CALCULATION OF THE DENSITY OF THE DISTRIBUTION OF ELECTRONIC STATES IN THE CONDUCTION BAND FROM THE FUNDAMENTAL ABSORPTION SPECTRA OF AMORPHOUS SEMICONDUCTORS

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INTRODUCTION

The region of fundamental absorption in the optical spectra of amorphous semiconductors is theoretically studied using the Davis-Mott approximation according to the Kubo-Greenwood formula. As is known, three types of optical transitions of the electron can be observed in the fundamental absorption region; from the tail of the valence band to the conduction band, from the valence band to the conduction band and from the valence band to the tail of the conduction band. For all these electronic transitions, analytical expressions of the partial absorption spectra are obtained from two different types of the Kubo-Greenwood formula. The width of the optical mobility gap and the proportionality coefficient were determined in the analytical form of the interband absorption spectrum by fitting them to the experimental interband absorption spectrum. A new method is presented for calculating the density of distribution of electronic states in the conduction band of amorphous carbon based on the experimental interband absorption spectrum and the analytical expression of the Kubo-Greenwood formula written for the interband absorption spectrum.

Keywords: Amorphous semiconductors; Optical absorption spectra; Davis-Mott approximation method; Kubo-Greenwood formula; Fundamental absorption spectrum; Partial absorption spectra; Interband absorption spectrum; Electronic state density distribution

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INTRODUCTION

The optical absorption coefficient of amorphous semiconductors is usually determined by the Kubo-Greenwood formula using the Davis-Mott approximation [1, 2]:

$$\alpha(\hbar \omega) = A \int g_t(\varepsilon) g_c(\varepsilon + \hbar \omega) \frac{d\varepsilon}{\hbar \omega}$$ (1)

or

$$\alpha(\hbar \omega) = A \int g_t(\varepsilon - \hbar \omega) g_c(\varepsilon) \frac{d\varepsilon}{\hbar \omega}$$ (2)

where $A$ - is the coefficient of proportionality, independent of the energy $(\hbar \omega)$ of absorbed photons, $g_t(\varepsilon)$, $g_c(\varepsilon - \hbar \omega)$ and $g_c(\varepsilon)$ are the densities of the initial and final electronic states during optical transitions in valence band and conduction band, respectively.

It can be seen from Formulas (1), (2) that the values of the absorption coefficient strongly depend on the distribution of the density of electronic states involved in optical transitions. Formula (1) is used when the initial electronic states involved in optical transitions play the main role. Therefore, in [3], using Formula (1), the distributions of the density of electronic states in the valence band were determined. And then the main role is played, the final electronic state uses the Formula (2). From this it follows that, it is possible to analytically investigate the distribution of the density of electronic states in the conduction band and the valence band separately. Therefore, this paper proposes a new method for determining the distribution of the density of electronic states in the conduction band from the Kubo-Greenwood formula (2). Since the integrals in Formula (1) and (2) are indefinite, they give a general solution. It was shown in [4] that in order to obtain own solutions of the spectra of the optical absorption coefficient from the Kubo-Greenwood Formula, the indefinite integral in this formula must be written in a certain form, and then formula (1) takes the form:

$$\alpha(\hbar \omega) = A \int_{\varepsilon_0}^{\varepsilon_0 + \hbar \omega} g_t(\varepsilon) g_c(\varepsilon + \hbar \omega) \frac{d\varepsilon}{\hbar \omega}$$ (3)

where $\varepsilon_0$ is the energy position of the intersection point of the exponentially decaying “tails” of allowed bands.

It is known that the energy of absorbed photons in the fundamental region is greater than the energy width $(E_g < \hbar \omega)$ of the mobility gap of amorphous semiconductors. It was shown in [5] that in amorphous semiconductors, upon absorption of photons with energies $E > E_g$, optical transitions of electrons from the “tail” of the valence band to...
the conduction band, from the valence band to the conduction band, and from the valence band to the “tail” of the conduction band are simultaneously observed. Therefore, by adapting Formula (3) to the above optical transitions, we obtain:

