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OPTICAL PROPERTIES OF ZINC SULPHIDE (ZnS)

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ABSTRACT

Optical properties of Zinc Sulphide (ZnS) 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 0.60 – 6.01eV. The calculated optical properties of ZnS indicate that it has promising applications in the fabrication of optoelectronic devices such as phosphors and catalysts, laser, sensor, infrared windows, the cathode ray tube, solar cells, blue light-emitting diodes, electro-optic modulators, electroluminescence device applications and Light emitting diodes (LED).

Key words: Complex Index of Refraction, Extinction Coefficient, Dielectric Constant, Transmittance, Absorption Coefficient, Reflectance, Semiconductor

INTRODUCTION

Zinc Sulphide is an important II-VI semiconductor material with a wide direct band gap of 3.68eV **(**Sooklal *et al*., 1996**)** at room temperature and a relatively large exciton binding energy (approximately 40meV) (Yamamoto *et al*, 2001; Bredol and Merichi, 1998; Vacassy *et al*, 1998). It exhibits a wide optical transparency from the ultraviolet (u v) to the infrared (IR) regions. This optical transparency combined with chemical and thermal stability makes ZnS one of the most widely used materials for optical windows (Uzar and Arikan, 2011; Rhadar *et al*, 2012). It has been studied due to its wide application as phosphors and catalysts (Zhu et al, 2003). ZnS is widely used for laser (Klimov *et al*, 2000), sensor (Wada *et al*, 2001; Ennaoui *et al*, 2003; Ozutok *et al*, 2012), infrared windows, the Cathode ray tube, solar cells, blue light emitting diodes (Coe *et al*, 2002), electro-optic modulators (Marquerdt *et al*, 1994), electroluminescence device applications (Calandra *et al*, 1999) and photovoltaic cells which enable wide application in the field of displays (Beard *et al*, 2002; Raffaelle et *al*, 2002; Nadeem and Ahmed, 2000). It is a potentially important material to be used as an antireflection coating for heterojunction solar cells (Bloss *et al*, 1988) for light emitting diode (Antony *et al*, 2005). ZnS is currently used as a shell or capping layerin core/shell nanoprobes such as CdSe/ZnS core/shell structures (Thakur and Fradin,2005).

In this work, optical properties of Zinc Sulphide (ZnS) have been investigated in the photon energy range 0.60 – 6.01eV. The rest of the paper is organized as follows: Section 2 describes the method of calculation of optical properties, section 3 presents the results and discussion, while conclusions are given in section 4.

METHOD OF CALCULATION

Kramers-Kronig analysis of measured refractive index and extinction coefficient data obtained by Schubert (2004) was carried out to obtain reflection coefficient and reflectance of ZnS using Eq. (1) and Eq. (2).

Reflection coefficient measures the fractional amplitude of the reflected electromagnetic field and it is given by (Fox, 2001)

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

where n is the refractive index and k is called 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)

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

The complex dielectric constant is a fundamental intrinsic property of the material. The real part of the dielectric constant shows how much it will slow down the speed of light in the material, whereas the imaginary part shows how a dielectric material absorbs energy from an electric field due to dipole motion. The knowledge of the real and the imaginary parts of dielectric constant provides information about the loss factor which is the ratio of the imaginary part to the real part of the dielectric constant (Bakr *et al*, 2011; Akinlami and Ashamu, 2013). The real and the imaginary parts of the dielectric constant can be estimated using the relations (Goswami, 2005)

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

$$\boxed{E_2 = 2nk} \qquad (4)$$

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

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

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

The transmittance is obtained from the relation

R + T + A = 1 (6)

where R, T and A represent the reflectance, transmittance and absorbance respectively. The sum of these macroscopic quantities which are usually known as the optical properties of the material 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 is mainly studied in terms of the optical conductivity (σ) which is given by the following relation (Sharma and Katyal, 2007) :

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

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 ZnS in the energy range 0.60eV to 6.01eV is shown in Figure 1. There is an increase in the refractive index in the energy range 0.60eV to 5.50eV, with a peak value of 3.18 at 5.50eV as shown in Figure 1. The refractive index decreases afterwards in the energy range 5.50 – 6.01eV. This decrease in refractive index indicates that ZnS shows normal dispersion behaviour.

