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The study of the optical properties of copper based chalcopyrite semiconductors

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Abstract

The dielectric constants and reflectance of $Cu_2ln_4Se_7$, $CuGa_3Se_5$ and $CuGa_5Se_8$ typical chalcopyrite belonging to the family of ordered defect compounds (ODC) were computed using $\varepsilon(\omega)=\varepsilon_1(\omega)+i\varepsilon_2(\omega)$ ***and*** $R=\frac{(n-1)^2}{(n+1)^2}$ ***obtained from the values of the experimental results of the refractive index n and the extinction coefficient*** κ***. The graphs plotted from the computed values of the dielectric function and the reflectance were analyzed and compared with experimentally measured values at the angles of*** 55^0 ***and*** 65^0 ***and they were found to be in tandem.***

Keywords
Dielectric function, Extinction coefficient, Reflectance, Refractive index, Optical properties, Chalcopyrite

1.0 Introduction

Wave propagated in materials like crystals such as thin film has been of interest to many researchers since the earlier works of [1, 2 and 3]. Their works made significant impact on the use of beam propagation method in study of properties of crystals. The applicability of this technique has been assessed and discovered to be of great technological importance and has been widely used as a modeling tool for integrated optics [9 and 10].

Electromagnetic wave incident normally or obliquely on the surface of a crystal is bound to experience attenuation as the field propagates through it [7 and 11]. The attenuation depends on the solid state properties of the crystal such as the refractive index and the dielectric function of the crystal. In determining the optical properties of $CulnSe_2$, and the related chalcopyrite type semiconductors, it has been found that the existence of an indium rich *n*-type material surface layer on the later enhances the absorption performance of thin films as it increases the efficiency of the film which makes it suitable for use as a solar cell [8].

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A typical ordered defect compound has been found to play an important role in the performance of the high efficiency of chalcopyrite type semiconductor based solar cells [4, 11]. There had been an evidence of band gap widening from the report on the surface properties of $CuGa_3Se_5$ thin film [6]. This makes the study of its optical properties essential.

To achieve this, the knowledge of the dielectric function over a wide range of wavelength is indispensable for many applications [13] coupled with the band gap as measured by [5].

In this work, the interest was on the use of the pseudo-dielectric functions of the samples comprising the ordered defects compound in computing the dielectric constants of the samples using the measured value of refractive index and the extinction coefficient as obtained using Spectroscopic Ellipsometry (SE) [5] and to relate the corresponding computed reflectance and the dielectric constants of each of the samples both at normal and oblique incident photon.

2.0 Experimental and theoretical procedure

The samples were specified as given below according to compound group.

A	B	C	$B1$	$C1$
$Cu_2In_4Se_7$	$Cu_2Ga_3Se_5$	$CuGa_3Se_7$	$CuGa_5Se_6$	$CuGa_5Se_8$

These samples were developed using Bridgman's method by the solid phase crystallization technique as a family of ordered defect compounds [5]. The values of the dielectric functions of the crystals were computed using the relations:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \tag{2.1}$$

which can be decomposed in terms of the refractive index and extinction coefficient as

$$\varepsilon_1(\omega) = n^2 - \kappa^2 \tag{2.2}$$

$$\varepsilon_2(\omega) = 2n\kappa \tag{2.3}$$

where $\varepsilon_1(\omega)$ is the real part of the dielectric and $\varepsilon_2(\omega)$ is the imaginary parts of the dielectric constant, n is the refractive index and κ, the extinction coefficient.

The computed results carried out on the ordered defect compounds (ODC) samples were measured by SE at room temperature in the photon energy range from $0.8eV$ to $3.8eV$. The measured refractive indices and extinction coefficient were determined using microscopic ellipsometer [5].

This computed dielectric were compared with the experimentally measured dielectric constant which was measured over incidence angles of 55^0 and 65^0 consistently in order to ensure a degree of accuracy in the determination of the dielectric constant. The reflectance of the crystals was also computed for normal incidence wave/field, which was simplified by considering the complex amplitude for the reflectance coefficient of an electromagnetic wave of frequency ω, given by

$$r(\omega) = R^{\frac{1}{2}} \exp i\alpha \tag{2.4}$$

The reflectance coefficient allows one to calculate the phase angle to wave propagating through the crystal by the equation:

$$\alpha(\omega) = \frac{1}{\pi}\int_0^{\infty} \log\left|\frac{\xi+\omega}{\xi-\omega}\right| \frac{d}{d\xi} \log\left[R\xi\right]^{\frac{1}{2}} d\xi \tag{2.5}$$

By limiting to the quasi – normal induce measurement done at ($\theta \approx 0$); we get the value of R as

$$R = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2} \tag{2.6}$$

which on simplification reduces to $$R = \frac{(n-1)^2}{(n+1)^2} \quad (2.7)$$

The energy band gap of the material was computed for the samples A, B, B1, C1 as specified at room temperature and was found to range from 0.8*eV* to 3.8*eV* from the relations

$$\alpha = 4\pi\kappa/\lambda \quad (2.8)$$

and

$$\alpha = \left(\frac{hc}{\lambda} - E_g \right)^2 \quad (2.9)$$

where α is the absorption co-efficient, *k* is the extinction co-efficient, E_g is the energy band gap while $\frac{hc}{\lambda}$ is the photon energy.

