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EXPONENTIAL ABSORPTION SPECTRUM AND DENSITY DISTRIBUTION OF ELECTRONIC STATES ON THE TAIL OF THE VALENCE ZONE OF AMORPHOUS SEMICONDUCTORS

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Abstract. *The analytical expression of the spectrum, derived for the region of exponential absorption of amorphous semiconductors, is investigated. The parameters in this expression that determine the slope of the tails of the allowed bands are determined by fitting to the exponential absorption spectrum, which are determined experimentally. For the Davis-Mott approximation, a new formula is derived from the Kubo-Greenwood formula, which determines the densities of electronic states at the tail of the valence band. Using these formulas and the experimentally determined exponential absorption spectrum, it is shown that it is possible to determine the density of electronic states at the tail of the valence band.*

Keywords: *amorphous semiconductors, tails of allowed bands, Kubo-Greenwood formula, Davies-Mott approximation method, electronic optical transitions, exponential absorption spectrum, energy gap width, parameters determining the slope of allowed band tails, distribution of the density of electronic states.*

ЭКСПОНЕНЦИАЛЬНЫЙ СПЕКТР ПОГЛОЩЕНИЯ И РАСПРЕДЕЛЕНИЕ ПЛОТНОСТИ ЭЛЕКТРОННЫХ СОСТОЯНИЙ НА ХВОСЕ ВАЛЕНТНОЙ ЗОНЫ АМОРФНЫХ ПОЛУПРОВОДНИКОВ

Аннотация. *Исследовано аналитическое выражение спектра, полученное для области экспоненциального поглощения аморфных полупроводников. Параметры в этом выражении, определяющие наклон хвостов разрешенных полос, определяются подгонкой к экспоненциальному спектру поглощения, который определяется экспериментально. Для приближения Дэвиса-Мотта новая формула выводится из формулы Кубо-Гринвуда, которая определяет плотности электронных состояний в хвосте валентной зоны. Используя эти формулы и экспериментально определенный экспоненциальный спектр поглощения, показано, что можно определить плотность электронных состояний в хвосте валентной зоны.*

Ключевые слова: *аморфные полупроводники, хвосты разрешенных зон, формула Кубо-Гринвуда, метод приближения Дэвиса-Мотта, электронно-оптические переходы, экспоненциальный спектр поглощения, ширина запрещенной зоны, параметры, определяющие наклон хвостов разрешенных зон, распределение плотности электронных состояний.*

INTRODUCTION

It is known that it is customary to study the spectra of the optical absorption coefficient of amorphous semiconductors by dividing it into the regions of fundamental (interband), exponential, and defect absorption [1].

The energy of photons absorbed in the region of exponential absorption will be less from the energy width of the mobility gap (E_g) and more from $\varepsilon_0 - \varepsilon_V$, i.e.

$\varepsilon_C - \varepsilon_V = E_g \succ \hbar\omega \succ \varepsilon_0 - \varepsilon_V$. Where ε_0 is the energy position of the point of intersection of the exponential tails of the allowed bands (Fig. 1), ε_V is the top of the valence band, and ε_C is the bottom of the conduction band. When such photons are absorbed, the following optical transitions of electrons occur simultaneously: from the tail of the valence band to the conduction band, from the tail of the valence band to the tail of the conduction band, and from the valence band to the tail of the conduction band [2].

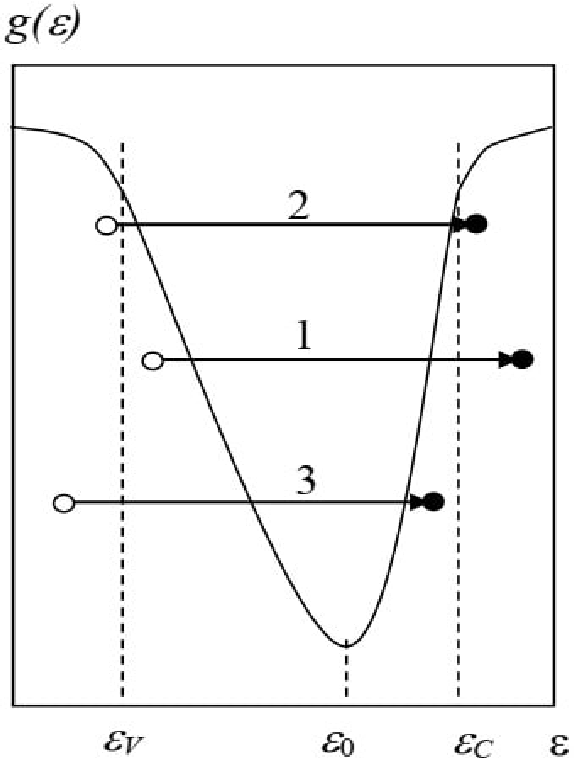

Fig. 1. Types of optical transitions of an electron, when the absorbed photons are in the interval $\varepsilon_0 - \varepsilon_V \prec \hbar\omega \prec \varepsilon_C - \varepsilon_V = E_g$ in amorphous semiconductors. 1 - from the tail of the valence band in the conduction band, 2 - from the tail of the valence band in the tail of the conduction band, 3 - from the valence band in the conduction band.