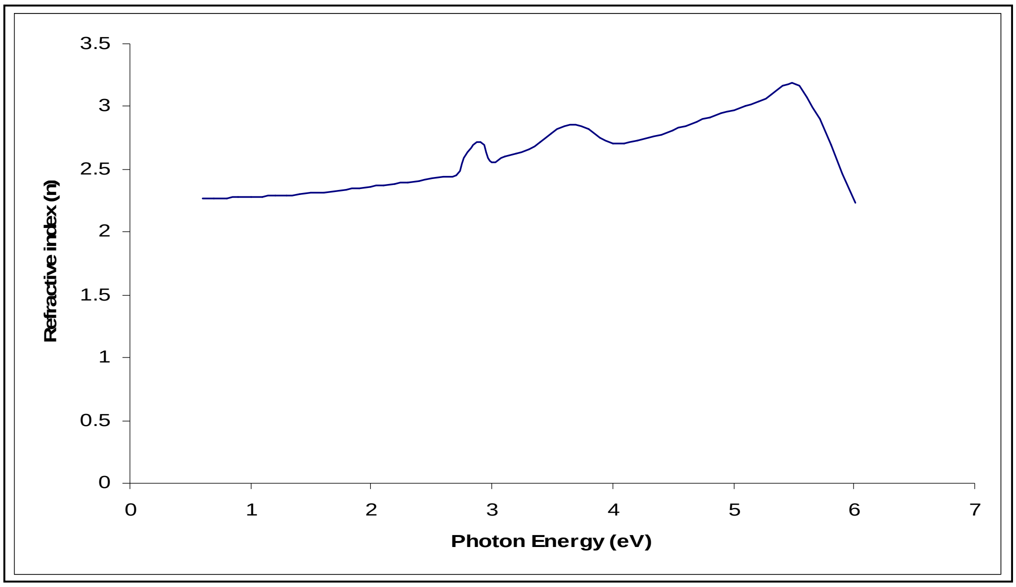

Figure 1: Refractive Index of Zinc Sulphide (ZnS)

Three peaks were observed at 2.9eV, 3.7eV and 5.5eV. The result for refractive index is in good agreement with 3.1 and 3.0 reported by Saeed (2011) and Thamizhmani *et al.* (2005), respectively, but it is higher than the value (2.4) reported by Hu and White (1983).The variation of refractive index with photon energy agrees with the result obtained by Nadeem and Ahmed (2000), Ndukwe (1996) and Polster (1952). With a refractive index of 3.18, ZnS can be used as a reflector.

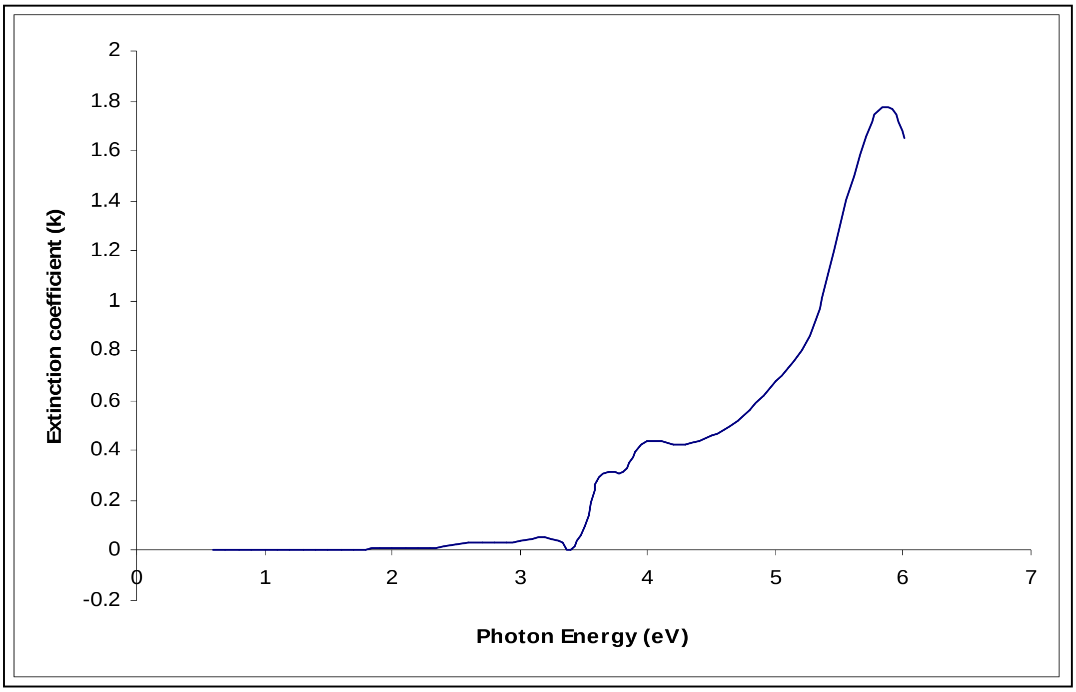

Figure 2: Extinction Coefficient of Zinc Sulphide (ZnS)

