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Analyzing Optical Reflectance of Semiconductors: An Application to Silicon

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Abstract: The optical parameters of Silicon (Si) were determined from available data of normal reflectance of single crystal silicon measured at 0.01 eV-30 eV range by unpolarized light. Kramers-Kronig Analysis relationship was used to determine the optical parameters from the reflectance data. The results obtained from the KKT analysis was found to be in a satisfactory agreement with the previous results and literatures with little disparity observed for some optical parameters, particularly extinction coefficient, which was as a result of approximation made in extrapolation method used in evaluating reflectance phase shift/angle. From the calculated values of optical parameters by KKT analysis, an overview of electronic band structure of silicon was given particularly from the optical transition strength and absorption edge spectral. The relationship between efficiency of devices made from silicon and its band structures were also established.

Key words: Optical constants, silicon single crystals, oscillator fit procedure, Kramers-Kronig analysis

INTRODUCTION

Electrons in crystal lattice are arranged in energy bands separated by forbidden regions or energy gap in which no electron energy states are allowed.

Photons absorption with electronic transitions from the valence band states to states in the conduction band can take place in an insulator or semiconductor, if the photon energy $\hbar\omega \geq E_g$; E_g is the minimum energy of the band gaps (Kiang, 1976). This is called Interband Transition. If $\hbar\omega \geq E_g$, interband transition cannot occur. Also for a degenerate semiconductor whose conduction band or valence band is partially filled with electrons or holes, respectively, Interband Transitions can occur (Kiang, 1976).

Exploring the optical behaviour of semiconductors is of fundamental importance in the study of the band structure of semiconductors and insulators.

Determination of optical constants is extremely useful in explaining and analyzing the behaviours of band parameters and structure of energy bands in real materials particularly silicon in this case, thus the relationship between the band parameters and efficiency of semiconductor made devices can be established in addition to obtaining the Energy gap (E_g).

The Kramer Kronig transformation analysis is thus extremely significant in determining and analyzing optical constants. We have adopted the Kramer-Kronig transformation analysis in this work using available reflectance data from Stanford University Physics Laboratory, measurement was carried out by Eden (1985) for his studies on Photoemission Studies of Band structures of Semiconductor: Si, Ga, As, GaP.

Various methods have been developed for this purpose comprising those based upon measurement of multiple reflections or transmission and absorbance in thin films while others are based on the measurement of reflectance from bulk materials only (Durmus *et al*., 2000). All these methods have differences with respect to their relative precision and the techniques with which they handle the experimental data (Durmus *et al*., 2000). Based on the method adopted, the optical constants are determined either only at the specified energy values or over some energy ranges.

MATERIALS AND METHODS

In this research, Kramer-kronig transformation analysis is used to compute optical constants from normal reflectance data over an energy range for silicon through application of numerical integration by Simpson 1/3 and integral transformation.

The reflectance data analyzed in this work was adapted from Stanford University Physics Laboratory as reported by (Eden, 1985) 'Photoemission Studies of Electronic Band Structures of Semiconductor'.

Theory: From Fresnel equation, in any solid material, the complex reflectance is given as

$$\vec{r}(w) = R^{1/2} e^{-i\theta(w)} \quad (1)$$

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Here, the R(w) is measured reflectance and θ(w) is phase shift arising from the reflection.
Taking logarithm of Eq. 1, one obtains

$$\ln\vec{r}(w) = \ln R^{1/2} + i\theta(w) \quad (2)$$

Applying one of the K.K relations on Eq. 2, the real and imaginary parts of it can be related to each other as:

$$\theta(w_o) = -\left(\frac{w_o}{\pi}\right) P\int_0^\infty \frac{\ln R(w)}{w^2 - w_o^2} dw \quad (3)$$

Where P denotes the principal value of the integral. Integrating Eq. 3 by parts, we have

$$\theta(w_o) = -\frac{1}{2\pi}\int_0^\infty \frac{d\ln R(w)}{dw} \ln\left|\frac{w + w_o}{w + w_o}\right| \quad (4)$$

In the process of performing the Kramer-kronig analysis, Eq. 3 is first applied to the measured normal reflectance, R(w) data taken between a certain w_a-w_b frequency range and θ(w) are calculated for each value (Greenaway *et al*., 1965). The integral corresponding to the measured range can be calculated using any numerical integration technique of choice. Thus to account for contributions from outside the range, extrapolation functions of different kinds can be applied, the commonest of the extrapolation functions is the Rossler's extrapolation function (Rossler, 1966) and this is used for this research.

