2.24 x 10^8 m^{-1} (22.4 x 10^4 cm^{-1}) at 5.3eV which is in agreement with that reported by Dean and Thomas (10^4 cm^{-1}) (Dean and Thomas, 1966), and Dean *et al* (10^4 cm^{-1} (Dean *et al*, 1967). The value of absorption coefficient then drops to a value of 1.39 x 10^8 m^{-1} at 6.01eV. This high value of the absorption coefficient is typical for interband absorption in semiconductors (Sturge, 1962.). It is important to emphasize that there is no absorption in the energy range 1.03 – 2.6eV which is the energy range of bandgap of GaP. That is, the energy at which the absorption starts corresponds to the direct band gap at 2.25eV (Panish and Casey, 1969). GaP shows no absorption below its band gap. The absorption coefficient shows two peaks at photon energies 3.78eV and 5.3eV, they are mainly due to Γ transition (Zhang et al; 2011).

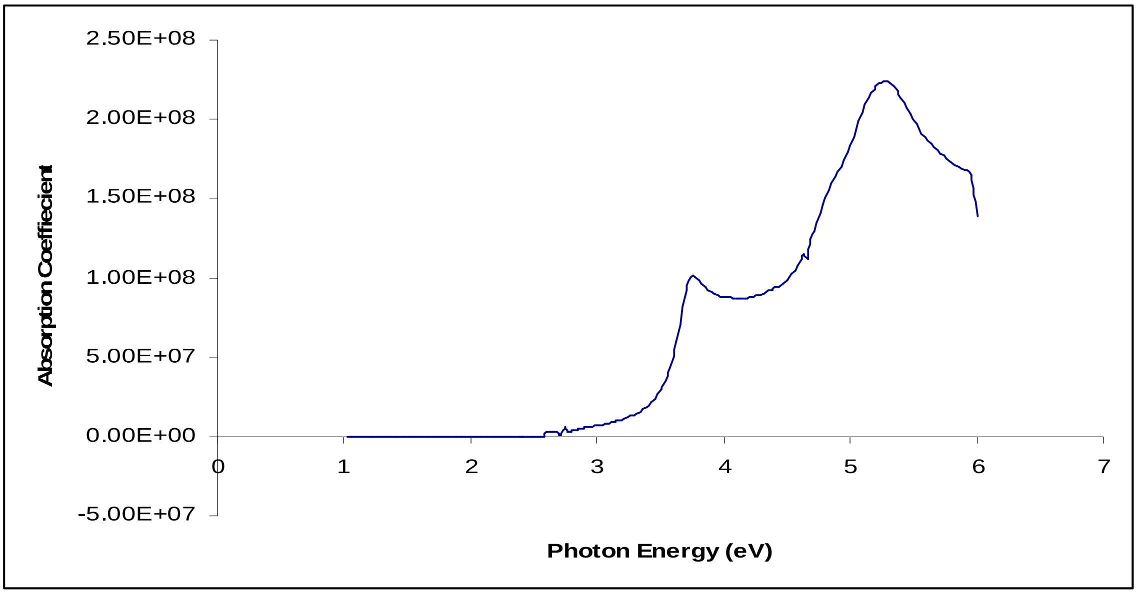

Figure 5: Absorption Coefficient of Gallium Phosphide (GaP)

The reflection coefficient of GaP is as shown Figure 6. It peaks at a value of 0.83 at 5.42eV which agreed with that obtained by Treideris *et al* (0.82) (Treideris *et al*, 2011). The high value of the reflection coefficient means that GaP is highly absorbing.

Figure 7 shows the reflectance of GaP. It has a maximum value of 0.69 at 5.39eV. Two peaks are observed at 3.70eV and 5.39eV, they are mainly due to Γ transition (Zhang et al; 2011) .