MATERIALS AND METHODS

In [3], based on the results of calculations, in determining the value of the exponential absorption coefficient, it was shown that the main role in this is played by optical electronic transitions from the tail of the valence band to the tail of the conduction band (Fig.1) and for these transitions the Kubo-Greenwood formula, for the approximation Davis-Motta [4] is written as follows:

$$\alpha(\hbar\omega) = A \int_{\varepsilon_V}^{\varepsilon_C - \hbar\omega} g_1(\varepsilon) g_2(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega}. \qquad (1)$$

Here the proportionality coefficient is $A = \frac{8\pi^4 e^2 \hbar^2 a}{nc(m^*)^2}$, where a is the average distance between the semiconductor atoms, n is the refractive index of the semiconductor, c is the speed of light in vacuum, m^* are the effective masses of electrons in the conduction and valence bands of the semiconductor, $\hbar$ is Planck's constant, ω is the frequency of absorbed photons, $g_1(\varepsilon)$ is the distribution of the density of electronic states at the tail of the valence band, and $g(\varepsilon+\hbar\omega)$ is the distribution of the density of electronic states at the tail of the conduction band.

In [5], the distributions of the densities of electronic states on the exponential tails of the allowed bands are written in the following forms: for the tail of the valence band

$$g_1(\varepsilon)=N(\varepsilon_V)\exp(-\beta_1(\varepsilon-\varepsilon_V)), \quad \text{where} \quad \varepsilon_V \prec \varepsilon \prec \varepsilon_0 \quad , \tag{2}$$

and for the tail of the conduction band

$$g_2(\varepsilon)=N(\varepsilon_C)\exp(\beta_2(\varepsilon-\varepsilon_C)),$$

where $\varepsilon_0 \prec \varepsilon \prec \varepsilon_C$ (3)

In these formulas, $N(\varepsilon_V)$ - and $N(\varepsilon_C)$- are the effective values of the density of electronic states of the valence and conduction bands, respectively, and they are equal to $N(\varepsilon_V)\approx$ $N(\varepsilon_C)\approx 10^{22}$ eV^{-1}cm^{-3} [6], β_1 - and β_2 are parameters that determine the slope of the tails of the valence and conduction bands, respectively.

By supplying (2) and (3) to (1), performing calculations, the following result is obtained:

$$\alpha(\hbar\omega)=\frac{B}{(\beta_2-\beta_1)\hbar\omega}\exp(\beta_1(\hbar\omega-E_g))\left[1-\exp((\beta_2-\beta_1)(\hbar\omega-E_g))\right], \tag{4}$$

here B is equal on $B=AN(\varepsilon_V)N(\varepsilon_c)$ [7].

In order to determine the analytical solutions of the exponential absorption spectrum using this formula, it is necessary to find the constants B, E_g, β_1, and β_2. For this we will use the results of the exponential absorption spectrum determined experimentally.

In [8], the spectral characteristics of the optical absorption coefficient of the amorphous selenium-gray compound $a-Se_xS_{1-x}$. are given. To determine the above constants, we choose the results of experiments performed for $a\text{-}Se_{0.5}S_{0.5}$.

RESULTS

We divide the selected spectral characteristics of the optical absorption coefficient into interband, exponential, and defect absorption regions (Fig. 2). In [9], the values of B and E_g were determined considering them as fitting parameters, comparing the results of calculations of the formula for the interband absorption coefficient obtained for the parabolic allowed bands with the experimental results: B = 7.5 * 10^5 cm^{-1} and E_g = 2, 25 eV.

To determine the numerical values of β_1 and β_2, we will consider them as adjustable parameters, compare the experimental results for the exponential absorption region with the results of calculations of formula (4). After these comparisons, values were obtained equal to β_1 = 16.2 eV^{-1} and β_2 = 19.8 eV^{-1} (Fig. 2, solid curve).

