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The High Energy Region of the Absorption Edge of a-Si:H, a Theoretical Study—III

Salwan Kamal Jamil Al-Ani*#, Abdullah Ibrahim, Subhi Saeed Al-Rawi

Physics Department, College of Science for Women, Baghdad University, Baghdad, Iraq.
Email: *salwan_kamal@yahoo.com

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ABSTRACT

In this paper we try to give a reasonable account for the origin of the experimental optical energy gap E_o of a-Si:H deduced from the plot due to Cody ($\varepsilon_2^{1/2}$ vs. E). Using a realistic model density of states diagram for a-Si:H and the constant dipole matrix element assumption, and a reasonable definition of the real optical energy gap E_G, a new theoretical equation for $\varepsilon_2(E)$ was derived. The plot of the square root of this function $\varepsilon_2^{1/2}$ as a function of the photon energy E for appropriate fitting parameters gives a straight line fit in the energy region of significance extrapolating to the energy axis at a value similar to the experimental optical gap but about 0.1 eV lower than the theoretical optical gap E_G proposed in our paper. We conclude that the experimental optical gap E_o does not necessarily coincide with any optical transition threshold in the density of states diagram of a-Si:H.

Keywords: High Energy; Absorption Edge

1. Introduction

In two previous papers [1,2], we concluded from the re-analysis of the experimental results of Jackson *et al.* [3] for the density of states convolution integral $J(E)$ as a function of photon energy E for GD a-Si:H in the energy range (1.6 - 3.7 eV), that the theoretical model due to Cody [4] is the suitable theoretical model for the interpretation of the optical data at the high absorption region of the optical absorption edge of this important material.

This model assumes a parabolic density of states (DOS) distribution near each of the valence and conduction band edges (similar to the Tauc [5] model), and a constant dipole matrix element (Tauc assumed a constant momentum matrix element).

The problem of the interpretation of the optical energy gap E_{opt} is still a matter of controversy in literature [4,6]. For example in the case of our analysis, the optical gap obtained from the plot attributed to Cody ($\varepsilon_2^{1/2}$ vs. E) which is ~1.68 eV does not match with the value of the mobility gap of Jackson *et al.* [3] samples *i.e.* ~1.93 eV. While the gap obtained from the famous Tauc plot ($E\varepsilon_2^{1/2}$ vs. E) ~1.89 eV is significantly closer to the value of the mobility gap for Jackson *et al.* samples.

In this paper we try to give a reasonable explanation for this problem, which we hope that it gives a possible clue towards the understanding of the problem of the interpretation of the optical energy gap problem in amorphous semiconductors.

2. Theory

The imaginary part of the dielectric constant $\varepsilon_2(E)$ for amorphous semiconductors is given by [3]:

$$\varepsilon_2(E) = \text{const}\ R^2(E) J(E) \tag{1}$$

where $R^2(E)$ is the normalized average dipole matrix element and $J(E)$ is defined as:

$$J(E) = \int N_V(E) N_C(E' + E)\,\mathrm{d}E \tag{2}$$

where $N_v(E')$ and $N_c(E')$ are the valence and conduction band density of states functions respectively and E' is the state energy.

It usually assumed that the density of states distribution near each of the valence and conduction band edges is some simple power law *i.e.* $N(E') \alpha E'^m$. If $R^2(E)$ also obeys a simple power law of the form $R^2(E) \alpha E^{-q}$. The general solution of Equation (1) using the above assumptions is [4]:

$$\varepsilon_2(E) = KE^{-q}(E - E_o)^r \tag{3}$$

where K is a constant, $r = 2m + 1$ (for symmetrical DOS), and E_o is a parameter usually identified with the optical energy gap E_{opt} ($E_o = E_{opt}$) though of course this is not

*Corresponding author.
#Present address: NCPW, P.O. Box (25777), Doha, Qatar.

necessarily true.

For the Tauc model [5] $N(E')\alpha E'^{1/2}$ and the momentum matrix element squared ($P^2(E)$) is constant, thus $q = 2$ and $r = 2$ in Equation (3), then the relation $E\varepsilon_2^{1/2} = A(E - E_o)$ gives a straight line with E_o as the Tauc gap.

For the Cody approach [4] the only variant with the Tauc approach is the assumption of a constant dipole matrix element $R^2(E)$ = const., Thus $q = 0$ and $r = 2$ in Equation (3), then the relation $\varepsilon_2^{1/2} = B(E - E_o)$ gives a straight line with E_o different from the Tauc gap usually lower.

The optical energy gap E_o is obtained from the extrapolation of the straight line to the photon energy axis.

In this paper our main concern is with interpretation of E_o using a detailed model density of states for a-Si:H assuming a reasonable theoretical optical energy gap in order to deduce a new equation for $\varepsilon_2(E)$.