The extinction coefficient spectrum in the energy range 0.60eV – 6.01eV is as shown in Figure 2. There is an increase in extinction coefficient in the energy range 1.8 – 5.91eV as shown in Figure 2. It has a peak value of 1.77 at 5.91eV and then decreases to a value of 1.65 at 6.01eV. The increase in extinction coefficient with increase in photon energy in the energy range 1.8 – 5.91eV 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 5.91 – 6.01eV shows that the fraction of light lost due to scattering and absorbance decreases in this energy region. Three peaks were observed at 3.8, 4.1 and 5.94eV. The extinction coefficient is zero in the photon energy range 0.60 – 1.80eV which means that ZnS is transparent in this energy region.

The real part of the dielectric constant spectrum in the energy range 0.60eV – 6.01eV is as shown in Figure 3. There is an increase in the real part of the dielectric constant in the energy range 0.6 – 5.41eV as shown in Figure 3. It peaks at a value of 8.79 at 4.51eV which is in good agreement with (9.0) reported by Thamizhmani *et al* (2005) and (8.8) by Saeed (2011). The increase in dielectric constant with increase in photon energy in the photon energy range 0.6 – 5.41eV shows that the loss factor increases with increase in photon energy in this energy range. The real part of the complex dielectric then decreases with increase in photon energy in the photon energy range 5.41 – 6.01eV with a minimum value of 2.30 at 6.01eV. This shows that the loss factor decreases with increase in photon energy in this energy range.

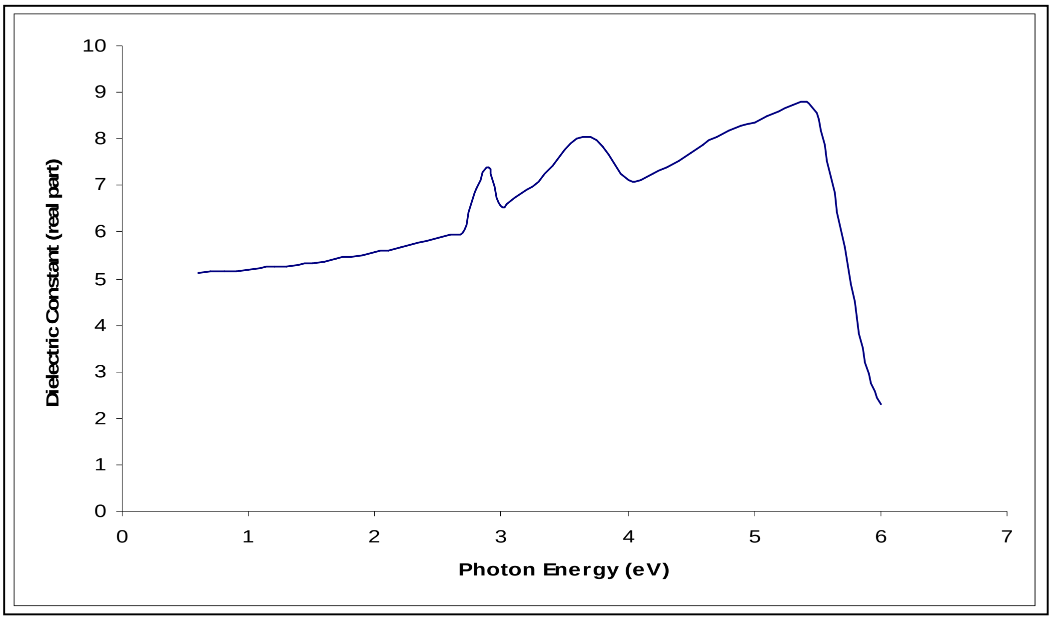

Figure 3: Complex Dielectric Constant (Real part) of Zinc Sulphide (ZnS)

