

# Calculation of the interband absorption spectra of amorphous semiconductors using the Kubo-Greenwood formula

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A new method is presented for calculating the interband absorption spectrum for amorphous semiconductors using the Kubo-Greenwood formula in accordance with the Davis-Mott approximation method. It is shown that the calculated spectrum of interband absorption explained the experimental results, and a method is recommended to reduce the indefinite integral in the Kubo-Greenwood formula to a definite integral. It is explained that the boundaries of a definite integral are determined according to the empirical Tauc model, written for the distribution of the density of electronic states in amorphous semiconductors.

**Keywords:** amorphous semiconductors, interband optical transitions of electrons, interband absorption spectrum, Kubo-Greenwood formula, Davis-Mott approximation method, empirical Tauc model.

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## 1. Introduction

It is known that the spectral characteristic of the optical absorption coefficient of non-crystalline semiconductors is investigated by dividing absorbed photons into energy regions in accordance with their energy. One of these areas is the region of interband absorption.

In these regions, an optical transition of electrons from the valence band to the conduction band occurs. The interband absorption spectrum for amorphous semiconductors is calculated using the Kubo-Greenwood formula in accordance with the Davis-Mott approximation method [1].

$$\alpha(\hbar\omega) = \frac{8\pi^4 e^2 \hbar^2 a}{m^2 n_0 c} \int \frac{g_V(\varepsilon) g_C(\varepsilon + \hbar\omega)}{\hbar\omega} d\varepsilon. \quad (1)$$

Methods for calculating Eq. (1) are given in [2, 3]. This formula is written as:

$$\alpha(\hbar\omega) = A \int \frac{g_V(\varepsilon) g_C(\varepsilon + \hbar\omega)}{\hbar\omega} d\varepsilon \quad (2)$$

here  $A = \frac{8\pi^4 e^2 \hbar^2 a}{m^2 n_0 c}$  proportionality coefficient.

The analytical form of the interband absorption spectrum of amorphous semiconductors is usually determined using several empirical models [4, 5] that establish the energy distribution of the density of electronic states in the valence band and in the conduction band.

In all these models, the distributions of the density of electronic states at the edges of the valence and conduction bands are chosen in a parabolic form.

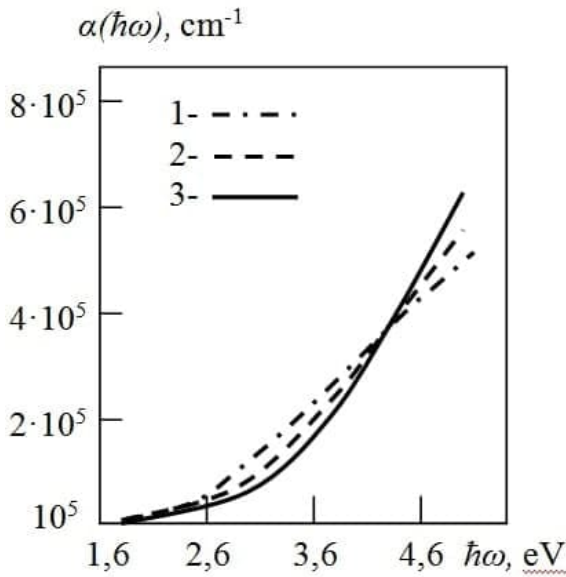
It was shown in [6] that the distributions of the density of electronic states at the boundaries of the valence and conduction bands have a power-law dependence: near the upper boundary of the valence band:

$$g_V(\varepsilon) = C_1 (\varepsilon_B - \varepsilon)^p, \quad \varepsilon \leq \varepsilon_B \quad (3)$$

near the lower boundary of the conduction band:

$$g_C(\varepsilon) = C_2 (\varepsilon - \varepsilon_A)^s, \quad \varepsilon_A \leq \varepsilon \quad (4)$$

Where  $C_1, C_2$  – constant values,  $p$  and  $s$  are constant numbers, which can take the values 1/2 and 1 [7], Since in



**Fig. 1.** Interband absorption spectra calculated by formulas 1- (18), 2- (19) and 3- (20).

formulas Eq. (3) and Eq. (4)  $\epsilon_A$  and  $\epsilon_B$  are the energy positions of the lower boundary of the conduction band and the upper boundary of the valence band, then

$$\epsilon_B = \epsilon_V, \epsilon_A = \epsilon_C, \epsilon_A - \epsilon_B = \epsilon_C - \epsilon_V = E_g$$

Where  $E_g$  - energy width of the mobility gap.