Thus, from known value of R(w) and $\theta(w_o)$ other optical constants are evaluated.
From Maxwell equation;

$$\vec{N}^2 = \vec{\varepsilon} \text{ and } \vec{N} = n + ik \quad (5)$$

Where, N is complex refractive index, $\vec{\varepsilon}$ is the complex dielectric constants, n = refractive index and k is the extinction coefficient. Solving the Fresnel equation explicitly, we obtain the following approximation for n (w) and k (w)

$$n(w) = \frac{1 - R(w)}{1 + R(w) - 2\sqrt{R(w)}\cos\theta(w)} \quad (6)$$

$$k(w) = \frac{-2\sqrt{R(w)}\sin\theta(w)}{1 + R(w) - 2\sqrt{R(w)}\cos\theta(w)} \quad (7)$$

The complex dielectric constants of a solid is given as:

$$\varepsilon(w) = \varepsilon_{1(w)} + i\,\varepsilon_{2(w)} \quad (8)$$

Using the relation in Eq. 5 the real and imaginary parts are given by

$$\varepsilon_{1(w)} = n^2(w) + k^2(w) \quad (9)$$

$$\varepsilon_{2(w)} = 2n(w)k(w) \quad (10)$$

Other optical constants estimated include Optical transition strength ($(h\nu)^2\,\varepsilon_2$):
Absorption Edge coefficient:

$$\alpha = \frac{2\omega k}{c} = \frac{4\pi k}{\lambda} \quad (11)$$

and Energy loss function:

$$-\mathrm{Im}\,\varepsilon^{-1} = \frac{\varepsilon_2}{(\varepsilon_1)^2 + (\varepsilon_2)^2} = \frac{2nk}{(n^2 + k^2)^2} \quad (12)$$

RESULTS AND DISCUSSION

The spectral dependence of the % reflectance for silicon obtained from available reflectivity data is found to be in satisfactory agreement with the ones presented by (Vina, 1984) and (Durmus *et al*., 2000) although, over a low energy range and the theoretical reflectance curve obtained by oscillator fit procedures.

It is observed that the refractive indices (n(w)) and extinction coefficient (k(w)) spectral obtained by KKT analysis has the same pattern with the one reported by (Durmus *et al*., 2000) and experimental values.

From Fig. 1 and 2, the three main peaks identified correspond with those in the optical reflectance spectrum and imaginary part of complex dielectric constant having energies, E_1 = 3.45eV, E_2 = 4.25eV and E_3 = 5.3eV.

The spectral dependence of the real and imaginary parts of dielectric constants was also found to agree with the existing literatures and theoretical values (Aspnes *et al*., 1983).

We found additional energy peaks as a revelation over previous work. The peak E_3 = 5.3 eV was found having extended the energy range compared to the previous work.

Also from Fig. 3, the three energy peaks E_1 = 3.45eV, E_2 = 4.25eV and E_3 = 5.3eV also correspond with the 3 main energy peaks in the optical reflectance spectrum.

