



# World Renewable Energy Congress 2006

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## The high Energy Region of the Absorption Edge of a-Si:H , An analytic study

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### Abstract

In this work , the authors used the experimental results due to Jackson et al for the density of states convolution integral  $J(E)$  vs. photon energy  $E$  for GD a-Si:H films in the energy range (1.6-3.7)eV . We plotted the square and the cubic roots of  $J(E)$  as a function of  $E$  , the square root plot  $J^{1/2}(E)$  exhibited a fairly linear behaviour in the energy range (-1.8-3.3)eV . Because  $J(E)$  depends only on the density of states distributions near the band edges of the valence and conduction bands , in contrast to the imaginary part of the dielectric function  $\epsilon_2(E)$  which depends also on the transition matrix element , we concluded that the density of states distribution near each band edge could be approximated by a parabolic law behaviour i.e  $N(E)\propto E^{1/2}$  . As Jackson et al found the electric dipole matrix element squared  $R^2(E)$  is constant in the energy range of for GD a-Si:H films , we conclude that the theoretical model due to Cody ( $N(E)\propto E^{1/2}$  ,  $R^2(E) = \text{constant}$ ) is in accord the above experimental findings .

Thus we recommend the plot due to Cody ( $\epsilon_2^{1/2}$  vs. $E$ ) as the most suitable plot to analyze  $\epsilon_2$  - data of the high absorption region of the optical absorption edge of high quality GD a-Si:H films , and Cody's theoretical model as the proper entry towards a possible future solution of the optical gap problem in this material at least .

### Introduction

It is well known , that the magnitude of the forbidden gap and its relation to the optical absorption edge is still a mystery in amorphous semiconductors [1] . Fundamentally , this is because that the optical absorption depends not on a convolution of the conduction band (CB) and valence band (VB) density of states but also on the transition matrix element [2] .

In order to possible solve this dilemma , two independent measurements of the density of states distributions close to both edges of the valence and conduction bands , and the optical absorption spectrum of the high photon energy region ( $\alpha \geq 10^4 \text{ cm}^{-1}$ ) where  $\alpha$  is the absorption coefficient of the absorption edge on the same samples or at least prepared at the same run , should be performed .

Because of the difficulties in achieving such kind of a project , it is seldom found in literature , except may be is the very important and it might be considered unique work of Jackson et al [2] about 20 years ago , where they determined the energy dependence of

the optical matrix element of GD- a-Si:H films using independent measurements results of the density of states and the  $\epsilon_2$  spectra . (where  $\epsilon_2$  is the imaginary part of the dielectric function ) in the energy range (~0.6-6eV) .

We think that the correct implications of this important and fairly accurate work are not well established in the scientific society , except for an important note stated by Cody some years ago [3] .

For this purpose , and on behalf of Jackson et al important work , the authors here studied it in more details , to make use of its full implications , in the hope of catching the right thread towards a possible solution of the optical gap problem in the near future at least for high quality GD a-Si:H films which are now very important optoelectronic materials .

### Theory

Following Jackson et al [2] , the imaginary part of the dielectric function an amorphous structure and unpolarized light is given by :

$$\epsilon_2(E) = \frac{(2\pi)^2}{3\rho_A} R^2(E) \int N_v(E'+E) dE' \text{----- (1)}$$

Where E is the photon energy ,  $E'$  is the state energy , e is the electron charge ,  $N_v(E')$  [ $N_c(E')$ ] is the valence (conduction ) band density of states ,  $\rho_A$  is the atomic density , and  $R^2(E)$  is the square of the normalized (with respect of the crystal) average dipole matrix element .

If for simplicity , we assume that the density of states distribution near the mobility edge of the valence (conduction) band is a simple power law ( $N(E') \propto E'^m$  i.e symmetrical DOS (an assumption which is usually not easy to justify in amorphous materials) we can define a theoretical optical energy gap  $E_o$  as seen in the following resulting expression [1]

$$E^q \epsilon_2(E) = K_m (E - E_o)^r \text{----- (2)}$$

Where :  $K_m$  is a theoretical prefactor , q is an index indicating the simple power dependence of the dipole matrix element (if possible) ( $R^2 \propto E^{-q}$ ), ( $r = 2m + 1$ ) and  $E_o$  exactly defined if the limits of the density of states convolution integral in eq.1 is equal to the zeros of the two functions inside it [4] .