\[
\alpha(h\omega) = A \int_{\epsilon_{v}}^{\epsilon_{c}} g_v(\epsilon) g_c(\epsilon + h\omega) \frac{d\epsilon}{h\omega} = A \int_{\epsilon_{c}}^{\epsilon_{v}} g_c(\epsilon) g_v(\epsilon + h\omega) \frac{d\epsilon}{h\omega} + \int_{\epsilon_{v}-h\omega}^{\epsilon_{c}} g_v(\epsilon) g_c(\epsilon + h\omega) \frac{d\epsilon}{h\omega}
\]

\[
(4)
\]

where \(\epsilon_v\) is the upper boundary of the valence band; \(\epsilon_c\) is the lower boundary of the conduction band; \(\alpha_f(h\omega), \alpha_s(h\omega), \alpha_3(h\omega)\) are partial absorption coefficients determined by optical transitions of electrons from the “tail” of the valence band to the conduction band, from the valence band to the conduction band (interband absorption spectrum), from the valence band to “tail” of the conduction band, respectively.

To calculate the partial spectra of fundamental absorption using Formula (4), the distributions of the density of electronic states in the valence band and in its tail, as well as in the conduction band and in its tail, must be known. Usually, in a theoretical study of optical absorption spectra, the density of electronic states of amorphous semiconductors at the boundaries of allowed bands is written with linear or parabolic distributions, and at the tails of allowed bands, with exponential distributions [6, 7]. In [4], for these distributions, it was proposed:

\[
g_v(\epsilon) = N(\epsilon_v) \left(\frac{E_c - \epsilon}{E_v}\right)^{n_v}, \quad n_v = 1/2, 1 \quad \text{and} \quad g_c(\epsilon) = N(\epsilon_c) \exp\left(-\beta_v (\epsilon - \epsilon_v)\right),
\]

\[
g_c(\epsilon) = N(\epsilon_c) \left(\frac{\epsilon - E_c}{E_c}\right)^{n_c}, \quad n_c = 1/2, 1 \quad \text{and} \quad g_c(\epsilon) = N(\epsilon_c) \exp\left(\beta_v (\epsilon - \epsilon_c)\right),
\]

where \(\beta_v\) and \(\beta_c\) are the parameters that determine the slopes of the exponential tails of the valence and conduction bands, \(N(\epsilon_v)\) and \(N(\epsilon_c)\) are the effective densities of electronic states in the valence and conduction bands.

Substituting the distribution in Formulas (5) and (6) into Formula (4), for partial absorption spectra, we obtain: for interband electronic transitions at \(n_1 = n_2 = 1/2\)

\[
\alpha_f(h\omega) = \frac{B}{4h\omega E_v} \left[2(h\omega - E_v)\sqrt{E_v-h\omega-(E_v-h\omega)^2} \arctan\left(\frac{E_v-h\omega}{2\sqrt{E_v(h\omega)}}\right)\right],
\]

\[
(7)
\]

for \(n_1 = n_2 = 1\)

\[
\alpha_f(h\omega) = \frac{B}{6h\omega E_v} (h\omega - E_v)(E_v + 4h\omega E_v + (h\omega)^2),
\]

\[
(8)
\]

For \(n_1 = 1, n_2 = 1/2\) or \(n_1 = 1/2, n_2 = 1\)

\[
\alpha_s(h\omega) = \frac{2B}{15h\omega E_v} \left[5(h\omega + E_v)\left(\sqrt{(h\omega)^2 - E_v^2}\right) - 3\left(\sqrt{(h\omega)^2 - E_v^2}\right)^3\right],
\]

\[
(9)
\]

where \(B = AN(\epsilon_v)N(\epsilon_c)\).

The results of calculation by Formulas (7)–(9) are shown in Fig. 1. Calculations were carried out for amorphous hydrogenated silicon \(B = 2.5 \times 10^4 \text{ cm}^{-1}\) and \(E_g = 1.8 \text{ eV}\) [1].

\[\alpha(h\omega), \text{ cm}^{-1}\]

\[\text{Figure 1. Partial spectra of fundamental absorption of amorphous semiconductors obtained by Formulas:}\]

1 - at \(n_1 = n_2 = 1/2\) (7); 2 - at \(n_1 = n_2 = 1\) (8); 3 - at \(n_1 = 1, n_2 = 1/2\); 4 - at \(n_1 = 1/2, n_2 = 1\) (9) and obtained from Formulas (10) and (11) and from numerical calculations, when 4 - \(n_1 = n_2 = 1\) and 5 - when \(n_1 = n_2 = 1/2\) electronic transitions from the tail of the valence band to the conduction band (a) and from the valence band to the “tail” of the conduction band (b).
Since at \( n_1 = n_2 = 1/2 \) it is impossible to obtain an analytical expression for partial absorption spectra determined by optical transitions of electrons (from the “tail” of the valence band to the conduction band, from the valence band to the “tail” of the conduction band), they are determined using numerical calculations.

