A Study of a-Si:H Absorption Edge Using Dunstan’s Model

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Abstract:

The optical absorption data of Hydrogenated Amorphous Silicon was analyzed using a Dunstan model of optical absorption in amorphous semiconductors. This model introduces disorder into the band-band absorption through a linear exponential distribution of local energy gaps, and it accounts for both the Urbach and Tauc regions of the optical absorption edge. Compared to other models of similar bases, such as the O’Leary and Guerra models, it is simpler to understand mathematically and has a physical meaning. The optical absorption data of Jackson et al and Maurer et al were successfully interpreted using Dunstan’s model. Useful physical parameters are extracted especially the band to the band energy gap $E_o$, which is the energy gap in the absence of disorder, that can be interpreted as the mobility gap of the material.

Keywords: Dunstan model, Localized states, Mobility gap, Tauc model, Urbach model.

Introduction:

The use of the Tauc model for optical absorption is the most common in researches to obtain the so-called the energy gap of semiconductors in general, and amorphous semiconductors in particular. It was a successful model in defining an effective optical gap for amorphous semiconductors, although its physical meaning is still somewhat obscure. Tauc model virtue is in its simplicity as known to researchers. However the disadvantage of Tauc model is its neglect of absorption due to band tails, it is a model of band to band absorption only, therefore it neglects the effect of disorder on the absorption edge which appears mainly in the Urbach tail of the semiconductors. Many researchers developed more sophisticated models which include the Urbach tail and its effect on the Tauc edge of amorphous semiconductors such as the O’Leary with various co-authors and Guerra et al. Their models accounted for both the Urbach and Tauc regions of the absorption edge, these researchers main achievement is that they introduced analytical models that can also be handled numerically to model the absorption edge of amorphous semiconductors to obtain useful model parameters, also they clarified the role of absorption due to tails on the Tauc edge itself. However, there is an older model due to Dunstan which accounted for the disorder through the Urbach edge which is simpler in mathematical form than O’Leary and Guerra models, but as claimed and investigated by Dunstan that his model accounted for most optical data he studied. With the exception of Frova and Selloni, this simple model seems to remain unexploited in literature although mentioned by Guerra et al, who developed a single poly-logarithm equation to fit Urbach and Tauc regions simultaneously which is very useful and is based on the same band fluctuation model of Skettrup adopted by Dunstan. The aim of this work is to use and further exploit Dunstan's model to analyze and model quality optical absorption data of a-Si:H due to Jackson et al and Maurer et al, which is in our opinion, a simple model and clear in its physical meaning, and can account satisfactorily for experimental data. We believe that Dunstan's model is unjustly neglected in literature and deserves further exploitation. We adopted this model because we believe it is the simplest analytical model beyond the Tauc model that can account satisfactorily for the effect of disorder on the absorption edge of amorphous semiconductors, and from which the mobility gap of the material could
be extracted, also further physical insight can be obtained beyond the Tauc approach.

**Theoretical Background:**

The original Tauc model is a model of the region of high optical absorption \( (\alpha \geq 10^3 \text{cm}^{-1}) \), where \( \alpha \) is the absorption coefficient of the absorption spectrum of amorphous semiconductors is given by the well-known Tauc equation \(^2\) \(^2\) \(^2\) \(^2\)

\[
\alpha E = B_{\text{Tauc}}(E - E_{\text{Tauc}})^2 \quad \ldots \quad 1
\]

Where \( E \) is the photon energy, \( E_{\text{Tauc}} \), the Tauc optical gap and \( B_{\text{Tauc}} \) is a pre-factor.

A more appropriate model to a-Si:H thin films, Cody et al.\(^2\)\(^2\)\(^2\) adopted Tauc model but with a slight modification, that is the constant dipole matrix element assumption\(^2\) instead of the constant momentum matrix element of Tauc, thus the Cody expression is given by:

\[
\alpha / E = B_{\text{Cody}} (E - E_{\text{Cody}})^2 \quad \ldots \quad 2
\]

Where \( E_{\text{Cody}} \) is the Cody model optical gap, and \( B_{\text{Cody}} \) is a pre-factor.