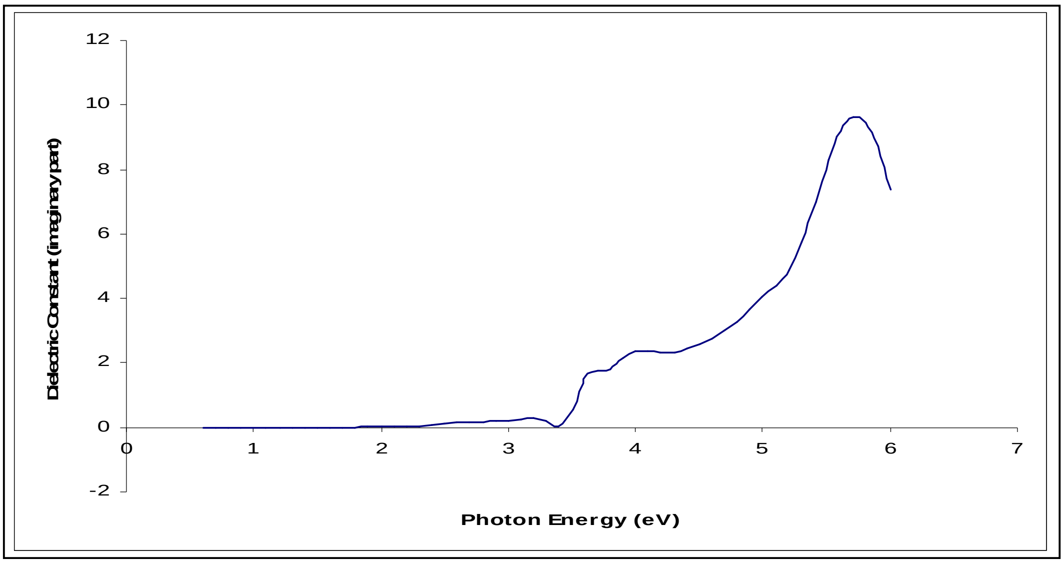

Figure 4: Dielectric Constant (Imaginary Part) of Zinc Sulphide (ZnS)

The imaginary part of the dielectric constant spectrum in the energy range 0.6eV – 6.01eV is shown in Figure 4. There is an increase in the imaginary part of the dielectric constant with increase in photon energy in the energy range 1.80 – 5.71eV as shown in Figure 4. It has a peak value of 9.63 at 5.71eV. The increase in imaginary part of the dielectric in the photon energy range 1.8 – 5.81eV shows that the loss factor increases with increase in photon energy in this energy range. The imaginary part of the dielectric constant decreases with increase in photon energy in the photon energy range 5.81 – 6.01eV which shows that the loss factor decreases with increases in photon energy in this energy range.

Figure 5 shows the transmittance spectrum for ZnS in the photon energy range 1.0 – 6.01eV. The transmittance increases with increase in photon energy in the energy range 0.6 – 5.81eV. It rises to a maximum value of 0.20 at 5.81eV 81eV and afterwards decreases with increase in photon energy in the energy range 5.81 – 6.01eV. A similar behaviour (rise and fall in the transmittance) is reported by Kim (1996). With a peak value of 20% (0.20) for transmittance it means that ZnS is a material for optoelectronic devices.