At \( n_1 = n_2 = 1/2 \), analytical expressions for partial absorption spectra determined by optical transitions of electrons from the “tail” of the valence band to the conduction band and from the valence band to the “tail” of the conduction band:

\[
\alpha_1(h\omega) = \frac{B \exp\left(-\beta_1 \left(\epsilon_e - \epsilon_i\right)\right)}{E \hbar \omega \beta_1} \left[ \left(\frac{1}{\beta_1} + h\omega\right) \exp\left(\beta_1 \left(\epsilon_e - \epsilon_i\right)\right) - \left(\epsilon_e - \epsilon_i + \frac{1}{\beta_1} + h\omega\right)\right], \tag{10}
\]

\[
\alpha_2(h\omega) = \frac{B \exp\left(\beta_2 \left(\epsilon_e - \epsilon_i\right)\right)}{E \hbar \omega \beta_2} \left[ \left(\frac{1}{\beta_2} + h\omega\right) \exp\left(\beta_2 \left(\epsilon_e - \epsilon_i\right)\right) - \left(\epsilon_e - \epsilon_i + \frac{1}{\beta_2} + h\omega\right)\right]. \tag{11}
\]

The results of calculation by Formulas (10), (11) and by the method of approximate calculation at \( n_1 = n_2 = 1/2 \) are shown in Fig. 1 (4- and 5- curve). The calculations were carried out for \( E_g = 1.8 \text{ eV}, \epsilon_C - \epsilon_0 = 0.7 \text{ eV}, \epsilon_0 - \epsilon_V = 1.1 \text{ eV}, \beta_1 = 16 \text{ eV}^{-1} \) and \( \beta_2 = 22 \text{ eV}^{-1} \).

To calculate the absorption coefficient using the above method, taking into account (2), we write the integral in the form of a definite integral:

\[
\alpha(h\omega) = A \int_{\epsilon_e}^{\epsilon_0} g_\tau(\epsilon - h\omega)g_\tau(\epsilon) \frac{d\epsilon}{h\omega}, \tag{12}
\]

Having adapted this Formula to the types of optical transitions of an electron, we divide it into partial absorption spectra:

\[
\alpha(h\omega) = A \int_{\epsilon_e}^{\epsilon_0} g_\tau(\epsilon - h\omega)g_\tau(\epsilon) \frac{d\epsilon}{h\omega} = A \int_{\epsilon_e}^{\epsilon_0} g_\tau(\epsilon - h\omega)g_\tau(\epsilon) \frac{d\epsilon}{h\omega} + A \int_{\epsilon_e}^{\epsilon_0} g_\tau(\epsilon - h\omega)g_\tau(\epsilon) \frac{d\epsilon}{h\omega} = \alpha_1(h\omega) + \alpha_2(h\omega) + \alpha_3(h\omega), \tag{13}
\]

where \( \alpha_1(h\omega), \alpha_2(h\omega), \alpha_3(h\omega) \) are partial fundamental absorption spectra.

From the calculation of the interband absorption coefficient according to Formula (13), the expressions are obtained:

For \( n_1 = n_2 = 1/2 \)

\[
\alpha_1(h\omega) = \frac{B}{4h\omega E_g} \left[ 2(h\omega - E_g) \sqrt{E_g + h\omega} - (E_g - h\omega)^2 \arctg \left( \frac{E_g - h\omega}{2\sqrt{E_g h\omega}} \right) \right], \tag{14}
\]

For \( n_1 = n_2 = 1 \),

\[
\alpha_2(h\omega) = \frac{B}{6h\omega E_g}(h\omega - E_g)(E_g^2 + 4h\omega E_g + (h\omega)^2), \tag{15}
\]

