The High Energy Region of the Absorption Edge of a-Si:H (II) , Derivative Methods Analysis

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Abstract

Using derivative methods for the analysis of ϵ_2 -data in the high absorption region of the absorption edge of high quality a-Si:H , taken from Jackson et al and Cody . An important result obtained in our previous paper is confirmed here , that the density of states distributions near the conduction and valence band edges can be approximated by a parabolic law , and the electric dipole matrix element is nearly constant

in the energy range (2-2.7 eV) and then slowly decreases with photon energy .

In addition , it was found that the Tauc plot is not suitable for the analysis of ϵ_2 (or α) data of high quality GD a-Si:H in the high absorption region of the absorption edge .

1.Introduction

In a pervious paper [1] ; we used the experimental data of Jackson etal [2] for the density of states convolution integral J(E) as a function of photon energy E for GD a-Si:H films in the energy range (1.6-3.7)eV .

J(E) depends only on the density of states distribution in contrast to the imaginary part of the dielectric function ϵ_2 (E) which depends also on the transition matrix element ; that aided us to conclude , from plotting $J^{1/2}$(E) vs. E and obtaining a straight line in the energy range (~1.8-3.3eV) , that the density of states near the conduction (valence) band edge can be fitted to a parabolic behaviour (i.e $N(E) \propto E'^{1/2}$ where E' is the state energy) .

This led us to conclude that the theoretical model due to Cody [3] ($N(E') \propto E'^{1/2}$; $R^2(E)$ = constant , where R is the electric dipole matrix element) is in accordance with experimental results of Jackson etal [2] .

Here , we extend our study of the high absorption region of the absorption edge of good quality , a-Si:H using derivative methods .

2-Theory

ϵ_2 (E) for amorphous semiconductors , is given by [2] :

$$\epsilon_2 (E) = \text{const.}\ R^2 (E)\ J(E) \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where $R^2(E)$ is the normalized average dipole matrix element squared , J(E) is defined as

$$J(E) = \int (N_v(E')\ N_c(E'+E)\ dE \quad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Where $N_v(E')$, $N_c(E')$ is the valence (conduction) band density of states function .

It is usually assumed but not necessarily correct the density of states distribution near the band edges a simple obeys power law i.e $N(E')\alpha E'^{m}$ where m is a positive constant . If $R^2(E)$ also obeys a simple power law of the form $R^2(E)\alpha E^{-q}$ where q is a constant . The general solution of (1) using the above assumptions is :

$$\epsilon_2 (E) = KE^{-q}(E-E_o)^r \quad \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Where K is a constant , r =2m+1 [4] for a symmetrical density of states for the conduction and valence bands , and E_o is a parameter usually identified as the optical energy gap i.e $E_o=E_{opt}$.

Tauc [5] assumed that $N(E') \propto E'^{1/2}$ and a constant momentum matrix element ($P^2(E)$ = const.) leading to

$$E^2 \epsilon_2 = A(E-E_{opt})^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

Where as Cody [2] assumed that the electric dipole momentum matrix element is constant keeping the same assumption for the density of states , leading to

$$\epsilon_2 = B(E-E_{opt})^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots (5)$$

A and B are constants

Thus either of the plots of $(E^2 \epsilon_2)^{1/2}$ or $\epsilon_2^{1/2}$ vs.E leads to a straight line with Eopt deduced from the extrapolation to the E-axis .

Both approaches or any similar approach are not conclusive in obtaing a dependable value for Eopt. This can be simply understood from eq.3 , because unless we know either q or / and r we cannot obtain a dependable value for Eopt for amorphous semiconductors .

This delimma stresses the great importance of Jackson etal [2] results as exploited more

fully (as hoped) by A. Ibrahim [6] and Al-Ani etal [7] .

In view of the above difficulties the derivative methods proposed by Al Ani [8] and Ray and Hogarth [9] are exploited here for the analysis of ϵ_2 - data of GD a-Si:H data taken from Jackson etal [2] and Cody [3] .

The derivative of eq.3 can be easily obtained by taking the log and deriving with respect to E [6,7] , leading to :

$$\left[\frac{\epsilon' 2}{\epsilon 2} + \frac{q}{E}\right]^{-1} = \frac{E - Eopt}{r} \quad \ldots\ldots\ldots\ldots\ldots\ldots (6)$$

Where $\epsilon'_2 \equiv d\,\epsilon_2/dE$

Because q has to be chosen in advance ; eq. (6) does not offer an independent method to obtain Eopt and r , but we hope that the higher sensitivity of the derivative function compared to the original function might lead to some important information although at the expense of accuracy because of known numerical problems .

3- Results and Discussion

ϵ_2 – data were taken from Jackson etal [2] and Cody [3] for high quality (solar cell grade) GD a-si:H films .

The numerical derivative was computed by fitting the (smooth) data to a fourth - order polynomial then taking the analytical derivative of the polynomial function with respect to E .

To further confirm our previous results concerning the analysis of Jackson etal [2] results mentioned in the introduction , we ploted ϵ_2/ϵ'_2 vs E in the range (2-3.3eV) (i.e for r=2 and q=0) in eq.3 for both Jackson etal [2] and Cody [3] data as shown in figures 1 and 2 .

It is clearly evident that this plot (in both cases) is fairly linear in the range (~2-2.6 eV) and the deviates significantly from linearity above 2.6eV .