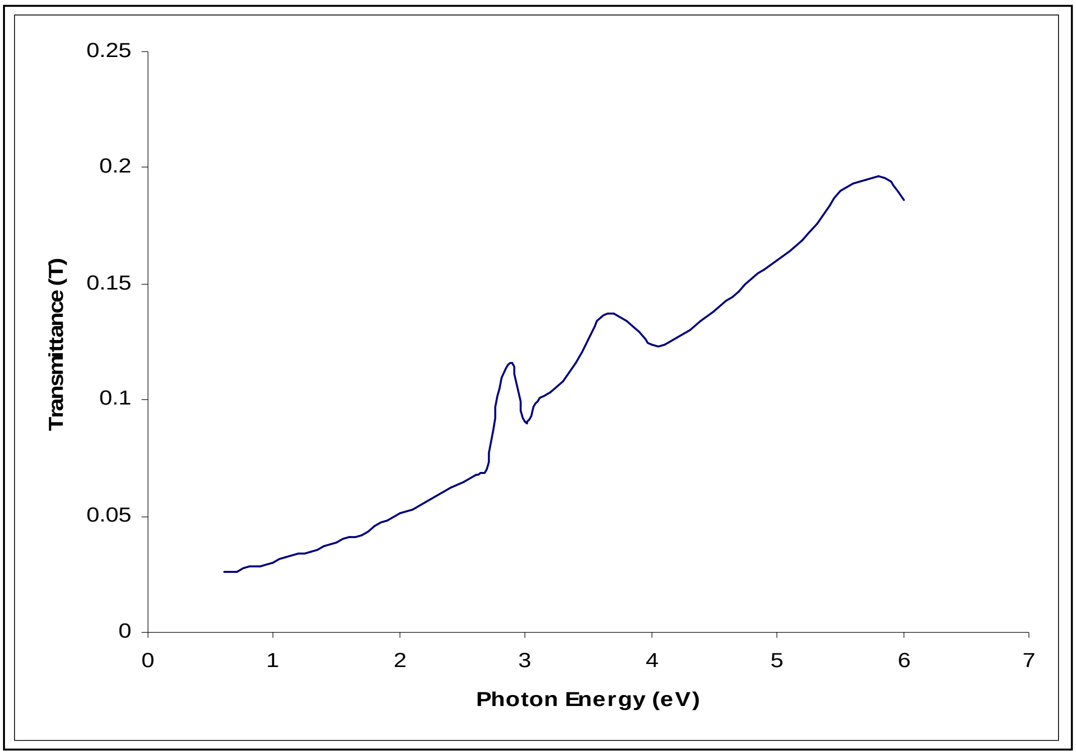

Figure 5: Transmittance of Zinc Sulphide (ZnS)

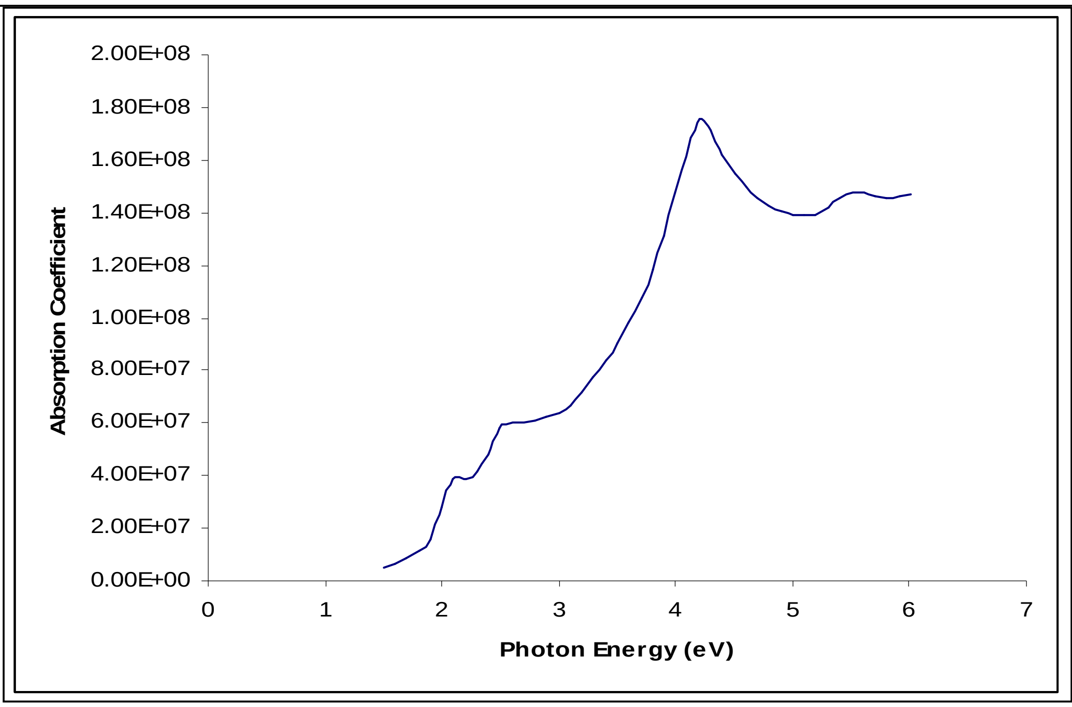

Figure 6: Absorption Coefficient of Zinc Sulphide (ZnS)

The absorption coefficient of ZnS is constant in the energy range 0.60 -1.80eV and it then increases with increase in photon energy in the energy range 1.80 – 5.91eV as shown in figure 6. It rises to a maximum value of 1.06 x 10^8 m^{-1} at 5.91eV which is twice (0.52 x 10^8 m^{-1}) reported by Saeed (2011). The value of absorption coefficient then drops to a value of 1.00 x 10^8 m^{-1} at 6.01eV. This high value of the absorption coefficient is typical for interband absorption in semiconductors (Sturge, 1962).