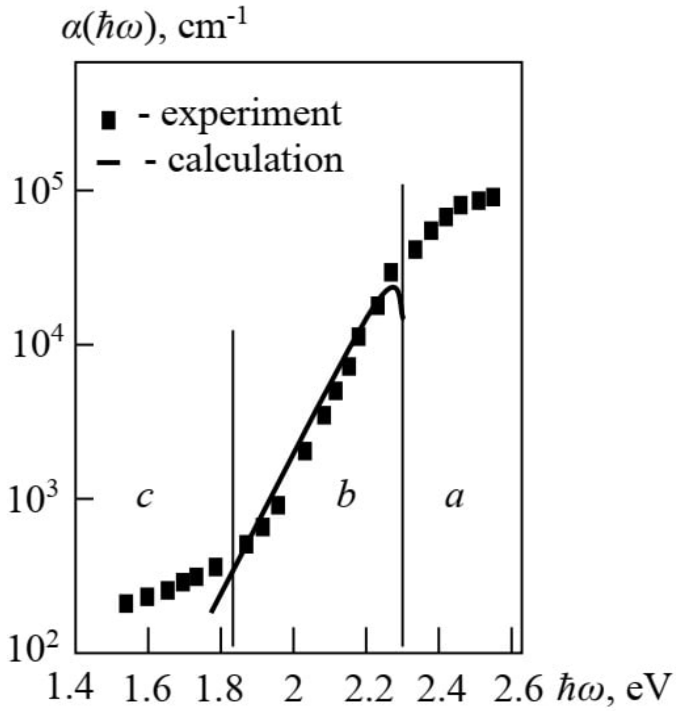

Fig. 2. Spectral characteristics obtained from experiment [8] for amorphous $Se_{0.5}S_{0.5}$ and formula (4). *a* - region of interband absorption, *b* - region of exponential absorption, *c* - region of defect absorption.

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

$$\frac{d}{dy}\int_{\alpha(y)}^{\beta(y)} f(x,y)dx = \int_{\alpha(y)}^{\beta(y)} \frac{\partial f(x,y)}{\partial y}dx + \frac{\partial\beta(y)}{\partial y} f(\beta(y),y) - \frac{\partial\alpha(y)}{\partial y} f(\alpha(y),y) \qquad (5)$$

Putting this formula in (7), we get the following expression:

$$\frac{\partial\alpha(\hbar\omega)}{\partial\hbar\omega} = \frac{\partial}{\partial\hbar\omega}A(\int_{\varepsilon_V}^{\varepsilon_C-\hbar\omega}(\frac{g_1(\varepsilon)g_2(\varepsilon+\hbar\omega)}{\hbar\omega})d\varepsilon =$$
$$= \frac{A}{\hbar\omega}\int_{\varepsilon_C-\hbar\omega}^{\varepsilon_V} g_1(\varepsilon)\frac{\partial}{\partial\hbar\omega}g_2(\varepsilon+\hbar\omega)d\varepsilon - \frac{\alpha(\hbar\omega)}{\hbar\omega} - \frac{A}{\hbar\omega}g_1(\varepsilon_C-\hbar\omega)g_2(\varepsilon_C). \qquad (6)$$

Putting (2) and (3) into this formula we get:

$$\frac{\partial\alpha(\hbar\omega)}{\hbar\omega} = \frac{A}{\hbar\omega}\int_{\varepsilon_C-\hbar\omega}^{\varepsilon_V} N(\varepsilon_V)N(\varepsilon_C)\exp(\beta_1\varepsilon_V)\exp(-\beta_1\varepsilon)\beta_2\exp(\beta_2(\varepsilon-\varepsilon_C+\hbar\omega))d\varepsilon - \frac{\alpha(\hbar\omega)}{\hbar\omega} -$$
$$-\frac{A}{\hbar\omega}N(\varepsilon_V)N(\varepsilon_C)\exp(-\beta_1(E_g-\hbar\omega)) = \qquad (7)$$
$$= \frac{B\beta_2}{\hbar\omega(\beta_2-\beta_1)}\exp(\beta_2(\hbar\omega-E_g)) - \frac{A}{\hbar\omega}\exp(-\beta_1(E_g-\hbar\omega))(\frac{\beta_2}{(\beta_2-\beta_1)}+1) - \frac{\alpha(\hbar\omega)}{\hbar\omega}$$

In expression (7) we denote:

$$g_1(\varepsilon) = N(\varepsilon_V)\exp(-\beta_1(\varepsilon-\varepsilon_V)) = N(\varepsilon_V)\exp(-\beta_1(E_g-\hbar\omega)) \qquad (8)$$