\( n_1=1, n_2=1/2 \) and \( n_1=1/2, n_2=1 \)

\[
\alpha_3(h\omega) = \frac{2B}{15h\omega E_g^2} \left[ 5(h\omega + E_g) \left( \sqrt{(h\omega)^2 - E_g^2} \right)^3 - 3 \left( (h\omega)^2 - E_g^2 \right) \right]. \tag{16}
\]

It can be seen that Formulas (7)-(9) and (14)-(16) are the same. This it follows that Formulas (3) and (12) can be used when determining the analytical expressions for the interband absorption coefficients using the Kubo-Greenwood formula.

Similarly, consider the calculation of \( \alpha_1(h\omega) \) and \( \alpha_3(h\omega) \) using Formula (13). Since at \( n_1 = n_2 = 1/2 \) it is impossible to obtain an analytical expression for the spectral dependences of partial absorptions determined by optical transitions of electrons from the “tail” of the valence band to the conduction band, from the valence band to the “tail” of the conduction band, they were determined using numerical calculations.

The obtained analytical expressions for the partial absorption spectra \( n_1=n_2 =1 \) had the form:

\[
\alpha_1(h\omega) = \frac{B \exp\left(-\beta_1 \left(\epsilon_e - \epsilon_i\right)\right)}{E \hbar \omega \beta_1} \left[ \left(\frac{1}{\beta_1} + h\omega\right) \exp\left(\beta_1 \left(\epsilon_e - \epsilon_i\right)\right) - \left(\epsilon_e - \epsilon_i + \frac{1}{\beta_1} + h\omega\right)\right], \tag{17}
\]

\[
\alpha_2(h\omega) = \frac{B \exp\left(\beta_1 \left(\epsilon_e - \epsilon_i\right)\right)}{E \hbar \omega \beta_1} \left[ \left(\frac{1}{\beta_2} + h\omega\right) \exp\left(\beta_2 \left(\epsilon_e - \epsilon_i\right)\right) - \left(\epsilon_e - \epsilon_i + \frac{1}{\beta_2} + h\omega\right)\right]. \tag{18}
\]
It can be seen from Formulas (10), (11) and (17), (18) that with the correctness of the chosen empirical model for the distribution of the density of electronic states in amorphous semiconductors and the limits of a definite integral in the Kubo–Greenwood formulas (3), (12), calculated partial absorption coefficients in the fundamental region will be the same.

RESULTS AND DISCUSSION

Figure 1 shows that the interband absorption spectrum plays the main role in the region of fundamental absorption, and at the edge of fundamental absorption, the values of the partial absorption spectra of the higher indicated optical transitions are almost equal [8]. It can be seen from Formulas (14)–(16) that in order to calculate the interband absorption coefficients, it is necessary to know the energy width of the mobility gap \( E_g \) and the coefficient of proportionality \( B \) in them. To determine these parameters, we use the experimental results for the interband absorption coefficient. In [9], the interband absorption spectrum of amorphous carbon is presented (Fig. 2).

Let us proceed to the calculation of the density of electronic states in the conduction band of amorphous carbon. To do this, from Formula (13) we select the interband absorption spectrum:

\[
\alpha_\varepsilon (\hbar \omega) = A \int_{\epsilon_c} e^{\epsilon_\varepsilon} \left( \epsilon - \epsilon_\varepsilon + \hbar \omega \right) \frac{d \epsilon}{\hbar \omega}, \tag{19}
\]

In [10], a Formula is given for the derivative of the integral of a function of two variables with respect to one variable:

\[
\frac{d}{d y} \int_{a(y)}^{b(y)} f(x,y) dx = \int_{a(y)}^{b(y)} \frac{\partial f(x,y)}{\partial y} dx + \frac{\partial b(y)}{\partial y} f(b(y),y) - \frac{\partial a(y)}{\partial y} f(a(y),y), \tag{20}
\]