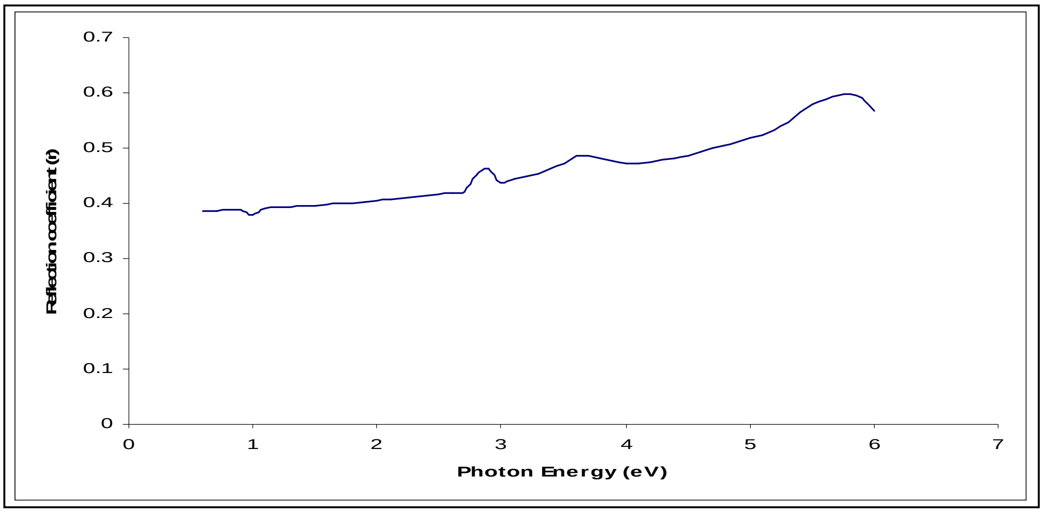

Figure 7: Reflection Coefficient of Zinc Sulphide (ZnS)

Figure 7 shows the reflection coefficient for ZnS. The reflection coefficient of ZnS increases with increase in photon energy in the energy range 0.60 – 5.81eV as shown in Figure 7. It has a peak value of 0.60 at 5.81eV. Three peaks were observed at 2.9eV, 3.7eV and 5.81eV.

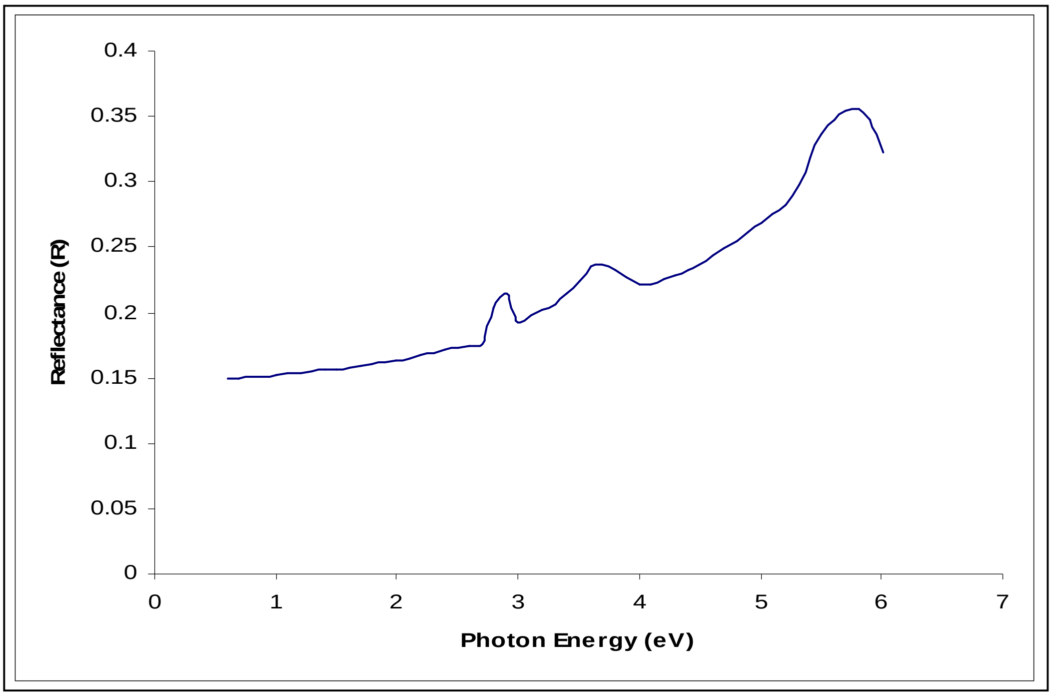

Figure 8: Reflectance of Zinc Sulphide (ZnS)