The straight line portions of the two plots are fitted to the equation below :

$$\frac{\epsilon 2}{\epsilon' 2} = \frac{E - 1.68}{2} \quad \ldots\ldots\ldots\ldots\ldots\ldots (7)$$

Where Eopt is chosen 1.68 eV, the value obtained in our previous paper [1] from the extrapolation of the straight line of $J^{1/2}$ vs. E plot for Jackson etal data . These results confirm our previous findings [1] that the model due to Cody [3] is the most suitable for high quantity GD a-Si:/H .

The deviation from linear behavior is attributed to a matrix element effect discussed in our previous paper [1] where the $R^2(E)$ vs.E plot for Jackson etal [2] results showed roughly a slight deviation from constancy above about 2.7eV .

The above useful conclusions were not obtained independently using the derivative methods but indeed consolidated our

previous important findings from the direct analysis of Jackson etal [2] results .

An independent benefit from these methods is also found here as shown below .

The Tauc plot (r=2 and q=2 in eq.3) was tested for good fit for ϵ_2- data of both Jackson etal [2] and Cody [3] .

Figures (3) and (4) shows the computed $[\epsilon'_{2/} \epsilon_{2+2/E]}^{-1}$ vs.E data for Jackson etal and Cody samples . The complete misfit between the above data and the data that should result from a Tauc plot $[[\epsilon'_{2/} \epsilon_{2+2/E]}^{-1} = E-1.86/2]$ is quite apparent for both samples .

The above result is an example evidence for the unsuitability of the Tauc plot for fitting with ϵ_2-data of the high absorption region of the absorption edge of high quality GD a-Si:H important is solar cell and other important opto – electronic applications .

References

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Figure Captions

Figure 1 , Computed $\epsilon_{2/}\epsilon'_2$ data for Jackson etal [2] GD a-Si:H samples .

Figure 2 , Computed $\epsilon_{2/}\epsilon'_2$ data for Cody's [3] GD a-Si:H samples .

Figure 3 , Computed $[\epsilon'_{2/} \epsilon_{2+2/E]}^{-1}$ data for Jackson etal [2] GD a-Si:H samples .

Figure 4 , Computed $[\epsilon'_{2/} \epsilon_{2+2/E]}^{-1}$ data for Cody's [3] GD a-Si:H samples

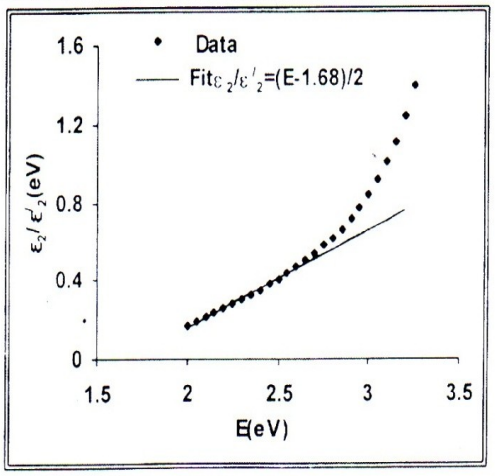

Fig.(1)

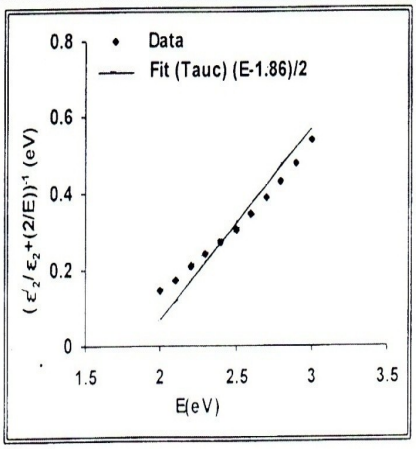

Fig.(3)

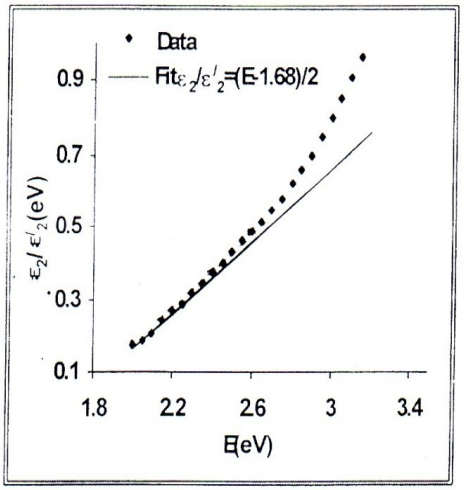

Fig.(2)

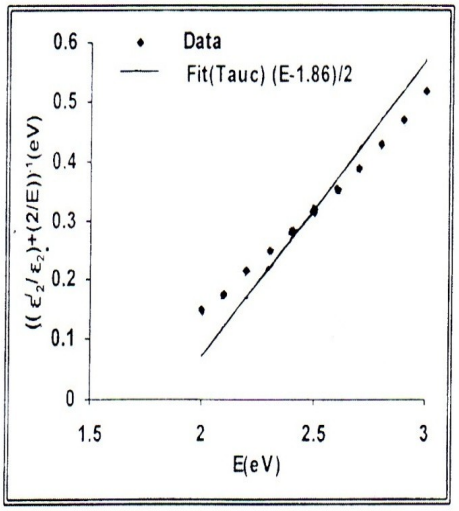

Fig.(4)