### 2. Discussion

In [7], Eq. (2) is written as follows:

$$\alpha(\hbar\omega) = A \int \frac{C_1 (\epsilon_B - \epsilon)^p C_2 (\epsilon - \epsilon_A + \hbar\omega)^s}{\hbar\omega} d\epsilon \quad (5)$$

By introducing the following notation:

$$y = \frac{\epsilon_A - \hbar\omega - \epsilon}{\epsilon_A - \hbar\omega - \epsilon_B}, \quad 0 \leq y \leq 1, \quad (6)$$

and differentiating it, the following expression is obtained:

$$dy = \frac{-1}{\epsilon_A - \hbar\omega - \epsilon_B} d\epsilon = \frac{1}{\hbar\omega - E_g} d\epsilon \quad (7)$$

By Eq. (6), the following expressions were obtained:

$$\epsilon - \epsilon_A = y (\hbar\omega - E_g) - \hbar\omega \quad (8)$$

$$\epsilon_B - \epsilon = (1 - y) (\hbar\omega - E_g) \quad (9)$$

Substituting Eqs. (7) to (9) into Eq. (5), we obtained:

$$\alpha(\hbar\omega) = AC_1C_2 \int \frac{(1 - y)^p y^s (\hbar\omega - E_g)^{p+s+1}}{\hbar\omega} dy = C \frac{(\hbar\omega - E_g)^{p+s+1}}{\hbar\omega} \int (1 - y)^p y^s dy. \quad (10)$$

Taking into account the limit of variation of  $y$ , this integral is written in the form:

$$\alpha(\hbar\omega) = C \frac{(\hbar\omega - E_g)^{p+s+1}}{\hbar\omega} \int_0^1 (1 - y)^p y^s dy \quad (11)$$

The integral solution of this expression using the gamma function is written in the following form:

$$\int_0^1 (1 - y)^p y^s dy = \frac{\Gamma(s + 1)\Gamma(p + 1)}{\Gamma(s + p + 2)} \quad (12)$$

Using this, the following expression was obtained for the interband absorption spectrum:

$$\alpha(\hbar\omega) = C \frac{\Gamma(s + 1)\Gamma(p + 1)}{\Gamma(s + p + 2)} \frac{(\hbar\omega - E_g)^{p+s+1}}{\hbar\omega} \quad (13)$$

In our opinion, there is no need to use the gamma function to calculate integral Eq. (12). Since  $p$  and  $s$  in this formula have values  $1/2$  and  $1$ , it is possible to obtain analytical solutions of the integral Eq. (12) [8]:

1. When  $p=1/2$  and  $s=1/2$ ,

$$\int_0^1 (1 - y)^{1/2} y^{1/2} dy = \frac{1}{4} \left( (2y - 1)\sqrt{y(1 - y)} + \arctg \sqrt{\frac{y}{1 - y}} \right) \Big|_0^1 = \frac{\pi}{8} \quad (14)$$

2. When  $p=1/2$  and  $s=1$ ,

$$\int_0^1 (1 - y)^{1/2} y^1 dy = - \frac{2(3y + 1)}{15} \sqrt{(1 - y)^3} \Big|_0^1 = \frac{4}{15} \quad (15)$$

3. When  $p=1$  and  $s=1/2$ ,

$$\int_0^1 (1 - y)^1 y^{1/2} dy = - \frac{4}{15} \sqrt{(1 - y)^5} \Big|_0^1 = \frac{4}{15} \quad (16)$$

4. When  $p=1$  and  $s=1$ ,

$$\int_0^1 (1 - y)^1 y^1 dy = \left( \frac{y^2}{2} - \frac{y^3}{3} \right) \Big|_0^1 = \frac{1}{6} \quad (17)$$

It can be seen from Eqs. (15) and (16) that when the distribution of the density of states at the boundaries of the allowed bands has a power dependence, the expression for the interband absorption spectrum does not change when these powers are rearranged. A similar result was obtained in [9].

It should be noted that the calculations performed using expression Eq. (12) give similar results. For example, when  $p = 1$  and  $s = 1$ , you can get the following result:

$$\int_0^1 (1-y)^1 y^1 dy = \frac{\Gamma(1+1)\Gamma(1+1)}{\Gamma(1+1+2)} = \frac{1}{6}$$

Substituting Eqs. (14) to (17) into expression Eq. (11), the following expressions for the interband absorption spectra were obtained.