The main peaks observed in Fig. 4 correspond to the peaks in the reflectance spectrum, having energy of

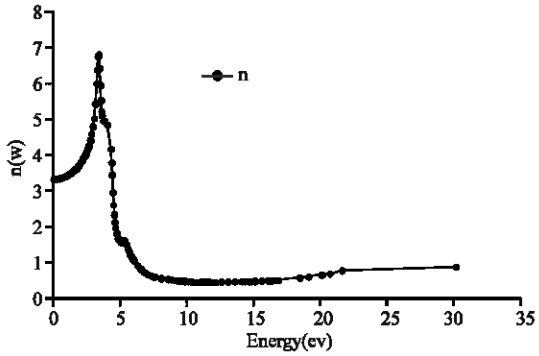

Fig. 1: Refractive index for silicon determind by KKT

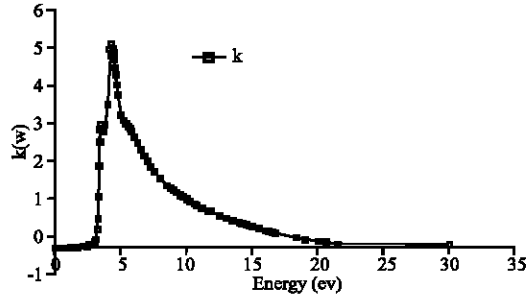

Fig. 2: Extinction coefficient for silicon determind by KKT

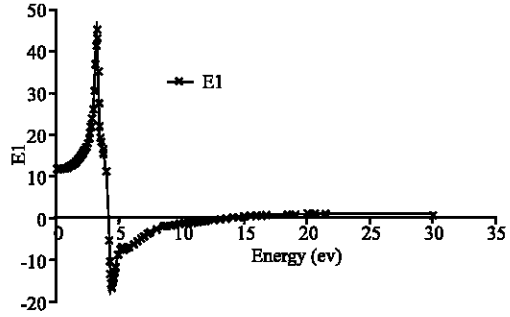

Fig. 3: Real part of complex dielectric contrast for silicon determind by KKT

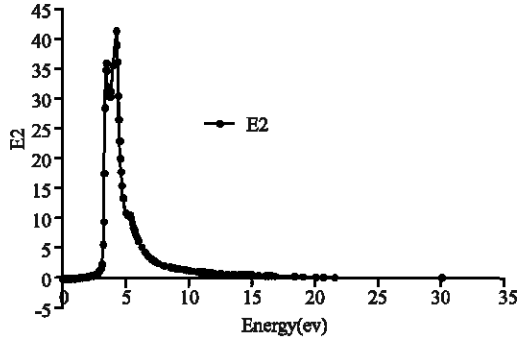

Fig. 4: Imaginary part of complex dielectric constant for silicon determind by KKT

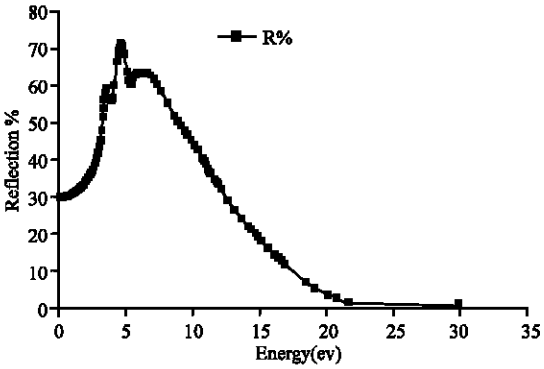

Fig. 5: Percentage optical reflectance

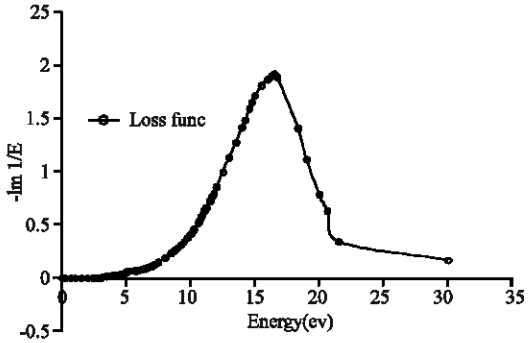

Fig. 6: Energy loss function for silicon determind by KKT

E_1 = 3.45 eV,E_2 = 4.25 eV and E_3 = 5.3eV. These peaks correspond to the peaks identified in the optical reflectance spectrum (Fig. 5).

The positions of these peaks are consistent with the literature and they have been associated with various interband transition (Vina *et al*., 1984).

The energy loss function and absorption edge spectral quite agree with the experimental values and the peaks in absorption spectral correspond with the main peak in extinction coefficient (Cohen *et al*., 1989) (Fig. 6 and 7).