Applying (20) to (19), we get:

\[
\frac{d \alpha_\varepsilon (\hbar \omega)}{d \hbar \omega} = \frac{d}{d \hbar \omega} A \int_{\epsilon_c} e^{\epsilon_\varepsilon} \left( \epsilon - \epsilon_\varepsilon + \hbar \omega \right) \frac{d \epsilon}{\hbar \omega} = A \int_{\epsilon_c} g_\varepsilon (\epsilon) \frac{d \epsilon}{\hbar \omega} - \frac{\alpha_\varepsilon (\hbar \omega)}{\hbar \omega}, \tag{21}
\]

Let us substitute in (21) the distribution functions in the chosen model:

\[
\alpha_\varepsilon (\hbar \omega) = A \int_{\epsilon_c} N(\varepsilon_\epsilon) \left( \frac{E_c - \epsilon + \hbar \omega \frac{1}{2}}{E_g} \right)^2 N(\varepsilon_\epsilon) \left( \frac{E_c - \epsilon - \hbar \omega \frac{1}{2}}{E_g} \right) d \epsilon. \tag{22}
\]

From here we obtain the derivative with respect to the photon energy

\[
\frac{d \alpha_\varepsilon (\hbar \omega)}{d \hbar \omega} = \frac{B}{E_g} \int_{\epsilon_c} \left( \epsilon - \epsilon_\varepsilon + \hbar \omega \right) \frac{1}{2} \frac{\partial}{\partial \hbar \omega} (\epsilon - \epsilon + \hbar \omega)^{1/2} d \epsilon + B \frac{\partial (E_c + \hbar \omega)}{\partial \hbar \omega} \frac{\partial (E_c - \epsilon - \hbar \omega + \hbar \omega)^{1/2}}{\partial \hbar \omega} \frac{1}{2} (\epsilon_\varepsilon + \hbar \omega - \epsilon_\varepsilon)^{1/2}
\]

\[
- B \frac{\partial \epsilon_c (\epsilon_c - \epsilon_c + \hbar \omega)^{1/2} (\epsilon_c - \epsilon_\varepsilon - \epsilon_\varepsilon)^{1/2}}{E_c h \omega} = \frac{B}{2 E_c h \omega} \frac{E_g - h \omega}{2 \sqrt{E_c h \omega}} \frac{\alpha_\varepsilon (h \omega)}{h \omega} + \frac{B (E_c h \omega)^{1/2}}{E_c h \omega} = \frac{B}{2 E_c h \omega} \frac{E_g - h \omega}{2 \sqrt{E_c h \omega}} \frac{\alpha_\varepsilon (h \omega)}{h \omega} + \frac{B (E_c h \omega)^{1/2}}{E_c h \omega}, \tag{22}
\]

where

\[
g_\varepsilon (\epsilon) = N(\varepsilon_\epsilon) \left( \frac{E_c - \epsilon}{E_g} \right)^{1/2} = N(\varepsilon_\epsilon) \left( \frac{\hbar \omega}{E_g} \right)^{1/2}. \tag{23}
\]
It follows from (23) that \( \epsilon - \epsilon_c = h\omega, \ \epsilon = \epsilon_c + h\omega \) this energy state is in the conduction band. Taking into account (23), we write (22)

\[
\frac{\partial \alpha (h\omega)}{\partial h\omega} = \frac{B}{2E_c h\omega} (E + h\omega) \arctan \left( \frac{E - h\omega}{2E_c h\omega} \right) \alpha (h\omega) + \frac{B}{N(\epsilon_c)} \frac{1}{h\omega} g_c (\epsilon),
\]

and find the distribution of the density of electronic states in the conduction band:

\[
g_c (\epsilon) = \frac{1}{B} \left( \frac{\partial \alpha (h\omega)}{\partial h\omega} - \frac{B}{2E_c h\omega} (E + h\omega) \arctan \left( \frac{E - h\omega}{2E_c h\omega} \right) \alpha (h\omega) + \frac{B}{E_c (h\omega_a + h\omega)} \right) \times
\]

\[
\times \arctan \left( \frac{2E_c (E + h\omega) + \alpha (h\omega_a + h\omega)}{2E_c h\omega_a + 2h\omega} \right) + \frac{\alpha (h\omega_a + h\omega)}{h\omega_a + h\omega},
\]

where \( \alpha (h\omega_a) \) and \( h\omega_a \) are the experimental values of the interband absorption coefficient and the energy of absorbed photons, respectively. The effective value of the density of electronic states in the mobility zone \( N(\epsilon_c) = 10^{21} \text{ eV}^{-1} \text{cm}^{-3} \).