3. Our Theoretical Analysis

Figure 1 depicts the model density of states diagram based mainly on the standard model applied for electronic quality a-Si:H. Here we take every possible detail into account accept for the effect of exponential tails on the resulting E_o which was studied previously by Malik and O'Leary [7]. In this figure we note the following:

1) The density of states distribution in the extended states near each of the valence and conduction band edges E_v and E_c respectively is parabolic ($N(E')\alpha E'^{1/2}$).

2) In the localized states regions just under the conduction band edge ($E_c - E_c' = \Delta E''$), and just above the valence band edge ($E_v' - E_v = \Delta E''$) the density of states distributions are also parabolic.

3) In the regions far away from each of the band edges, the density of states distributions is exponential in nature.

4) The energy interval (ΔE) in **Figure 1** is ($E_c - E_A = E_B - E_v$) *i.e.* the density of states diagram is assumed to be symmetric.

5) The energy interval ($\Delta E'$) in the same figure is ($E_c' - E_A = E_B - E_v'$).

6) The real optical energy gap which is defined as E_G represents in this diagram the assumed threshold for optical transitions responsible for the high energy region of the absorption edge which is ($E_c' - E_v$ or $E_c - E_v'$).

This last definition of E_G is based on the experimental findings of Jackson *et al.* [3] that the matrix element is nearly the same for localized-extended and extended-extended transitions. We call E_G the real optical gap because it is defined from the density of states diagram and not from the analysis of optical data *i.e.* E_{opt}, there is no a priori necessity or assuming them equal.

According to **Figure 1**:

$$N_V(E') = N(E_V')\{E_B - E'/\Delta E_V\}^{1/2} \quad (4a)$$

$$N_C(E') = N(E_C')\{E' - E_A/\Delta E_C\}^{1/2} \quad (4b)$$

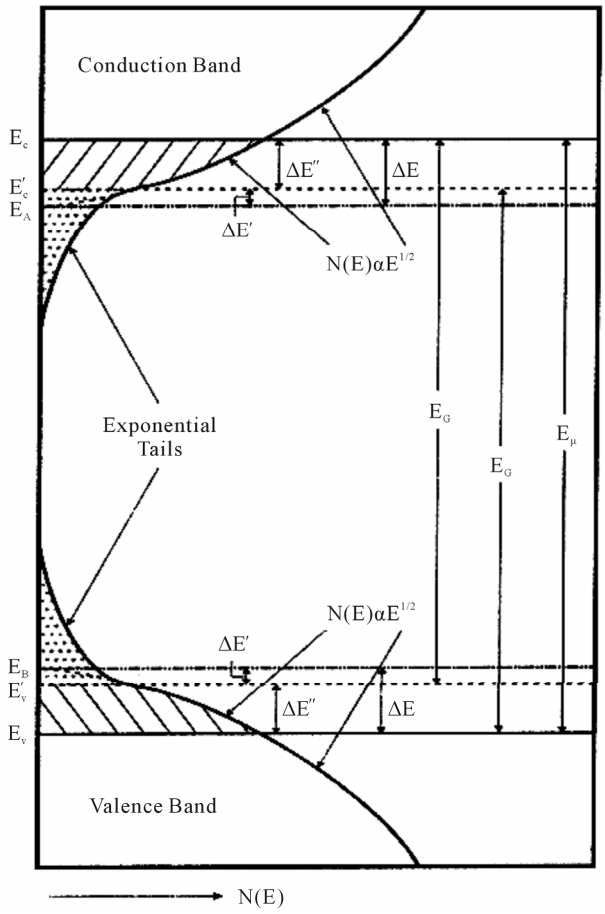

Figure 1. The model density of states diagram of a-Si:H.

where $N(E_v')$ and $N(E_c')$ are the densities of states at the valence and conduction band edges respectively.

For amorphous silicon and un-polarized light the prefactor in Equation (1) is equal to $(2\pi e)^2R^2(E)/3\rho_A$ [3] where ρ_A is the atomic density, taking this into account we substitute Equations (2) and (4) in Equation (1) to get [6]:

$$\varepsilon_2(E) = \frac{(2\pi e)^2 R^2(E) N^2(E_C')}{3\rho_A \Delta E}(E - E_G)^2 \cdot f(E) \quad (5)$$

where:

$$f(E) = (E - E_G)^2\left[\frac{b(E)-2}{4}\sqrt{b(E)+c(E)-1} - \frac{b(E)}{4}\sqrt{c(E)} - \left(\frac{b^2(E)+4c(E)}{8}\right)\right] \sin^{-1}\left[\frac{2-b(E)}{\sqrt{b^2(E)+4c(E)}}\right] + \sin^{-1}\left[\frac{b(E)}{\sqrt{b^2(E)+4c(E)}}\right] \cdot (6-a) \quad (6a)$$

$$b(E)=1-\frac{\Delta E-\Delta E'}{E-E_G} \quad (6b)$$

$$c(E)=\frac{\Delta E}{E-E_G}\left[1+\frac{\Delta E'}{E-E_G}\right] \quad (6c)$$

We see that Equation (5) includes three main parameters of the model density of states of **Figure 1** $E_G, \Delta E$ and $\Delta E'$, $\Delta E-\Delta E'$ in Equation (6b) is just $\Delta E''$.