1. When  $p = 1/2$  and  $s = 1/2$

$$\alpha(\hbar\omega) = C_0 \frac{(\hbar\omega - E_g)^2}{\hbar\omega} \quad (18)$$

2. When  $p = 1/2$  and  $s = 1$ ;  $p = 1$  and  $s = 1/2$

$$\alpha(\hbar\omega) = C_0 \frac{(\hbar\omega - E_g)^{5/2}}{\hbar\omega} \quad (19)$$

3. When  $p = 1$  and  $s = 1$

$$\alpha(\hbar\omega) = C_0 \frac{(\hbar\omega - E_g)^3}{\hbar\omega} \quad (20)$$

The plots of the interband absorption spectra calculated using expressions Eqs. (18) to (20) are shown in Fig. 1. The calculations were carried out for the specified values of  $E_g = 1.8\text{eV}$  and  $C_0 = 2.5 \cdot 10^5 \text{ cm}^{-1}$ , given in [9] for amorphous hydrogenated silicon ( $a - Si : H$ ).

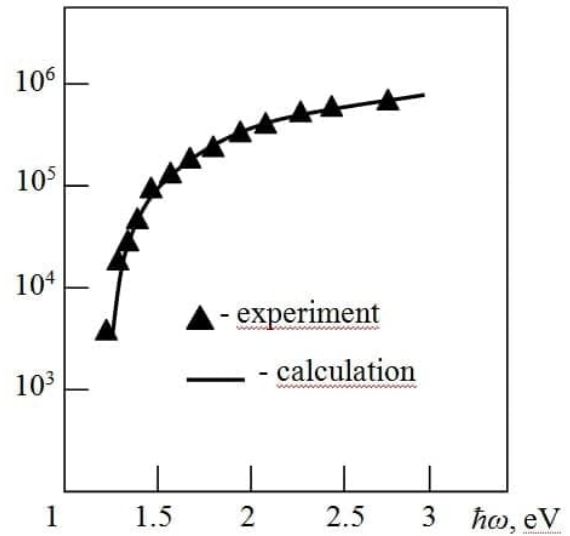
When calculating these plots, a point equal to a  $\alpha(\hbar\omega) = 5 \cdot 10^5 \text{ cm}^{-1}$  was chosen as the initial point of the interband absorption spectrum, when  $\hbar\omega = E_g = 1.8\text{eV}$  [10].

Experiments with amorphous semiconductors and calculations performed by other methods show that the graphs of the interband absorption spectra should be, first, convex, and, second, the values of these spectra should increase with an increase in the degree of the distribution of the density of electronic states of the allowed bands [11]. For example, Fig. 2 shows the interband absorption spectrum of amorphous carbon obtained in [12]. As can be seen from Fig. 1, the graphs calculated by expressions Eqs. (18) to (20) do not satisfy the experimental results.

### 3. Calculation

In our opinion, to overcome this drawback, the integral in Eq. (5) should be expressed in a certain form using expression Eq. (6).

$\alpha(\hbar\omega), \text{ cm}^{-1}$



**Fig. 2.** Interband absorption spectra of amorphous carbon obtained from the experiment [12] and calculated data obtained by formula (24).

For this, from expression Eq. (6) when  $y = 0$  for the lower limit of the integral  $\epsilon_1$  in Eq. (5), we obtain the equation:

$$0 = \frac{\epsilon_A - \hbar\omega - \epsilon_1}{\epsilon_A - \hbar\omega - \epsilon_B}, \epsilon_A - \hbar\omega - \epsilon_1 = 0, \epsilon_1 = \epsilon_A - \hbar\omega \quad (21)$$

For the upper limit of this integral  $\epsilon_2$ , when  $y = 1$ , we obtain the following equation:

$$1 = \frac{\epsilon_A - \hbar\omega - \epsilon_2}{\epsilon_A - \hbar\omega - \epsilon_B}, \epsilon_A - \hbar\omega - \epsilon_2 = \epsilon_A - \hbar\omega - \epsilon_B, \epsilon_2 = \epsilon_B \quad (22)$$

Using them, we write Eq. (5) in the following form:

$$\alpha(\hbar\omega) = \frac{C}{\hbar\omega} \int_{\epsilon_A - \hbar\omega}^{\epsilon_B} (\epsilon_B - \epsilon)^p (\epsilon - \epsilon_A + \hbar\omega)^s d\epsilon \quad (23)$$

Since the integral in Eq. (11) and the integral in Eq. (23) are equivalent, if  $p$  and  $s$  are known, an analytical solution of the interband absorption spectra can be obtained. Using [13], we obtain the following expressions:

