

A new method for determining the density distribution of electronic states on the tail of the valence band of amorphous semiconductors $\text{Se}_x\text{S}_{1-x}$

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The analytical expression and the experimental curve of the spectrum of the exponential absorption of amorphous selenium-sulfur solid solution ($\text{Se}_{0.5}\text{S}_{0.5}$ and $\text{Se}_{0.7}\text{S}_{0.3}$). Analytical parameters the expression for the exponential absorption spectrum, which determine the curvature of the exponential tails allowed bands are found by approximating the experimental curve. Using the approximation Davis - Mott, using the Kubo–Greenwood formula for the exponential absorption spectrum, a new formula that determines the density of electronic states in the tail of the valence band. Using this formula and the experimentally determined spectrum of exponential absorption shows the possibility of determination of the density of electronic states in the tail of the valence band.

Keywords: Amorphous semiconductors, allowed band tails, Kubo-Greenwood formula, Davis-Mott approximation method, optical electronic transitions, exponential absorption spectrum, parameters determining the slope of the allowed band tails, distribution of the density of electronic states.

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As it is known, the analytical spectrum of optical absorption of amorphous semiconductors is calculated by the Davis-Mott method from the Kubo-Greenwood formula [1]:

$$\alpha(\hbar\omega) = A \int g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega}. \quad (1)$$

Here A is the frequency independent proportion factor of the absorbed photon, equal to $A = \frac{8\pi^4 e^2 \hbar^2 a}{nc(m^*)^2}$, where e is electron charge, a is average distance between atoms of amorphous semiconductor, n is refraction index, c is speed of light in vacuum, m^* is electron effective weight, \hbar is Planck's constant, ω is frequency of absorbed photons, $g(\varepsilon)$ and $g(\varepsilon + \hbar\omega)$ are initial and final densities of electronic states of electrons involved in optical transitions, respectively.

The formula (1) shows that the optical absorption spectrum depends on the density distribution of electronic states involved in optical transitions. Therefore, in this paper, a new method for determining the density distribution of the electronic states in the tail of the valence band from the experimental exponential absorption spectrum.

In the region of exponential absorption the Urbach rule and the conditions for the absorbed photons energy $\varepsilon_C - \varepsilon_V = E_g > \hbar\omega$ is met, where E_g is energy width of mobility gap [2]. Here 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, and

from the valence band to the tail of the conduction band (Fig. 1).

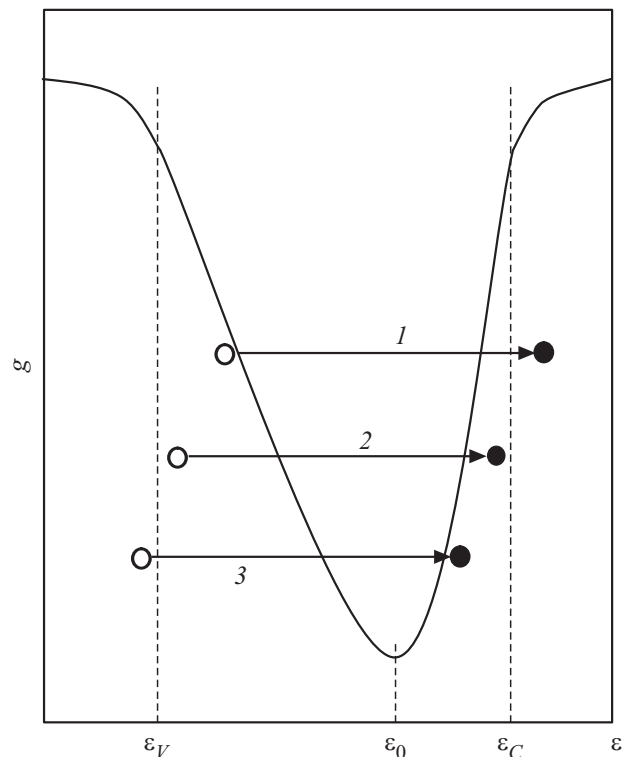


Figure 1. Types of optical transitions in amorphous semiconductors, at which the energy of absorbed photons lies in the range $\hbar\omega < \varepsilon_C - \varepsilon_V = E_g$: from the tail of the valence band to the conduction band (1), from the tail of the valence band to the tail of the conduction band (2), from the valence band to the tail of the conduction band (3).