For a-Si considering ρ_A is that for c-Si, Equation (5) becomes:

$$\varepsilon_2(E)=0.43\times10^{-44}R^2(E)\frac{N^2(E_C)}{\Delta E}f(E) \quad (7)$$

where $R^2(E)$ is in units of Å^2, E in eV, and $N(E_c)$ is in units of eV^{-1}·cm^{-3}

4. Results and Discussion

The function $f(E)$ is plotted for chosen parameters ($X = E_G$) = 1.78 eV, ($Y = \Delta E$) = 0.18 eV and ($Z = \Delta E'$) = 0.03 eV and the result is depicted in **Figure 2**.

If we plot the square root of this function *i.e.* $\sqrt{f(E)}$ as function of E, then **Figure 3** gives a straight line that fits the equation 0.654E−1.68, we see that the extrapolation to the x-axis is equal to ~1.68 eV which is equal to that for Jackson *et al.* [3] samples.

Thus although the assumed real optical gap E_G in our model was 1.78 eV the optical gap that results from the $(f(E))^{1/2}$ vs. E) plot is 1.68 eV which 0.1 eV smaller. Thus we conclude that the experimental optical energy gap E_{opt} is not an accurate marker of the energy gap responsible for the threshold of optical transitions responsible for the high energy region of the absorption edge.

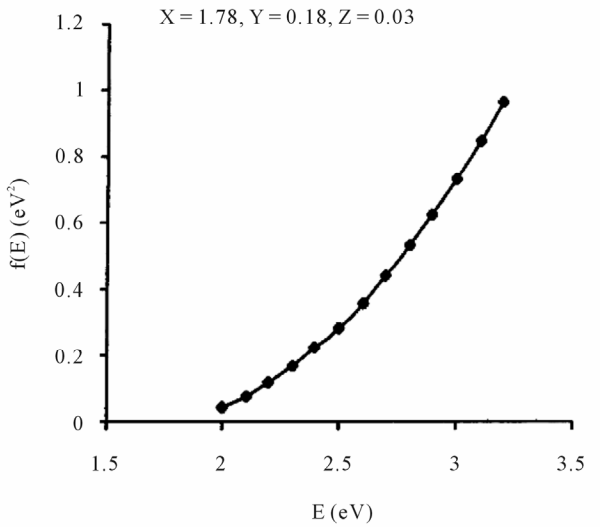

Figure 2. Plot of the function $f(E)$ vs. E for the fitting paramers $X = E_G = 1.78$ eV, $Y = \Delta E = 0.18$ eV, $Z = \Delta E' = 0.03$ eV.

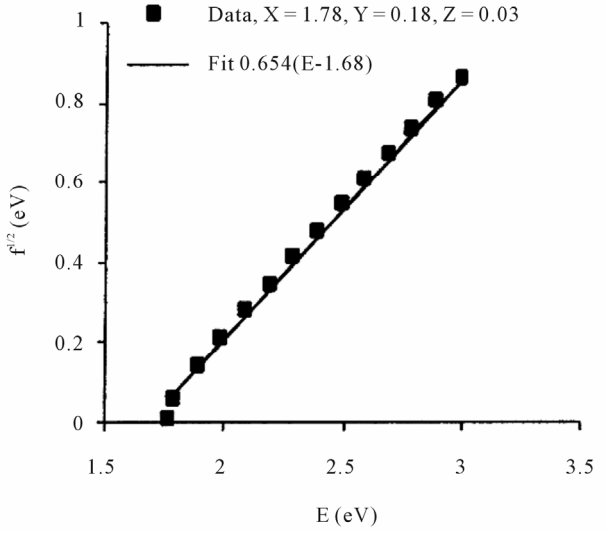

Figure 3. Plot of $f^{1/2}(E)$ vs. E for the fitting parameters X = 1.78 eV, Y = 0.18 eV, Z = 0.03 eV. It is fitted to the straight line equation 0.654(E−1.68).

Malik and O'Leary [7] also reached a similar conclusion albeit for a different reason which is the exponential band tailing at the valence and conduction band edges.

We may also conclude and suggest that may be by joining the two approaches *i.e.* accounting for exponential band tailing suggested by Malik and O'Leary [7] and our suggestion that the real optical gap does not necessarily start at the valence and conduction bands edges as suggested originally by Tauc (5) might be the right clue to account for the physical origin and the value of the experimental optical energy gap (E_{opt}) deduced from the plot due to Cody [4] $\in_2^{1/2}$ vs. E if it is adopted to analyze $\in_2$ data of a-Si-H in the high energy region of the absorption edge.

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