As Tauc and Cody models do not take into account optical transitions due to tail states, they tend to underestimate the energy gap proposed by their models\(^2\). Dunstan’s model\(^2\) is an old and unjustly neglected model which accounts for the effect of tail states on the obtained optical gap. Dunstan considered that static and thermal disorders lead to a distribution of local energy gaps \( E_g \) which have the form:

\[
P(\eta) = \frac{1}{E_u} e^{-\frac{\eta}{E_u} \eta} \geq 0 \quad \ldots \quad 3
\]

Where \( \eta \) is a disorder parameter responsible for taking \( E_g \) a distribution of values \( E_0 - \eta \) \( E_0 \) is the energy gap in the absence of disorder \), and \( E_u \) is the Urbach energy. If the absorption in the local regions is given by a function of the general form, \( \alpha(E) = f(E - E_g) \) \ldots 4

Then the absorption coefficient is expressed by integrating \( f(E-E_g) \) which is the local band to band absorption overall values of \( E_g \), i.e.

\[
\alpha(E) = \int_0^\infty \eta P(\eta) f(E - E_0 + \eta) d\eta \quad \ldots \quad 5
\]

Where the lower limit of the integration \( \ell \) is zero for \( E \geq E_0 \), and is \( E - E_0 \) for \( E \leq E_0 \). Eq.5 represents the general form of Dunstan’s model. For the special case that \( f(E - E_g) \) takes the special form of the Tauc law i.e.

\[
\alpha(E) = \alpha_0 (E - E_0)^2 / E \quad \ldots \quad 6
\]

Eq.5 can be solved analytically to obtain, \( 11,12 \)

\[
\alpha(E) = \frac{2a_\text{Cody}^2 E}{E} \exp \left\{ \frac{E - E_0}{E_u} \right\} \quad \text{for} \ E < E_0 \quad \ldots \quad 7-a
\]

\[
\alpha(E) = \frac{a_\text{Cody}^2}{E^2} \left\{ (E - E_0)^2 + 2E_u(E - E_0) + 2E_u^2 \right\} \quad \text{for} \ E > E_0 \quad \ldots \quad 7-b
\]

Dunstan based his model on the Skettrup model\(^1\). Frova and Selloni\(^1\) neglected conduction band tails which is a suitable approximation for a-Si:H and Si related thin films\(^2\). In eq.7-b, apart from the common factor, the 1st term concerns the contribution of band to band absorption and the 2nd and 3rd terms concern tail states related absorption.

**Figure 1.** A schematic density of states diagram suitable for a-Si:H, which shows the characteristic energy gap parameters \( E_{\alpha}, E_g, \) and \( E_{opt} \).

In Fig.1, we sketch an approximate density of state model suitable for a-Si:H related materials. Here the conduction band tails are neglected; \( E_g \) is the extrapolated bandgap to the zero density of states, which is the energy gap proposed by the Tauc model\(^1\), but due to the neglect of optical transitions originating from tail states in this model, the experimentally obtained optical energy gap \( E_{opt} \) is smaller than \( E_g \) i.e. \( E_{opt} < E_g \). \( E_g \) in fact, is the bandgap extracted from the O’Leary model when conduction band tails are neglected\(^3\). \( E_g \) is the energy gap between the band edges \( E_g = E_v - E_c \) which is the energy gap parameter deduced from Dunstan or Guerra models, it might be interpreted as the mobility gap of the material. Another important result derived by Dunstan\(^1\), is from the inversion of eq.5 without imposing any specific form for the band to band absorption \( f(E - E_0 - \eta) \). He obtained the following result.

\[
f(E) = \alpha(E) \left\{ \alpha(E) - \dot{\alpha}(E)E_u f \text{or} \ E > E_0 \right\} \quad \ldots \quad 8
\]

Where \( \dot{\alpha}(E) = d\alpha/dE \).
Thus by evaluating the numerical derivative of the absorption data in the Tauc region, the band to band absorption function \( f(E) \) can be calculated from eq.8. Thus if \( f(E) \) obeys the Tauc power law the plot of \( \{Ef(E)\}^{1/2} \) vs \( E \) gives a straight line with an extrapolated gap \( E_0 \), the bandgap in the absence of disorder.