Because the dependence of  $\epsilon_2(E)$  on both the values of q and r , there is no unique way to define the exact value of the optical gap  $E_o$  only if an independent measurement of the density of states near the mobility edge is accomplished for the sample under study which is a very hard task . According to our knowledge , only Jackson et al [2] succeeded in doing for GD a-Si:H samples , the energy dependence of  $R^2(E)$  in the energy range (~0.6-5.9)eV was determined from combined measurements of the optical absorption and

the density of states distribution in the appropriate energy range for GD a-Si:H samples prepared by the above authors .

They found that the dipole matrix element ,  $R^2(E)$  , the constant within the errors of their experiment for energy up to 3.4eV and decreases roughly as  $E^{-5}$  above this energy .

This is in partial accordance with the assumption of Cody [1] that the dipole matrix element is constant (to ~ 20eV) and not the momentum matrix element  $P^2(E)$  as proposed previously by Tauc [5] .

In accord with to equation (2) ,with  $q=0$  as the above mentioned experimental results indicated , Cody [1] found that this data of  $\epsilon_2^{1/2}$  for a-SiH<sub>x</sub> (x=0.09) as a function of E fits excellently to the linear equation [ $\epsilon_2^{1/2} = 3.06 (E-1.64)$ ] in the board energy range (1.6-3)eV , this means that r should equal to 2 in eqn. 2 in order to conform with the experimental results of Jackson et al [i.e  $q=0$ ] , which means that  $N(E')$  could be well approximated to a parabolic dependence on the state energy  $E'$  [i.e  $N(E') \propto E'^{r/2}$ ] .

In order to check for that , we found the density of states convolution integral data announced by Jackson et al for GD a-Si:H in the energy range (0.6-5.9)eV most beneficial as we shall see below .

### Results and Discussion

Fig.1 shows the main Jackson et al results [2] for  $\epsilon_2(E)$  , J(E) (the density of states integral) and  $R^2(E)$  in the photon energy range[-1.5-5.9]eV.

We have replotted Jackson et al J(E) data as  $J^{1/2}(E)$  and  $J^{1/3}(E)$  as a function of E in the wide range (1.6 – 3.7) eV as shown in fig . 2 , which covers the high energy region of the optical absorption edge of a-Si:H in full .

We note and conclude the following from these plots .

(1)The function  $J^{1/2}(E)$  extracted from experimental J(E) data highly correlates to a linear behaviour in the range (~1.78-3.25)eV a range which covers the high energy region of the absorption edge , and because J(E) does not depend on  $R^2(E)$  and they depends only the density of state distributions of the valence and conduction bands (in contrast to  $\alpha(E)$  or  $\epsilon_2(E)$  which depend on both) therefore according to eq.2 :

$$J(E) \propto (E - E_0)^{2m+1} \text{ -----(3)}$$

As  $r=2m+1 = 2$  according to eq.2 then m should equal to  $1/2$  , which means that we can approximate the density of state distributions of the valence and conduction bands to a parabolic behaviour (i.e  $N(E) \propto E^{1/2}$ ) . We note from fig.2 that  $J^{1/3}(E)$  data does not behave linearly with E at all excluding the narrow energy range (~1.78-2) eV .

(2) The extrapolation of the straight line fit to  $J^{1/2}(E)$  to the energy axis (J=0) gives us  $E_0 \sim 1.68$  eV , while the extrapolation of the short  $J^{1/3}(E)$  line is ~ 1.57 eV .

(3) We conclude the following from the above important notions :

a) The density of states distributions of the valence and conduction bands edges of Jackson et al GD a-Si:H films (which are electronic grade films) can be approximated by a parabolic function i.e with  $m=1/2$  in eq.2 ( $r=2m+1$ ), this is in accordance with the original assumption of Tauc [5] that  $N(E)\propto E^{1/2}$  near the band edges of amorphous semiconductors similar to (at least) crystal semiconductors but for the special case of electronic grade GD a-Si:H films of least.