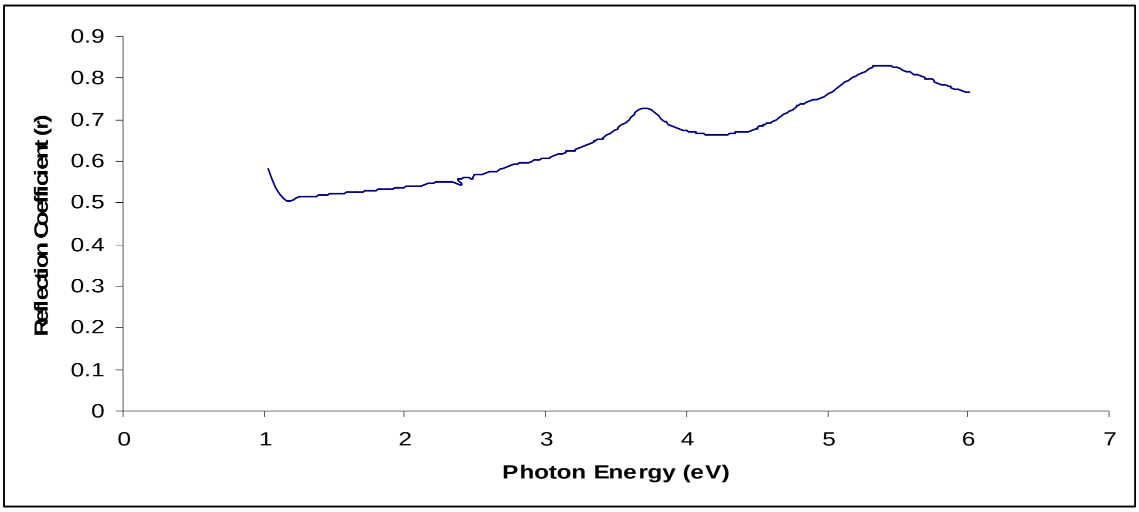

Figure 6: Reflection Coefficient of Gallium Phosphide (GaP)

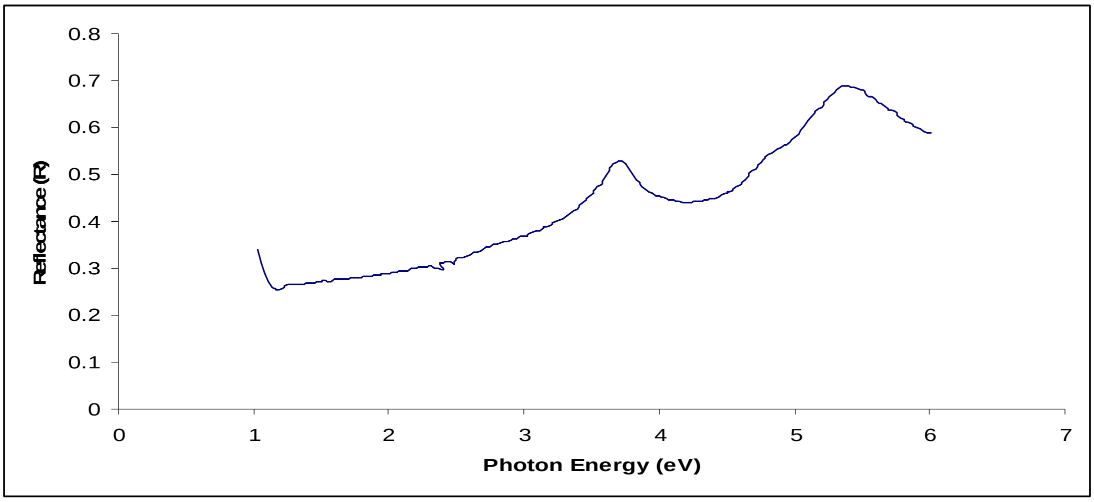

Figure 7: Reflectance of Gallium Phosphide (GaP)

The optical conductivity of GaP is as shown in Figure 8. The real part of the optical conductivity of GaP is constant in the photon energy range 1.03–2.58eV which means that GaP do not conduct in this energy range. There is an increase in the real part of the optical conductivityin the energy range 2.58–5.07eV. It peaks at a value of 16.5 x 10^{15} at 5.07eV. The increase in the real part of optical conductivity in the photon energy range 2.58–5.07eV can be attributed to the increase in absorption coefficient in this energy range. The real part of the optical conductivity shows two peaks at 3.73 and 5.07eV, they are mainly due to Γ transition (Zhang et al; 2011).

There is a decrease in the imaginary part of the optical conductivity of GaP in the energy range 1.03–3.61eV from a value of -1.30 x 10^{15} at 1.16eV to a minimum value of -1.20 x 10^{16} at 3.61eV as shown in Figure 8. The negative value of the imaginary part of the optical conductivity is due to the increase in extinction coefficient and it implies that there is reduction in the conductivity of GaP in this energy range. It has a maximum value of 8.09 x 10^{15} at 5.34eV.