**Results and Discussion:**

The optical absorptions data of device quality a-Si:H films prepared by Jackson et al18 which are given in terms of the imaginary part of the dielectric function \( \varepsilon_2(E) \) are analyzed here. Fig.2 shows the plots of \( \varepsilon_2^{1/2} \) and \( f^{1/2}(E) \) vs. \( E \) in a wide data range (\( E \approx 1.5-3 \) eV). Here the Cody model is adopted for the \( \varepsilon_2 \) data and also to the band to band absorption \( f(E) \) extracted using eq.8 (\( f(E) = \varepsilon_2(E) - \varepsilon_2(E)E_u \)) was obtained from the Urbach plot of Jackson et al data in the Urbach region giving \( E_u = 50 \) meV, and \( \varepsilon_2 = d\varepsilon_2/dE \) were numerically calculated in the photon energy range (\( \sim 1.7-3 \) eV). The energy gap parameters obtained are \( E_{Cody} = 1.627 \) eV in the fitting range (\( \sim 1.7-3 \) eV) and \( E_0 = 1.68 \) eV. It is obvious from the results that (\( E_0 = 1.68 \) eV) is larger by about 0.05 eV than \( E_{opt} \approx 1.63 \) eV. Two points are noticed is (1) \( E_0 \approx E_{Cody} + E_u \) as was originally claimed by Dunstan according to his model, but it should be mentioned that this is true only for low disorder films such as the one by Jackson et al here. For large \( E_u \) the relation between \( E_0 \) and \( E_{Cody} \) is slightly nonlinear (frova1985), (2) the \( E_0 \) value obtained for Jackson et al18 a-Si:H sample (\( \sim 1.68 \) eV) is the same as the value obtained by Orapunt et al 2011 from the O’Leary model, which they suggested as the value of the mobility gap of Jackson et al a-Si:H samples. The three parameters obtained here for a-Si:H films, \( E_u = 0.05 \) eV, \( E_0 = 1.68 \) eV and the slope value of \( f^{1/2} vs. E \) plot i.e. \( 3.067 \) eV \(^{-1}\) are substituted in Dunstan eqs.7-a & 7-b but here for the Cody constant dipole matrix element instead of the constant momentum matrix element model of Tauc.

![Figure 2. Linear fits for \( \varepsilon_2^{1/2} \) and \( f^{1/2} \) vs. photon energy of Jackson et al18 a-Si:H samples.](image)

The result is shown in Fig.3. First we see that the Dunstan model fits well the \( \varepsilon_2 \) data of a-Si:H of Jackson et al in the wide range of photon energy (\( \sim 1.5-3 \) eV) using the model parameters deduced from the Cody-like linear fitting of \( f^{1/2}(E) vs. E \). Second, the contributions of the band to band absorption and the tail to band absorption are shown. It is seen that the tail to band absorption is dominant in the range \( E = E_0 = 1.68 \) eV to \( E \sim 1.82 \) eV at the intersection point, then band to band increasingly dominates. This result of the Dunstan model is similar to the O’Leary model prediction illustrated in Fig.3 of ref18.

![Figure 3. Direct Dunstan model fit for Jackson et al18 a-Si:H samples.](image)

Optical Absorption data prepared by Maurer et al19 were also analyzed here they used Plasma Enhanced Chemical Vapor Deposition (PECVD) method to prepare their samples. They irradiated them with pulsed laser at \( \lambda = 532 \) nm in a highly controlled manner to study the effects of controlled hydrogen out-diffusion resulting from laser heating for short times. One of their important results is the determination of the optical absorption

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spectra of their samples as a function of the maximum heating temperature $T_{\text{max}}$ in a wide photon energy range. In our analysis here, the constant dipole matrix element approximation of Cody is used.

Figure 4. Linear fits for $(F/E)^{1/2}$ vs photon energy of a-Si:H samples at five $T_{\text{max}}$ values.

Figure 4 shows the plot of $(f(E)/E)^{1/2}$ vs. $E$ for Maurer et al a-Si:H samples for five $T_{\text{max}}$ values ranging from 407°C to 655°C. The data were linearly fitted using the least squares method. The extrapolated $E_o$ values tend to decrease with increasing $T_{\text{max}}$. $E_{\text{Cody}}$ of the samples showed a similar trend as depicted in Table I. The Dunstan model parameters are obtained from the linear fittings of Fig. 4. In order to assess the validity of the linear fitting results. The optical data were nonlinearly fitted to the direct Dunstan model equations (i.e. eqs. 7a & 7b but using the constant dipole model approximation). Fig. 5 shows the fitting results. It is obvious that the Dunstan model is capable of capturing the main features of the optical absorption data of a-Si:H samples prepared by Maurer et al.