The integral in formula (1) is indefinite; therefore, only a general solution can be obtained from this formula, but not eigensolution. Therefore, in the paper [3] the Kubo-Greenwood formula is written as a definite integral in the following form:

$$\alpha(\hbar\omega) = A \int_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega}, \quad (2)$$

where ε_0 is the energy position of the intersection point of the exponential tails of the allowed bands (Fig. 1). This formula was divided into partial absorption coefficients corresponding to the above optical transitions:

$$\begin{aligned} \alpha(\hbar\omega) &= A \int_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} \\ &= A \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_0} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} \\ &\quad + A \int_{\varepsilon_V}^{\varepsilon_C - \hbar\omega} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} \\ &\quad + A \int_{\varepsilon_0 - \hbar\omega}^{\varepsilon_V} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} \\ &= \alpha_1(\hbar\omega) + \alpha_2(\hbar\omega) + \alpha_3(\hbar\omega). \end{aligned} \quad (3)$$

The calculation results of values of these partial absorption coefficients show that the main role in determining the exponential absorption coefficient is played by optical electronic transitions from the tail of the valence band to the tail of the conduction band, i.e. $\alpha_1(\hbar\omega)$ (Fig. 2).

Therefore, in the paper [4] for the spectrum of the exponential absorption coefficient, the Kubo-Greenwood formula in the Davis-Mott approximation is written as follows:

$$\alpha(\hbar\omega) = A \int_{\varepsilon_V}^{\varepsilon_C - \hbar\omega} g_1(\varepsilon)g_2(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega}, \quad (4)$$

where $g_1(\varepsilon)$ is the density distribution of electronic states in the tail of valence band, and $g_2(\varepsilon + \hbar\omega)$ is the density distribution of electronic states in the tail of the conduction band.

In the paper [5] the density distributions of the electronic states in the exponential tails of the allowed bands is written as

$$g_1(\varepsilon) = N(\varepsilon_V) \exp(-\beta_1(\varepsilon - \varepsilon_V)), \quad (5)$$

where $\varepsilon_V < \varepsilon < \varepsilon_0$, for the tail of the valence band and

$$g_2(\varepsilon) = N(\varepsilon_C) \exp(\beta_2(\varepsilon - \varepsilon_C)), \quad (6)$$

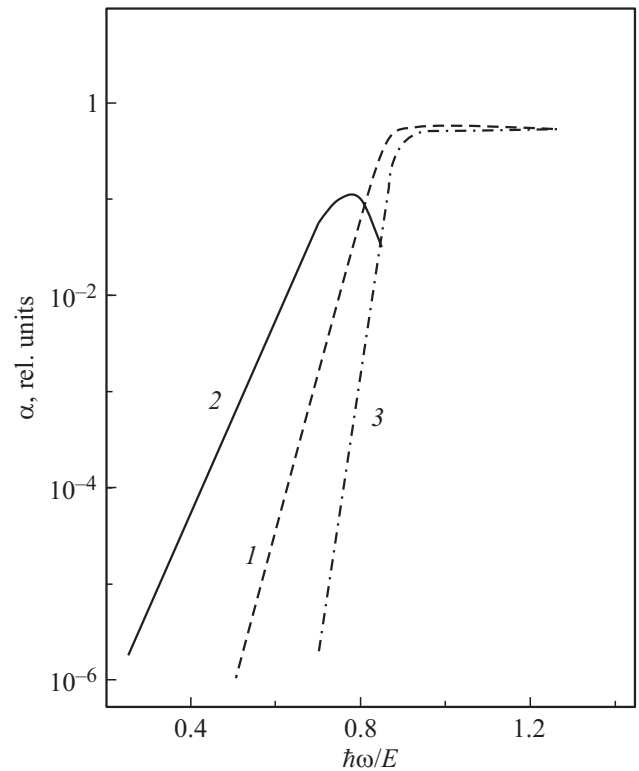


Figure 2. Spectral dependences of partial absorption coefficients corresponding to optical transitions of electrons, at which the energy of absorbed photons lies in the range $\hbar\omega < \varepsilon_C - \varepsilon_V = E_g$: α_1 — from the tail of valence band to the conduction band (1), α_2 — from the tail of valence band to the tail of conduction band (2), α_3 — from the valence band to the tail of the conduction band (3) [3].

where $\varepsilon_0 < \varepsilon < \varepsilon_C$ for the tail of the conduction band.

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, $N(\varepsilon_V) \approx N(\varepsilon_C) \approx 10^{22} \text{ eV}^{-1} \text{ cm}^{-3}$ [6], β_1 and β_2 are the parameters that determine the curvature of the exponential tails of the valence and conduction bands, respectively.