b) As  $E_0 \sim 1.68$  eV for  $J^{1/2}(E)$  plot, combined with experimental finding of Jackson et al that  $R^2(E)$  is constant in the energy range of interest and that  $N(E)\propto E^{1/2}$  near the band edges of valence and conduction bands of Jackson et al films, and noting that the  $\epsilon_2^{1/2}(E)$  vs.  $E$  plot for Jackson et al films is linear in the energy range of interest ( $\sim 1.6-3$ ) eV with extrapolation to  $E$ -axis giving  $E_0 \sim 1.64$  eV as given by Jackson et al in their paper which is close to the 1.68 eV for the  $J^{1/2}(E)$  extrapolation. We conclude that the most proper theoretical model that should be adopted as the correct start towards a possible understanding of the high energy region of the absorption edge problem in a-Si:H, is the one that is due to Cody [1] who proposed  $R^2(E)$  to be constant and  $N(E)\propto E^{1/2}$  near the band edges for a-Si:H films, excluding Tauc model which is not appropriate for GD a-Si:H films because he proposed that the momentum matrix  $P(E)$  to be constant and not the dipole matrix element in contradiction to the experimental finding of Jackson et al, and the Klazes et al [6] assumptions for a-Si:H films of  $N(E)\propto E^{1/2}$  and  $P^2(E)$  is constant.

Stated in another and more practical way  $E \propto \epsilon_2^{1/2}$  (or  $(\alpha/E)^{1/2}$ ) plot attributed to Cody [1] should be adopted for a-Si:H films and not  $(E^2 \epsilon_2)^{1/2}$  (or  $(\alpha/E)^{1/2}$ ) attributed to Tauc [5] or  $(E^2 \epsilon_2)^{1/3}$  (or  $(\alpha/E)^{1/3}$ ) attributed to Klazes et al [6] because the last two do not conform with the experimental findings of Jackson et al for GD a-Si:H at least. At the end, we think that our conclusions could be considered conclusive for the correct plot to adopt for  $\epsilon_2$  or  $\alpha$  data of good energy gap problem in this material at least is automatically solved, and a correct physical meaning for  $E_{opt}$  defined as the extrapolation of  $\epsilon_2^{1/2}$  plot to the  $E$ -axis, should be searched for. Our attempts toward a possible solution of this problem will be published later.

### References

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**Figure Captions**

- (1) Figure (1) : Jackson etal results , for GD a-Si:H [2] (a)  $\epsilon_2$  vs. $E$  on a linear plot .  
(b)  $\epsilon_2$  ,  $J$  , and  $R^2$  vs. $E$  on a semi logarithmic plot .
- (2) Figure (2) :  $J^{1/2}$  and  $J^{1/3}$  vs. $E$  plotted using Jackson etal  $J(E)$  data [2] in the energy range (1.6-3.7)eV .



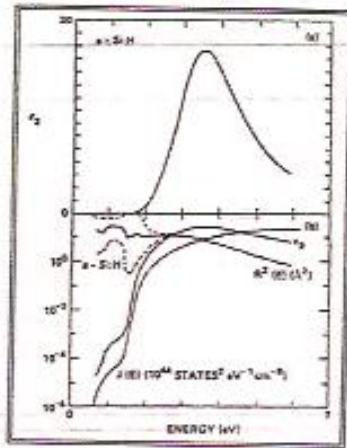


Figure (1) : Jackson et al result , for GD a-Si:H [2] (a)  $\sigma_2$  vs.E on a linear plot . (b)  $\sigma_2$  , J , and  $R^2$  vs.E on a semi logarithmic plot .

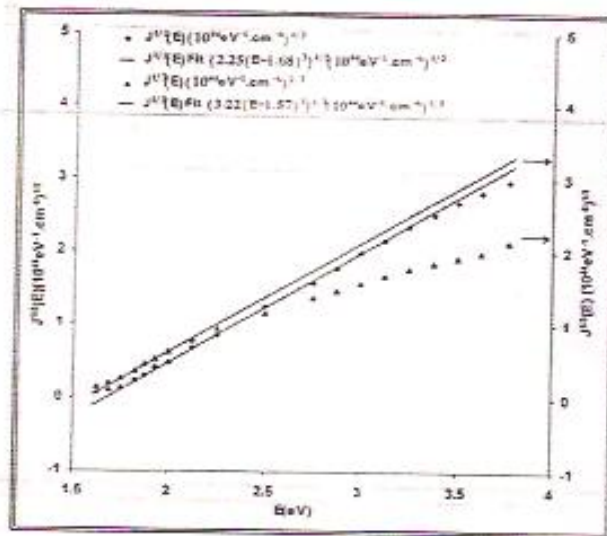


Figure (2) :  $J^{1/2}$  and  $J^{1/3}$  vs.E plotted using Jackson et al  $J(E)$  data [2] in the energy range (1.6-3.)eV .