Figure 5. Direct Dunstan model fits (eqs. 7a and 7b) for Maurer et al a-Si:H samples using parameters extracted from the Urbach plot ($E_u$), and $(F/E)^{1/2}$ vs $E$ plots ($E_o, \alpha_o^{1/2}$).

Figure 6 shows a comparative plot of $E_{\text{Cody}}$ vs $T_{\text{max}}$ and $E_o$ vs $T_{\text{max}}$ of Maurer et al a-Si:H data. The linear trend of the data is estimated from least squares fitting. Both $E_{\text{Cody}}$ and $E_o$ decreases with increasing $T_{\text{max}}$ indicating the effect of out-diffusion of hydrogen in decreasing the energy gap. $E_o$ linear trend is relatively slower than $E_{\text{Cody}}$. This means that part of the dependence of $E_{\text{Cody}}$ on Tmax can be attributed to the increase of tail to extended states optical transitions, this interpretation is facilitated by the use of the Dunstan model, while the other part can be attributed to the actual decrease of the mobility gap-related parameter $E_o$ with increasing hydrogen out-diffusion due to increasing $T_{\text{max}}$. Dunstan’s model in its general form eq.5 can also be applied to crystalline semiconductors and nanomaterials.
Conclusion:

In conclusion, in both the Urbach and the Tauc regions, Dunstan model was shown to be successful in fitting and interpreting optical absorption data. More physics can be extracted from the optical data; using this simple model which takes into account tail statescontribution to optical absorption; than the famous Tauc model which neglects these transitions. Dunstan regions, Tauc model due to Dunstan is relatively simpler in form than the important O’Leary and Guerra models, this can assist the experimenter to analyze the optical absorption data of amorphous semiconductors by relatively simple linear or/and nonlinear modeling, and we think it deserves more serious attention, and it should be further studied to assess its validity to wide variety of amorphous materials other than a-Si:H.

Table 1. Model parameters obtained in this paper of a-Si:H samples prepared by Maurer et al. It includes a comparison between Cody and Dunstan models fitting results.

<table>
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<tr>
<th>$T_M$°C</th>
<th>$E_u$ (eV)</th>
<th>$E_{Cody}$ (eV)</th>
<th>$B_{Cody}$(cm$^{-1}$eV$^{-2}$)</th>
<th>$E_*$ (eV)</th>
<th>$\alpha_*$ (cm$^{-1}$eV$^{-3}$)</th>
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<tr>
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<td>1.493</td>
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<td>1.647</td>
<td>110153.43</td>
</tr>
</tbody>
</table>

Authors’ declaration:

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours, have been given the permission for republication attached with the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in University of Baghdad.

Authors’ contributions statement:
The first author analyzed the data, and the 2nd author suggested and developed the project. Both authors participated in writing the paper.

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13. Guerra JA, Tejada A, Töfllinger JA, Grieseler R,


دراسة حافة الأمتصاص الى a-Si:H باستخدام نموذج دونستان

نا فاروق سهل
قسم الفيزياء، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق.

الخلاصة:

تم استخدام نموذج الامتصاص البصري في أشباه الموصلات غير المتبلورة المنسب Dunstan لتحليل بعض بيانات الامتصاص البصري لـ a-Si:H. يقدم هذا النموذج اضطرابًا في امتصاص حزمه الى حزمه من خلال التوزيع الأسي الخطي لفجوة الطاقة الموضعيه، والذي يمكن أن يفسر كلا من منطقتي Urbach و Tauc من حافه الامتصاص البصري. مقارنة بالنماذج الأخرى ذات الأسس المماثلة، مثل نموذجي O’Leary و Guerra، فهو أبسط في الشكل الرياضي وله معنى فيزيائي مباشر. نموذج دونستان نجح في تفسير بيانات الامتصاص البصري لـ Jackson et al و Maurer et al. تم استخراج معلمات فيزيائية مهمة خاصة فجوه الطاقة E° المتعلقة بأنتقالات حزمه الى حزمه والتي هي فجوة الطاقة في حالة عدم وجود اللانتظام، والتي يمكن تفسيرها على أنها فجوة التحركية للمادة.

الكلمات الافتتاحية: نموذج دونستان، الحالت الوضعية، فجوة التحركية، نموذج O’Leary، نموذج Guerra.