1. When  $p = 1/2$  and  $s = 1/2$ :

$$\begin{aligned} \alpha(\hbar\omega) &= C \int_{\epsilon_A - \hbar\omega}^{\epsilon_B} \frac{(\epsilon_B - \epsilon)^{1/2} (\epsilon - \epsilon_A + \hbar\omega)^{1/2}}{\hbar\omega} d\epsilon = \\ &= \frac{C_0}{\hbar\omega} \left( 2(\hbar\omega - E_g) \sqrt{E_g \hbar\omega} + \left( (E_g + \hbar\omega)^2 \operatorname{arctg} \left( \frac{E_g - \hbar\omega}{\sqrt{4E_g \hbar\omega}} \right) \right) \right), \end{aligned}$$

$$C_0 = \frac{C}{4} \quad (24)$$

2. When  $p = 1/2$  and  $s = 1$ :

$$\begin{aligned} \alpha(\hbar\omega) &= \frac{C}{\hbar\omega} \int_{\varepsilon_A - \hbar\omega}^{\varepsilon_B} (\varepsilon_B - \varepsilon)^{\frac{1}{2}} (\varepsilon - \varepsilon_A + \hbar\omega)^1 d\varepsilon = \\ &= \frac{C_0}{\hbar\omega} \left( 5(\hbar\omega + E_g) \left( \sqrt{(\hbar\omega)^3} - \sqrt{E_g^3} \right) - \right. \\ &\quad \left. \left( 3 \left( \sqrt{(\hbar\omega)^5} - \sqrt{E_g^5} \right) \right) \right), \\ C_0 &= \frac{2C}{15} \end{aligned} \quad (25)$$

3. When  $p = 1$  and  $s = 1/2$ :

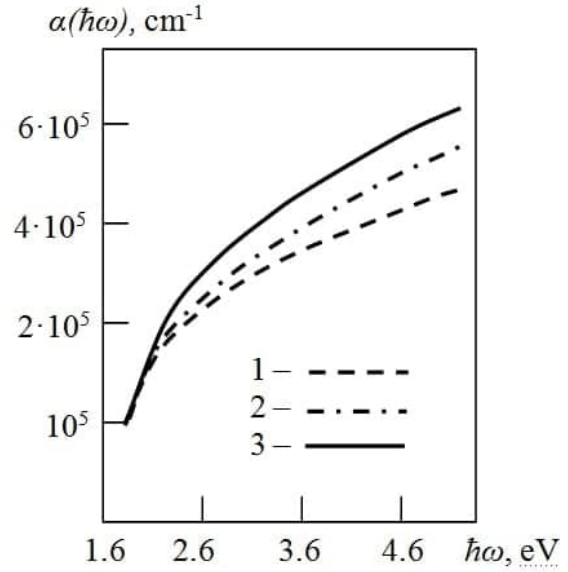
$$\begin{aligned} \alpha(\hbar\omega) &= \frac{C}{\hbar\omega} \int_{\varepsilon_A - \hbar\omega}^{\varepsilon_B} (\varepsilon_B - \varepsilon)^1 (\varepsilon - \varepsilon_A + \hbar\omega)^{\frac{1}{2}} d\varepsilon = \\ &= \frac{C_0}{\hbar\omega} \left( 5(\hbar\omega + E_g) \left( \sqrt{(\hbar\omega)^3} - \sqrt{E_g^3} \right) - \right. \\ &\quad \left. \left( 3 \left( \sqrt{(\hbar\omega)^5} - \sqrt{E_g^5} \right) \right) \right), \\ C_0 &= \frac{2C}{15} \end{aligned} \quad (26)$$

4. When  $p = 1$  and  $s = 1$ :

$$\begin{aligned} \alpha(\hbar\omega) &= \frac{C}{\hbar\omega} \int_{\varepsilon_A - \hbar\omega}^{\varepsilon_B} (\varepsilon_B - \varepsilon)^1 (\varepsilon - \varepsilon_A + \hbar\omega)^1 d\varepsilon = \\ &= \frac{C_0}{\hbar\omega} (\hbar\omega - E_g) \left( E_g^2 + 4\hbar\omega E_g + (\hbar\omega)^2 \right), \\ C_0 &= \frac{c}{6} \end{aligned} \quad (27)$$

The plots of the calculated interband absorption spectra Eq. (24), Eq. (26), and Eq. (27) for amorphous hydrogenated silicon ( $a-Si:H$ ) ( $E_g = 1.8\text{eV}$  and  $C_0 = 2.5 \cdot 10^5 \text{ cm}^{-1}$ ) are shown in Fig. 3. As can be seen from the figure, all these spectra are convex and agree well with the experimental results. In addition, the values of the interband absorption coefficient increase with an increase in the degree of distribution of the density of electronic states in the allowed bands. Hence it follows that when calculating the interband absorption spectrum using the Kubo-Greenwood formula, the integral in this formula must be a definite integral.