In the paper [7] by substituting (5) and (6) into (4) for the analytical solution of the exponential absorption spectrum, the following result was obtained:

$$\begin{aligned} \alpha(\hbar\omega) &= \frac{B}{(\beta_2 - \beta_1)\hbar\omega} \exp(\beta_1(\hbar\omega - E_g)) \\ &\quad \times [1 - \exp((\beta_2 - \beta_1)(\hbar\omega - E_g))], \end{aligned} \quad (7)$$

where $B = AN(\varepsilon_V)N(\varepsilon_C)$.

It can be seen that to determine the value of the analytical solutions of the exponential absorption spectrum by formula (7), it is necessary to determine the constants B , E_g , β_1 , and β_2 . To do this, we will use the results of the spectral characteristics of the exponential absorption coefficient determined experimentally.

The paper [8] presents the experimental results of the spectral characteristics of the optical absorption coefficient

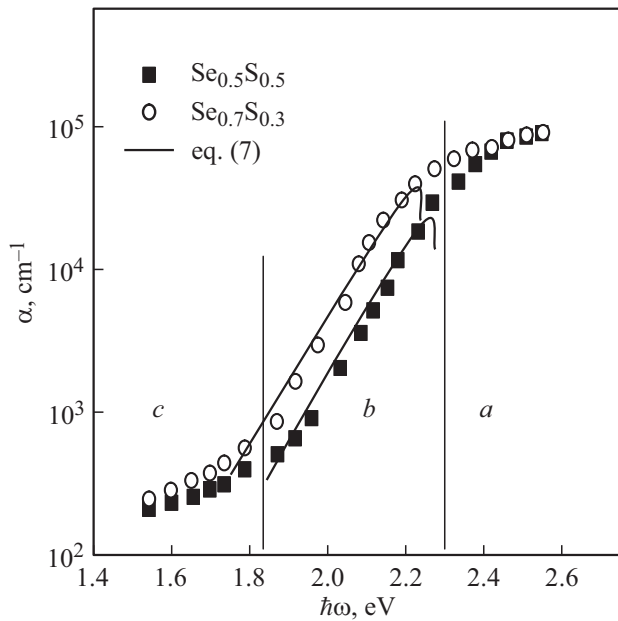


Figure 3. Spectrum obtained for amorphous $\text{Se}_{0.5}\text{S}_{0.5}$ and $\text{Se}_{0.7}\text{S}_{0.3}$ from experiment (circles and squares) [8], and also according to formula (7) (solid lines): regions of interband (a), exponential (b), defective absorption (c).

of an amorphous solid solution ($a-\text{Se}_x\text{S}_{1-x}$) obtained by thermal spraying in vacuum. To determine the above constants, we select the experimental results obtained for $a-\text{Se}_{0.5}\text{S}_{0.5}$ and $a-\text{Se}_{0.7}\text{S}_{0.3}$.

These optical absorption spectra are divided into interband, exponential and defect regions (Fig. 3) [9].

In the paper [10] the values of B and E_g are determined by considering them as adjustable parameters, comparing the results of calculations of the analytical form of the interband absorption spectrum obtained for parabolic allowed bands with the experimental results. For $a-\text{Se}_{0.5}\text{S}_{0.5}$ $B = 7.5 \cdot 10^5 \text{ cm}^{-1}$ and $E_g = 2.25 \text{ eV}$, and for $a-\text{Se}_{0.7}\text{S}_{0.3}$ $B = 7.1 \cdot 10^5 \text{ cm}^{-1}$ and $E_g = 2.2 \text{ eV}$. To determine the numerical values of β_1 and β_2 , considered as adjustable parameters, the experimental results for the region of exponential absorption are compared with the results of calculations using formula (7) (Fig. 3, solid lines). As a result, the values $\beta_1 = 16.2 \text{ eV}^{-1}$ and $\beta_2 = 19.8 \text{ eV}^{-1}$ for $a-\text{Se}_{0.5}\text{S}_{0.5}$, $\beta_1 = 16.3 \text{ eV}^{-1}$ and $\beta_2 = 19.7 \text{ eV}^{-1}$ for $a-\text{Se}_{0.7}\text{S}_{0.3}$.