The plasma frequency/resonance which is the maximum (peak) point in spectral dependence of the energy loss function is estimated to be 16.5 eV and for the standard plasma-dispersion relation ($\varepsilon_1 = 0$), it is 15 eV. These are found to be in line with the existing literatures (Aspnes *et al*., 1983).

In Fig. 8 spectral of optical transition strength shows relevant peaks and the peaks also correspond to the peaks observed in the reflectance spectral.

Conclusively, from the combined spectral dependence of ε_1, ε_1 and -1m $1/\varepsilon$) three distinguishable spectral are observed.

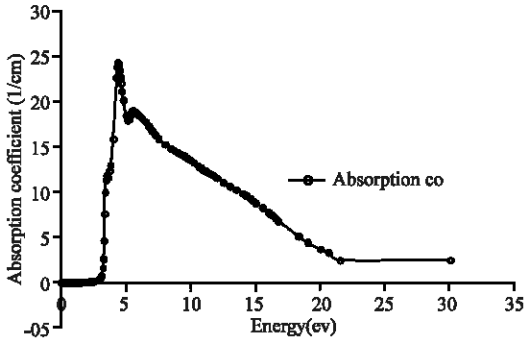

Fig. 7: Optical obsorption Edge for silicon

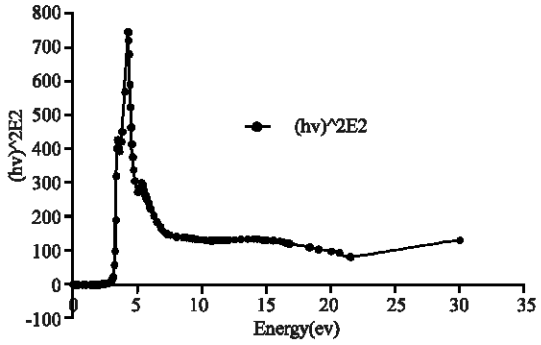

Fig. 8: Optical transition strength for silicon determind by KKT

The first region extending to about 7-10 eV is characterized by sharp structure associated with interband transition (states in valence band to empty state in conduction band).

The second region extending to about 16 eV which is referred to as "metallic" region is marked by a rapid decrease of the reflectance that is reminiscent of the behaviour of certain metals in the ultraviolet region. In this region we have sharp maximum of the function (-1m 1/ε)which describes the energy loss of fast electrons traversing the material and it is associated with the existence of plasma oscillation (Kittel, 1996).

The third region indicates the onset of additional optical absorptions and lies in the energy range, >20 eV. This structure is associated with transitions between filled bands lying below the valence band and empty conduction bands states.

Obviously we found out the sharp edges and peaks corresponding to interband transitions, the peaks are often attained in the low energy range as depicited in figures, precisely in the energy range 0 = E = 5eV and thus correspond to the energy band gap or width. This indicates and further buttress the point that semi-

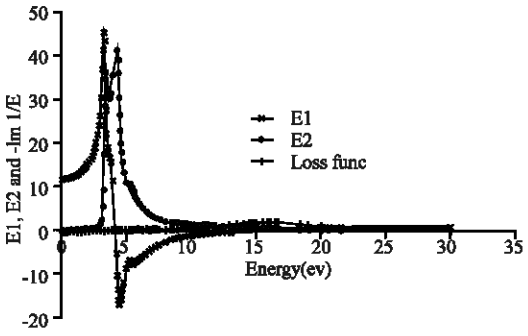

Fig. 9: The spectral dependence of E1, E2 and energy loss function

onductor materials with low energy band gap are essential and often used for practical application.

Previous works were done within a lower energy range compared with the present study, the energy range 0.01-30 eV was considered in contrast to earlier workdone by Durmus *et al.* (2000) in which the energy range 0.5-5.6 eV was considered.

Although the energy ranges earlier considered revealed the essential features characterizing interband transitions and some important spectral and sharp edges. A further revelation of this work is the existence of a third region, above the energy range (>20eV). It is depicted by fairly steady linear part of the curve which represents the onset of additional optical absorptions. This structure is associated with transitions between filled bands lying below the valence band and empty conduction band states as shown in Fig. 9.

