Exploring Optical Transition Strength of Silicon by Kramers-Kronig Tansformation

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Abstract: The optical transition strength of silicon (Si) was determined from available data of normal reflectance of single crystal silicon measured at 0.01eV – 30eV range by unpolarized light. Kramers – Kronig Analysis relationship was used to determine the optical transition strength 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 in the optical parameters, 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 spectrum. The relationship between efficiency of devices made from silicon and its band structures can be established.

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1.0 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 $\hbar\omega \leq E_g$, 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.

2.0 Methodology

In this work, Kramer-kronig transformation analysis is used to compute determine the optical transition strength and reveal significant interband energy transitions from data over an energy range for silicon through application of numerical integration by Simpson 1/3 and integral transformation.

3.0 Theory

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

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

Here, the $R(w)$ is measured reflectance, and $\theta(w)$ is phase shift arising from the reflection.
Taking logarithm of Equation (1), one obtains

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

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

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

where P denotes the principal value of the integral.
Integrating equation (3) by parts, we have

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

In the process of performing the Kramer-kronig analysis, Equation (3) is first applied to the measured normal reflectance, R(w) data taken between a certain $w_a - w_b$ frequency range and $\theta(w)$ 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 work.

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

From Maxwell equation;

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

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)

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

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

The complex dielectric constants of a solid is given as

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

Using the relation in equation (5) the real and imaginary parts are given by

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

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

Other optical constants estimated include Optical transition strength $((hv)^2 \varepsilon_2)$:

Absorption Edge coefficient: $\alpha = \frac{2\omega k}{c} = \frac{4\pi k}{\lambda}$ …(11)

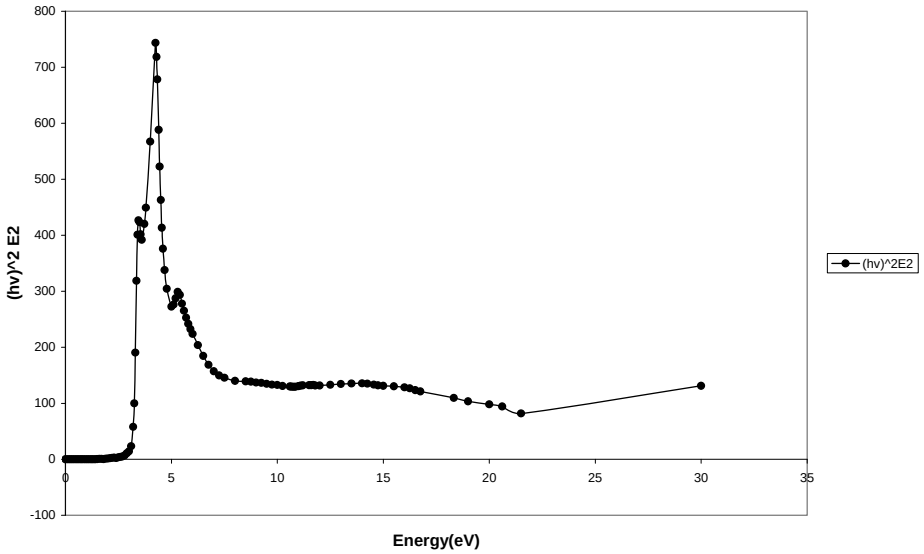
and Energy loss function: $-\mathrm{Im}\,\varepsilon^{-1} = \dfrac{\varepsilon_2}{(\varepsilon_1)^2 + (\varepsilon_2)^2} = \dfrac{2nk}{(n^2 + k^2)^2}$ … (12)

4.0 Results and Discussion

The spectral dependence of the optical transition strength for silicon obtained from available reflectivity data is found to be in satisfactory agreement with the ones presented by (Adewole et al, 2007), over an extrapolated energy range and the theoretical curve agree with experimental values.

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

Fig.8: Optical Transition Strenght for Silicon determined by KKT



The first region adjacent to 5 eV and 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 the figure, 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-conductor materials with low energy band gap are essential and often used for practical application.

In the present study, the energy range 0.01-30 eV was also considered (Adewole et al, 2007) but in contrast to earlier work done by (Durmus et al ,2000) in which the energy range 0.5-5.6 eV was considered and more significant features were revealed. 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 the above figure (8.0).

5.0 Deductions from Optical Constants of Silicon (Si)

The spectral dependence of reflectance, optical transition strength and absorption edge reveals the transition in electron excited from the valence band to conduction band. Absorption of photon energy approximately equal to energy gap (E_g) called fundamental absorption which obviously corresponds to the main peaks and sharp absorption edges that could be indicated in 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.

$$h\nu = E_c(k) - E_v(k) = E_g \text{ ....} (13)$$

where c is an empty band and v is a filled band. The relations in (eqn 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; $Grad\left[E_c(k) - E_v(k)\right] = 0$.

6.0 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 (hν) equals the energy gap (E_g). E_g is estimated 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.

7.0 CONCLUSION/SUMMARY

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

1) Optical constants 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 equation (13) above.
2) 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 equation (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.
3) 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.
4) The extrapolation outside the specified or experimental measurement is a limitation to the precision of the analyzed values due to possible errors but tremendous improvement can be made with the extrapolation method.

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