3.0 Results and discussion

Figures la and 1b show the computed real and imaginary $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ components of the dielectric of *A, B, C, B1* and *C1* from the numerical values of the refractive index *n* and the extinction coefficient κ. The real and imaginary refractive index *n* and extinction coefficient κ are the fundamental properties. To assess properly the influence of the chalcopyrite optical properties on the solar cell device properties, the optical absorption coefficient is important. The spectral dependence of $\alpha = 4\pi k/\lambda$ where λ is the wavelength of light in the vacuum is presented for the samples. The *n* values in the transparency region of the studied samples decrease with increasing wavelength. The spectra of the imaginary and real components of the complex dielectric function of the samples in figures 3.la and 3.1b show peaks that correspond to various values of energy transitions of the electronic band structure in accordance with the report of [15]. In the region below 2*eV*, the fundamental energy gap $E_o = E_g$ is well identified for each case and in the region below 3.8*eV*.

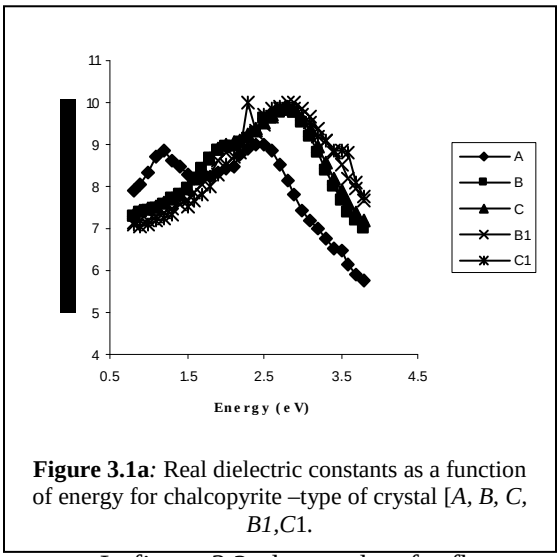

Figure 3.1a*:* Real dielectric constants as a function of energy for chalcopyrite –type of crystal [*A, B, C, B1,C*1.

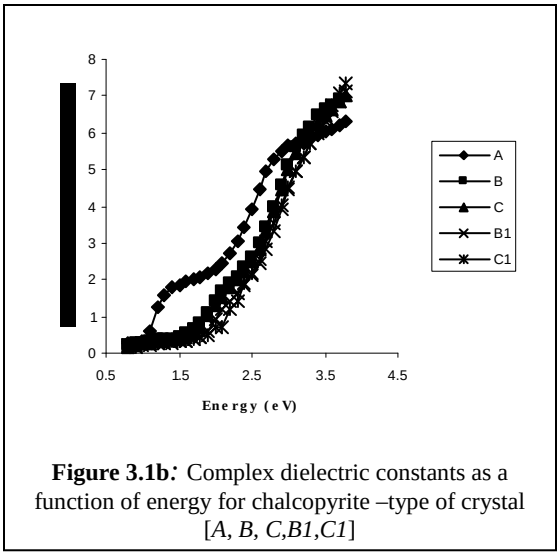

Figure 3.1b*:* Complex dielectric constants as a function of energy for chalcopyrite –type of crystal [*A, B, C,B1,C1*]

In figure 3.2, the graphs of reflectance with respect to the energy were plotted and it was observed that all the samples appear to have the same reflectance behaviour. That is the reflectance of the compound no matter how they are grown are the same. The structures observed

in the dielectric spectra are likened to the inter–band critical points, which is related to the region of the band structure with large, or singular point electronic density of states as explained by [5] and [14] in their work respectively. This structure was analyzed in terms of standard analytic line shape. The experimental spectra of the imaginary and real components of

the complex dielectric functions have slightly different shapes at different crystal photon energy as compared to the computed values.

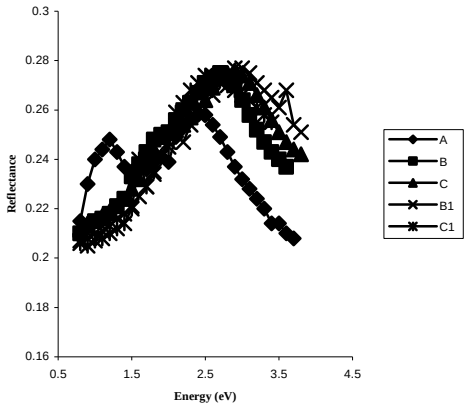

Figure 3.2*:* Reflectance behaviour as a function of energy-band for chalcopyrite –type of crystals [*A, B, C*, *B1*, *C1*]

4.0 Conclusion

In this work, the properties of copper based chalcopyrite semiconductors have been computed using measured refractive indices and extinction co-efficient from microscopic ellipsometer. The computed dielectric constant and reflectance tend to agree with the experimentally measured values apart from the peak that is observed in the computed real dielectric. From this work, the efficacy in the use of mathematical approach in computation of some solid state and optical properties of semiconductor materials is clearly demonstrated and is seen to be workable.

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