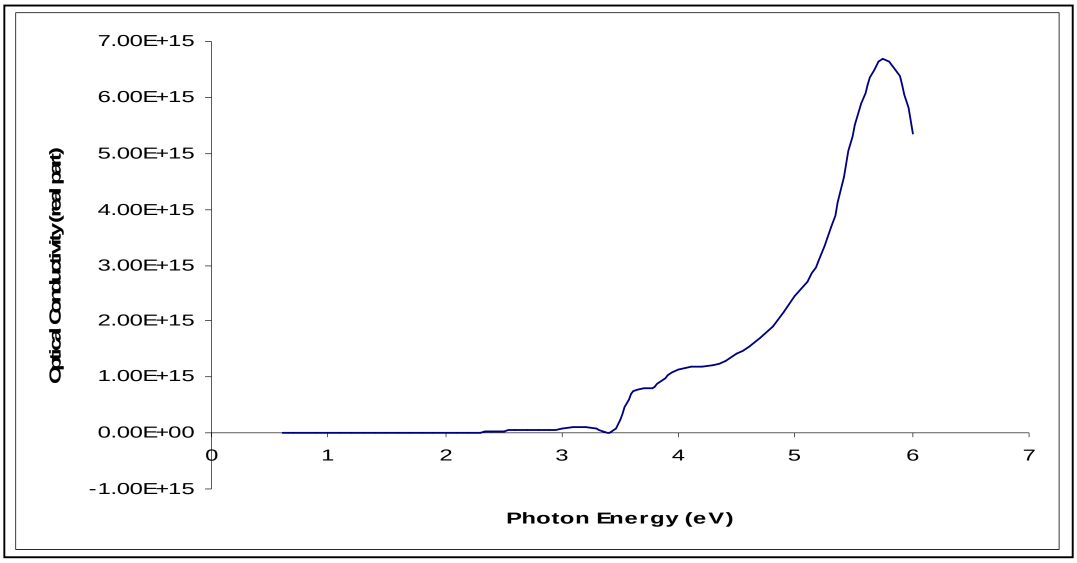

Figure 9: Optical Conductivity (Real part) of Zinc Sulphide (ZnS)

Figure 8 shows the reflectance for ZnS. The reflectance of ZnS increases with increase in photon energy in the energy range 0.6 – 5.91eV as shown in Figure 8. It has a peak value of 0.35 at 5.91eV which is in agreement with that reported by Saeed (0.42) (Saeed, 2011). Three peaks were observed at 2.9, 3.7 and 5.91eV. Reflectance exhibit similar feature to that reported by Memon and Tanner (1989).

Figure 9 shows the real part of the optical conductivity for ZnS. The real part of the optical conductivity of ZnS is constant in the energy range 0.6 – 1.8eV and then increases with increase in photon energy in the energy range 1.8 – 5.81eV as shown in figure 9. It rises to a maximum value of 6.65 x 10^{15} at 5.81eV. The increase in the real part of optical conductivity in the photon energy range 1.8 – 5.81eV can be attributed to the increase in absorption coefficient in this energy range. The real part of the optical conductivity shows three peaks at 3.7, 4.2 and 5.81eV. The real part of optical conductivity of ZnS decreases with photon energy in the photon energy range 5.81 – 6.01eV.

Figure 10 shows the imaginary part of the optical conductivity for ZnS. The imaginary part of the optical conductivity of ZnS first decreases with increase in photon energy in the energy range 0.60 – 5.41eV from a value of -3.72 x 10^{14} at 0.6eV to a minimum value of -5.74 x 10^{15} at 5.41eV as shown in figure 10. 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 ZnS in this energy range. It then increases with increase in photon energy in the photon energy range 5.41 – 6.01eV with a maximum value of -3.72 x 10^{14} at 0.6eV.