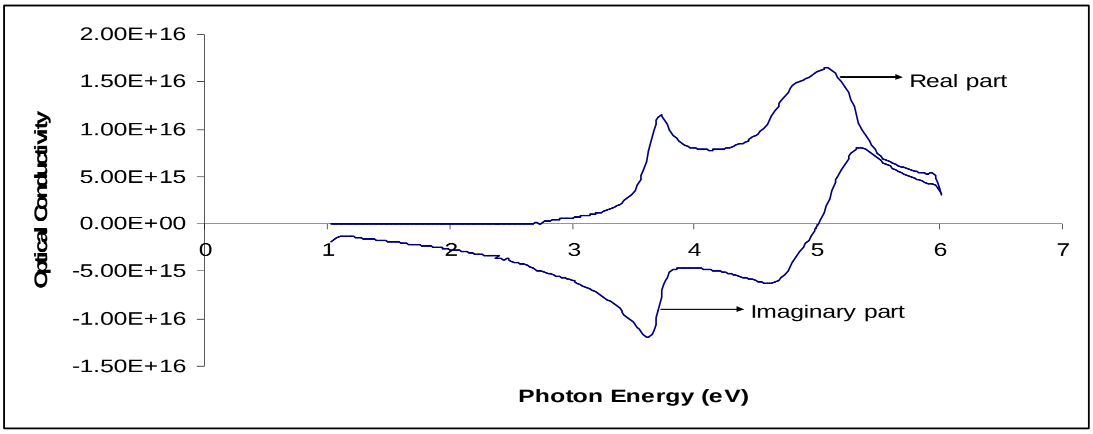

Figure 8: Optical Conductivity of Gallium Phosphide (GaP)

CONCLUSIONS

In conclusion, we have investigated theoretically the optical properties of Gallium Phosphide (GaP) in the energy range 1.03eV–6.01eV. The refractive index has a maximum value of 5.50 at 3.65eV. The refractive index decreases with increase in photon energy in the energy range 3.65-6.01eV. This decrease in refractive index indicates that GaP shows normal dispersion behaviour.

The increase in extinction coefficient with increase in photon energy in the photon energy range 2.7–5.7eV shows that the fraction of light lost due to scattering and absorbance increases in this energy range and the decrease in the extinction coefficient in the photon energy range 5.7–6.01eV shows that the fraction of light lost due to scattering and absorbance decreases in this energy region. The extinction coefficient is zero in the photon energy range 1.03–2.7eV which means that GaP is transparent in this energy region.

The real part of the complex dielectric constant has a maximum value of 27.4 at 3.61eV. The increase in dielectric constant with increase in photon energy in the photon energy range 1.1–3.61eV shows that the loss factor increases with increase in photon energy in this energy range. The decrease in the real part of the complex dielectric with increase in photon energy in the photon energy range 3.61–6.01eV shows that the loss factor decreases with increase in photon energy in this energy range.

The imaginary part of the complex dielectric constant has a maximum value of 26.9 at 5.07eV. The increase in imaginary part of the complex dielectric in the photon energy range 2.6–5.07eV shows that the loss factor increases with increase in photon energy in this energy region. The decrease in the imaginary part of the complex dielectric constant with increase in photon energy in the photon energy range 5.07–6.01eV shows that the loss factor decreases with increase in photon energy.

The transmittance has a maximum value of 0.20 at 4.63eV which shows that GaP is not a good transmitter of electromagnetic wave in this energy region. The absorption coefficient has a maximum value of 2.24×10^{8} m^{-1} (22.4×10^{4} cm^{-1}). This high value of the absorption coefficient is typical for interband absorption in semiconductors. GaP shows no absorption below its band gap.

The reflection coefficient has a maximum value 0.83 at 5.42eV which is in good agreement with that reported by Treideris *et al* (2011). With a value of 0.83 for reflection coefficient it means GaP is highly absorbing. The reflectance has a maximum value of 0.69 at 5.39eV.

The real part of the optical conductivity has a maximum value of 16.5×10^{15} at 5.07eV. The increase in the real part of optical conductivity in the photon energy range 2.58–5.07eV can be attributed to the increase in absorption coefficient in this energy range. At low energies between 1.3eV and 2.58eV, the conductivity is zero, which means that GaP do not conduct in this energy range.

The imaginary part of the optical conductivity has a minimum value of -1.20×10^{16} at 3.61eV and a maximum value of 8.09×10^{15} at 5.34eV. The negative value of the imaginary part of the optical conductivity is due to the increase in extinction coefficient and it implies that there is reduction in the conductivity of GaP in this energy range.

The values obtained for the optical properties of GaP over the energy range 1.03–6.01eV are essentially important for emerging GaP applications such as the design of optoelectronic devices, electronic and photonic devices.

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