And in [14], the experimentally obtained spectrum of interband absorption of amorphous carbon Fig. 2 is compared with the spectrum calculated by formula Eq. (24), considering  $E_0$  and  $E_g$  as adjustable parameters. Agreement between the experimental and calculated results was obtained at the values  $C_0 = 1.253 \cdot 10^5 \text{ cm}^{-1} \text{ eV}^{-1}$  and



**Fig. 3.** Interband absorption spectra of amorphous hydrogenated silicon ( $a-Si:H$ ) calculated by formulas 1 - (24), 2 - (25), and 3 - (27).

$E_g = 1.235\text{eV}$ . The results of these calculations are also shown in Fig. 2 (solid line).

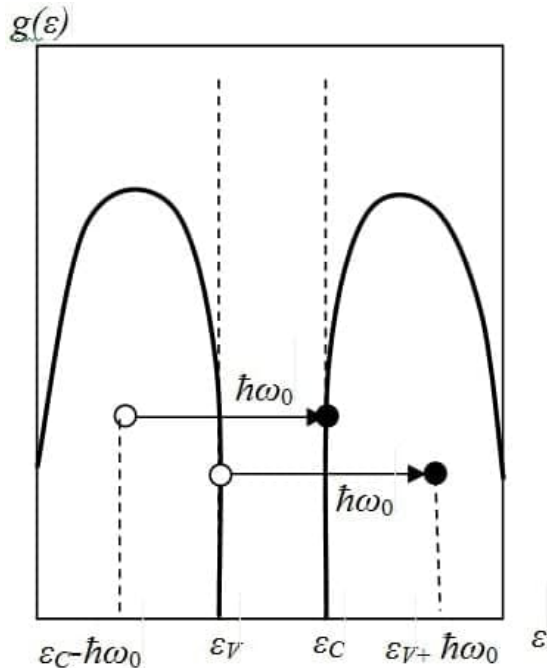
Let us now consider how the boundaries of a definite integral in the Kubo-Greenwood formula are found. For this, we will choose the distribution of the density of electronic states in the form of the empirical Tauc model [15]. According to this model, the distributions of the density of electronic states at the tails of the allowed bands of amorphous semiconductors are not taken into account.

$$g_V(\varepsilon) = C_1 \begin{cases} 0, & \varepsilon > \varepsilon_V \\ (\varepsilon_V - \varepsilon)^{1/2}, & \varepsilon \leq \varepsilon_V \end{cases}$$

$$g_C(\varepsilon) = C_2 \begin{cases} (\varepsilon - \varepsilon_C)^{1/2}, & \varepsilon \geq \varepsilon_C \\ 0, & \varepsilon < \varepsilon_C \end{cases}$$

Consequently, only optical transitions of electrons from the valence band to the conduction band occur. It is known that for this the energy of absorbed photons must be no less than the energy width of the mobility gap ( $\hbar\omega_0 \geq E_g$ ). The electron participating in the optical transition in the state with the highest energy must be located at the upper boundary of the valence band. This is due to the fact that if the energy state of an electron participating in the optical transition is higher than the energy state at the upper boundary of the valence band, then this electron passes from the tail of the valence band to the conduction band.

When photons with energy  $\hbar\omega_0$  are absorbed, the electron in the state with the lowest energy should be lower by  $(\varepsilon_C - \hbar\omega_0)$ , the energy state of the lower boundary of the



**Fig. 4.** Optical transitions of electrons when the energy of absorbed photons is equal to  $\hbar\omega_0$  according to the empirical Tauc model.

conduction band Fig. 4.

If the energy state of an electron participating in the optical transition is less than the energy interval  $\varepsilon_C - \hbar\omega_0$ , then it passes from the valence band to the tail of the conduction band. In these cases, the optical transitions of the electron are not interband. Therefore, when calculating the interband absorption coefficient using the Kubo-Greenwood formula, the upper limit of the definite integral in this formula should correspond to the upper limit of the valence band  $\varepsilon_V$  and the lower limit to the energy state  $\varepsilon_C - \hbar\omega_0$ .

#### 4. Conclusions

In this paper, the lower and upper bounds of the integral in the Kubo-Greenwood formula written by the Davis-Mott method are determined. It is shown that for consistency of the experimental spectra of interband absorption and those calculated using the Kubo-Greenwood formula using the Davis-Mott approximation method, the integral in the Kubo-Greenwood formula must be transformed into a definite integral. The determination of the upper and lower boundaries of this integral for the interband absorption spectra is explained using the empirical Tauc model.

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