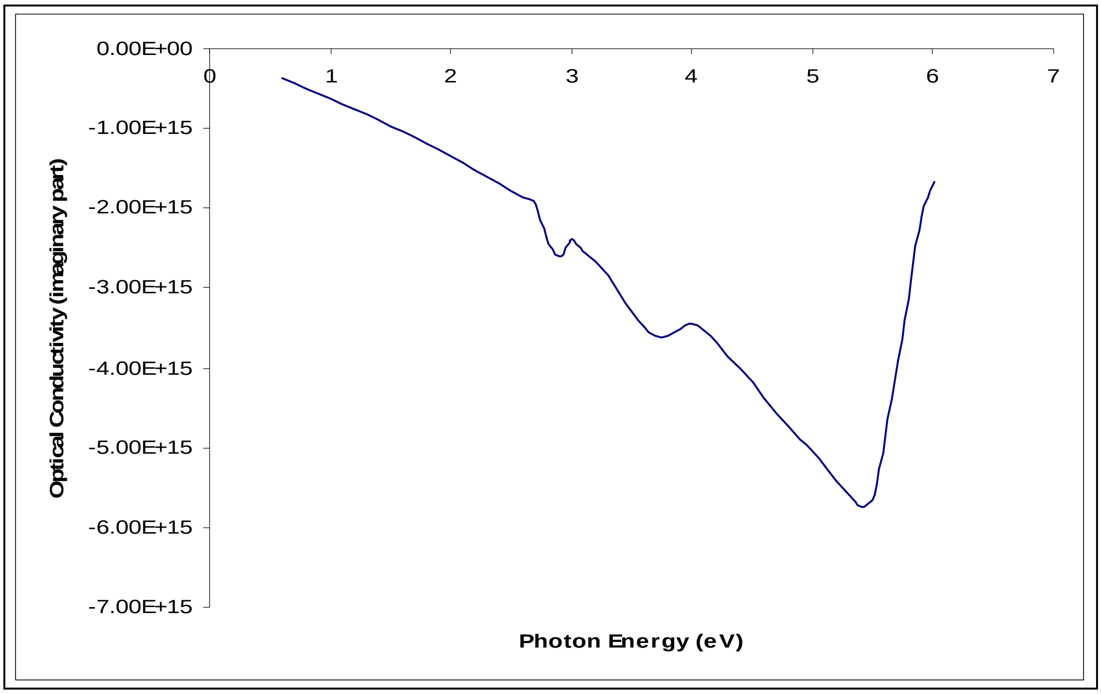

Figure 10: Optical Conductivity (Imaginary Part) of Zinc Sulphide (ZnS)

CONCLUSION

In conclusion, the optical properties of Zinc Sulphide (ZnS) have been investigated theoretically in the energy range 0.60eV – 6.01eV. The refractive index has a peak value of 3.18 at 5.51eV. The refractive index decreases with increase in photon energy in the energy range 5.51 – 6.01eV. This decrease in refractive index indicates that ZnS shows normal dispersion behaviour. With a refractive index of 3.18, ZnS can be used as a reflector. The extinction coefficient has a peak value of 1.77 at 5.91eV and it increases with increase in photon energy in the photon energy range 1.80 – 5.91eV which shows that the fraction of light lost due to scattering and absorbance increases in this energy range. The real part of the dielectric constant has a peak value of 8.79 at 5.41eV. It increases with increase in photon energy in the photon energy range 0.60 – 5.41eV which shows that the loss factor increases with increase in photon energy in this energy range. The imaginary part of the dielectric constant has a peak value of 9.63 at 5.71eV and it increases with increase in the photon energy range 1.80 – 5.71eV which shows that the loss factor increases with increase in photon energy in this energy region. The transmittance has a peak value of 0.20 at 5.81eV which shows that ZnS is a material for optoelectronic device. The absorption coefficient has a peak value of 1.06 x 10^8 m^{-1}. This high value of the absorption coefficient is typical for interband absorption in semiconductors. The reflection coefficient has a peak value 0.60 at 5.81eV. The reflectance has a peak value of 0.35 at 5.91eV. The real part of the optical conductivity has a maximum value of 6.65 x 10^{15} at 5.81eV. The increase in the real part of optical conductivity in the photon energy range 1.80 – 5.81eV can be attributed to the increase in absorption coefficient in this energy range. The imaginary part of the optical conductivity has a minimum value of -5.74 x 10^{15} at 5.41eV and a maximum value of -3.72 x 10^{14} at 0.6eV. 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 ZnS in this energy range. The values obtained for the optical properties of ZnS over the energy range 0.60 – 6.01eV indicate that ZnS has promising applications in the fabrication of optoelectronic devices such as phosphors and catalysts, laser, sensor, infrared windows, the cathode ray tube, solar cells, blue light-emitting diodes, electro-optic modulators, electroluminescence device applications and Light emitting diodes (LED).

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