Averaging the energy of absorbed photons and the interband absorption coefficient, we write (25) in the form

\[
g_c (\epsilon) = \frac{N(\epsilon_c)}{B} \left( \frac{\partial \alpha (h\omega)}{\partial h\omega} - \frac{B}{2E_c h\omega} (E + h\omega) \arctan \left( \frac{E - h\omega}{2E_c h\omega} \right) \alpha (h\omega) + \frac{B}{E_c (h\omega_a + h\omega)} \right) \times
\]

\[
\times \arctan \left( \frac{2E_c (E + h\omega) + \alpha (h\omega_a + h\omega)}{2E_c h\omega_a + 2h\omega} \right) + \frac{\alpha (h\omega_a + h\omega)}{h\omega_a + h\omega},
\]

where \( \alpha (h\omega_a) \) and \( h\omega_a \) are the experimental values of the interband absorption coefficient and the energy of absorbed photons, respectively. The effective value of the density of electronic states in the mobility zone \( N(\epsilon_c) = 10^{21} \text{ eV}^{-1} \text{cm}^{-3} \).

It can be seen from Formula (26) that the distributions of the density of electronic states in the conduction band should be overestimated from \( E_g \) and \( B \). We determine them, assuming fitting parameters according to Formula (14), adapt the theoretically calculated spectra (solid line in Fig. 2) to the experimental spectra of interband absorption. The latest calculations showed that the best agreement between the calculation value of Formula (14) and the experimental results is obtained at \( E_g = 1.25 \text{ eV} \) and \( B = 6.1 \cdot 10^5 \text{ cm}^{-1} \). Further calculations showed that these parameters do not have a very strong effect on the final result.

On Figure 3 presents the results of calculations performed with the substitution of experimental data for the interband absorption coefficient (Fig. 2) and the energy of absorbed photons into Formula (26), the density of electronic states in the conduction band of amorphous carbon.

**CONCLUSIONS**

Thus, in this work, the region of fundamental absorption of the optical absorption coefficient of amorphous semiconductors has been theoretically investigated and the following results have been obtained:

1. The analytically calculated and experimental determination of the interband absorption spectra is adapted by considering the mobility gap and the proportionality factor in the analytically determined Formula for interband absorption as fitting parameters.
2. For the first time, a method is shown for determining the density of electronic states in the conduction band from the experimental spectrum of interband absorption of amorphous semiconductors.
3. A new Formula is found that determines the density of electronic states in the conduction band, from the Kubo-Greenwood formula written for the interband absorption spectrum of amorphous semiconductors.
4. The density of electronic states in the conduction band of amorphous carbon was determined from the experimental spectrum of interband absorption.

**REFERENCES**


**Розрахунок щільності розподілу електронних станив у зоні провідності з фундаментального спектру поглинання аморфних напівпровідників**

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Теоретично досліджено область фундаментального поглинання в оптичних спектрах аморфних напівпровідників з використанням наближення Девіса-Мотта за формулою Кубо-Грінвуда. Як відомо, в області фундаментального поглинання можна спостерігати три види оптичних переходів електрона: від хвоста валентної зони до зони провідності, від валентної зони до зони провідності та від валентної зони до хвоста зони провідності. Для всіх цих оптичних переходів аналітичні вирази спектрів часткового поглинання отримані з двох різних типів формул Кубо-Грінвуда. Ширину забороненої зони оптичної рухливості та коефіцієнт пропорційності визначали в аналітичній формі спектра міжзонного поглинання шляхом їх підгонки до експериментального спектру міжзонного поглинання. Представлена новий метод розрахунку щільності розподілу електронних станів у зоні провідності аморфного вуглецю на основі експериментального спектру міжзонного поглинання та аналітичного виразу формул Кубо-Грінвуда, записаної для спектра міжзонного поглинання.

**Ключові слова:** аморфні напівпровідники; спектри оптичного поглинання; метод апроксимації Девіса-Мотта; формула Кубо-Грінвуда; фундаментальний спектр поглинання; часткові спектри поглинання; спектр міжзонного поглинання; електронний розподіл густини стану