We discovered an additional energy peak E_2 = 5.3ev compared to previous studies (Durmus *et al.*, 2000) evidence from extension of energy range.

From the various figures considered encompassing the optical parameters(Absorption coefficient), complex dielectric constants E2, refractive index N(w), three corresponding main energy peaks, E_1 = 3.45ev, E_2 = 4.25 ev and E_3 = 5.3 eV were found in unison.

The seemingly exception to this significant observation is Fig. 6 where the loss function has only one peak at about 0.5 eV and in the energy range 0-5ev.

Also work noting is the fact, from Fig. 5-8 there is a coincidence in the energy range. The optical parameters specifically, Extinct co-efficient K(w). The coincidence of extinction co-efficient, h (w) and the optical absorption edge h (w) indicates that if extinction co-efficient is zero there is no absorption.

Deductions from optical constants of Silicon (Si): The spectral dependence of reflectance, optical transitive positive strength, imaging dielectric constants and

absorption edge reveals the transition in electron excited from the valence band to the conduction band with absorption of photon energy approximately equal to energy gap (Eg) called fundamental absorption which obviously correspond to the main peaks and sharp absorption edges indicated in the various graphs of optical parameters.

Apart from the above transition, direct interband absorption of photon will occur at all points in the brillouin zone for which energy is conserved.

$$hv = E_c(k) - E_v(k) = E_g \quad (13)$$

Where c is an empty band and v is a filled band. The relations in (Eq. 13) include spectral structure in a crystal because transition accumulate at frequencies for which the bands c and v are parallels, i.e at frequencies where;

$$Grad\left[E_c(k) - E_v(k)\right] = 0$$

Band/energy gap determination: Band or Energy gap (E_g) is defined as the minimum energy required for the transition of an electron from the highest filled valence band state to the lowest unfilled conduction band state.

Perhaps, the most important band parameter that can obtain from optical spectroscopy is the Energy gap (E_g).

The absorption edge spectrum is characterized by a sharp increase when the photon energy ($h\nu$) equals the Energy gap (E_g).

From Fig. 7,E_g is deduced to fluctuate between 1.15 (3.55-2.40), 1.02(4.57-3.55) and 1.09 (5.66-4.57), hence E_g = 1.09 eV.

CONCLUSION

From KKT analysis of the reflectance data to determine optical constants of Silicon, the following conclusions were established/drawn

- Optical constants are extremely useful in determining are extremely useful in determining the various band parameters like the energy gap (Eg), width of silicon was determined from optical absorption edge spectrum as supported by Eq. 13 above.
- Also various interband transitions energy can be determined from reflectance and optical transition strength spectral. The energy band gaps correspond to various peaks of the optical and sharp edges due to maximum optical absorption as justified by Eq. 13. It is also interesting to note that the determination of the optical constants are extremely useful in explaining interband and various intraband transitions which is very crucial to the technology of various semiconductor devices.
- Based on these deductions, various devices such as transistors, tunnel diode, photodiode, gun diode, integrated circuit etc are designed. Most of these devices depend on the width of energy gap, for instance semiconductors with energy gap between 1.1 and 1.6eV is most suitable for solar cells that why silicon is most preferred in this regard even to GaAs, InSb etc.
- In this research, we extended the energy range, thus covering 0.01-30ev which is quite different from previous literatures, interestingly, the results agree with previous literatures within their energy ranges. We anticipate that the extrapolation outside the specified or experimental measurement makes precision of the analyzed values due to possible errors a limitation. Also obvious is the little disparity observed particularly for the extinction co-efficient due to approximation in the extrapolation method used in evaluating reflectance phase shift/angle.
- We proffer extension of energy ranges in future investigations as this may help to desalinate more optical behaviours that could be significant to band structure analysis. Also recommended for future investigation/work is improvement on the extrapolation function to be adopted essentially to minimize as much as possible errors due to extrapolation.

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