Using (8), we calculate which energy position determines. $E_g - \hbar\omega$

$$\varepsilon - \varepsilon_V = E_g - \hbar\omega : \qquad \varepsilon = \varepsilon_C - \varepsilon_V - \hbar\omega + \varepsilon_V = \varepsilon_C - \hbar\omega \tag{9}$$

Since in this expression, $E_g > \hbar\omega > \varepsilon_0 - \varepsilon_V$, $\varepsilon_V \prec 0$, ε in formula (9) determines the energy position at the tail of the valence band. Therefore, from equality (7) we obtain the following expression:

$$\frac{\partial\alpha(\hbar\omega)}{\partial\hbar\omega} = \frac{B\beta_2}{\hbar\omega(\beta_2-\beta_1)}\exp(\beta_2(\hbar\omega - E_g)) - \frac{B}{\hbar\omega N(\varepsilon_V)} g_1(\varepsilon)(\frac{\beta_2}{(\beta_2-\beta_1)}+1) - \frac{\alpha(\hbar\omega)}{\hbar\omega} \tag{10}$$

From the latter, the output is:

$$g_1(\varepsilon) = \frac{\hbar\omega N(\varepsilon_V)(\frac{B\beta_2}{\hbar\omega(\beta_2-\beta_1)}\exp(\beta_2(\hbar\omega - E_g)) - \frac{\partial\alpha(\hbar\omega)}{\partial\hbar\omega} - \frac{\alpha(\hbar\omega)}{\hbar\omega})}{B(\frac{\beta_2}{(\beta_2-\beta_1)}+1)} \tag{11}$$

We rewrite expression (11) by averaging the absorption coefficient and the energy of absorbed photons in the following form:

$$g_{1i}(\varepsilon) = \frac{(\hbar\omega_{i+1}+\hbar\omega_i)N(\varepsilon_V)(\frac{2B\beta_2}{(\hbar\omega_{i+1}+\hbar\omega_i)(\beta_2-\beta_1)}\exp(\beta_2(\frac{(\hbar\omega_{i+1}+\hbar\omega_i)}{2} - E_g)))}{2B(\frac{\beta_2}{(\beta_2-\beta_1)}+1)} - \\ - \frac{(\hbar\omega_{i+1}+\hbar\omega_i)N(\varepsilon_V)(\frac{\alpha_{i+1}(\hbar\omega)-\alpha_i(\hbar\omega)}{\hbar\omega_{i+1}-\hbar\omega_i} + \frac{\alpha_{i+1}(\hbar\omega)+\alpha_i(\hbar\omega)}{\hbar\omega_{i+1}+\hbar\omega_i})}{2B(\frac{\beta_2}{(\beta_2-\beta_1)}+1)} \tag{12}$$

Here $\alpha_i(\hbar\omega)$ - and $\hbar\omega_i$ are the absorption coefficient and the energy of absorbed photons, determined experimentally. Submitting the experimental results to (12), let us calculate the distribution of the density of electronic states at the tail of the valence band. The calculation results are shown in Fig. 3 (solid curve).

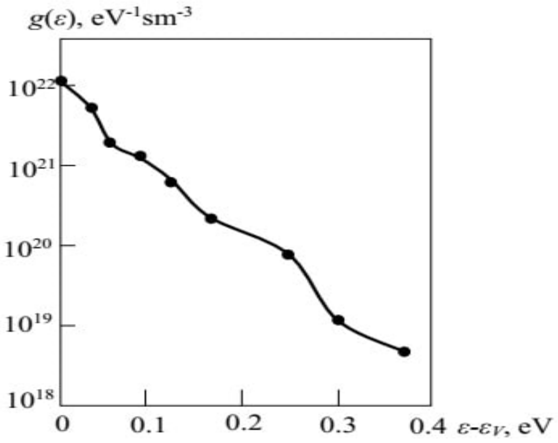

Fig. 3. The distribution of the density of electronic states at the tail of the valence band for amorphous $Se_{0.5}S_{0.5}$ was obtained from formula (12).

In the present work, the exponential absorption spectra are compared, the analytical expression obtained and those determined experimentally. These comparisons show the possibility of finding the parameters that determine the steepness of the tails of the valence and conduction bands. Using the Kubo-Greenwood formula by the Davis-Mott approximation method, for the region of exponential absorption, a new formula is derived that determines the distribution of the density of electronic states at the tail of the valence band. It is shown that this formula makes it possible to determine the distributions of the density of electronic states at the tail of the valence band from the experimental spectra of exponential absorption.

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