In the paper [11] for the derivative with respect to one variable of the integral of function of two variables, the following expression is given:

$$\frac{d}{dy} \int_{\alpha(y)}^{\beta(y)} f(x, y) dx = \int_{\alpha(y)}^{\beta(y)} \frac{\partial f(x, y)}{\partial y} dx + \frac{\partial \beta(y)}{\partial y} f(\beta(y), y) - \frac{\partial \alpha(y)}{\partial y} f(\alpha(y), y). \quad (8)$$

Substituting (2) into this formula, we obtain the following expression:

$$\begin{aligned} \frac{\partial \alpha(\hbar\omega)}{\partial \hbar\omega} &= \frac{\partial}{\partial \hbar\omega} A \left(\int_{\varepsilon_V}^{\varepsilon_C - \hbar\omega} \left(\frac{g_1(\varepsilon)g_2(\varepsilon + \hbar\omega)}{\hbar\omega} \right) d\varepsilon \right) \\ &= \frac{A}{\hbar\omega} \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_V} g_1(\varepsilon) \frac{\partial}{\partial \hbar\omega} g_2(\varepsilon + \hbar\omega) d\varepsilon \\ &\quad - \frac{\alpha(\hbar\omega)}{\hbar\omega} - \frac{A}{\hbar\omega} g_1(\varepsilon_C - \hbar\omega)g_2(\varepsilon_C). \end{aligned} \quad (9)$$

Substituting (3) and (4) into this formula, we obtain

$$\begin{aligned} \frac{\partial \alpha(\hbar\omega)}{\partial \hbar\omega} &= \frac{A}{\hbar\omega} \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_V} N(\varepsilon_V)N(\varepsilon_C) \exp(\beta_1 \varepsilon_V) \\ &\quad \times \exp(-\beta_1 \varepsilon) \beta_2 \exp(\beta_2(\varepsilon - \varepsilon_C + \hbar\omega)) d\varepsilon - \frac{\alpha(\hbar\omega)}{\hbar\omega} \\ &\quad - \frac{A}{\hbar\omega} N(\varepsilon_V)N(\varepsilon_C) \exp(-\beta_1(E_g - \hbar\omega)) \\ &= \frac{A\beta_2}{\hbar\omega(\beta_2 - \beta_1)} \exp(\beta_2(\hbar\omega - E_g)) - \frac{A}{\hbar\omega} \\ &\quad \times \exp(-\beta_1(E_g - \hbar\omega)) \left(\frac{\beta_2}{(\beta_2 - \beta_1)} + 1 \right) - \frac{\alpha(\hbar\omega)}{\hbar\omega}. \end{aligned} \quad (10)$$

In expression (10) we denote

$$\begin{aligned} g_1(\varepsilon) &= N(\varepsilon_V) \exp(-\beta_1(\varepsilon - \varepsilon_V)) \\ &= N(\varepsilon_V) \exp(-\beta_1(E_g - \hbar\omega)). \end{aligned} \quad (11)$$

Using (11), we calculate

$$\varepsilon - \varepsilon_V = E_g - \hbar\omega, \quad \varepsilon = \varepsilon_V + E_g - \hbar\omega. \quad (12)$$

Since in this expression $E_g > \hbar\omega$, $\varepsilon_V < 0$, in formula (10) ε determines the energy position on the tail of the valence band. Therefore, from equality (10) we obtain the following expression:

$$\begin{aligned} \frac{\partial \alpha(\hbar\omega)}{\partial \hbar\omega} &= \frac{B\beta_2}{\hbar\omega(\beta_2 - \beta_1)} \exp(\beta_2(\hbar\omega - E_g)) \\ &\quad - \frac{B}{\hbar\omega N(\varepsilon_V)} g_1(\varepsilon) \left(\frac{\beta_2}{(\beta_2 - \beta_1)} + 1 \right) - \frac{\alpha(\hbar\omega)}{\hbar\omega} \end{aligned} \quad (13)$$

and further

$$g_1(\varepsilon) = \frac{\hbar\omega N(\varepsilon_V) \left(\frac{B\beta_2}{\hbar\omega(\beta_2 - \beta_1)} \exp(\beta_2(\hbar\omega - E_g)) \right) - \frac{\partial \alpha(\hbar\omega)}{\partial \hbar\omega} - \frac{\alpha(\hbar\omega)}{\hbar\omega}}{B \left(\frac{\beta_2}{(\beta_2 - \beta_1)} + 1 \right)}. \quad (14)$$

In formula (14) $\frac{\partial \alpha(\hbar\omega)}{\partial \hbar\omega} \approx \frac{\Delta \alpha(\hbar\omega)}{\Delta \hbar \omega} = \frac{\alpha(\hbar\omega_{i+1}) - \alpha(\hbar\omega_i)}{\hbar\omega_{i+1} - \hbar\omega_i}$. Using the average values of the exponential absorption coefficient

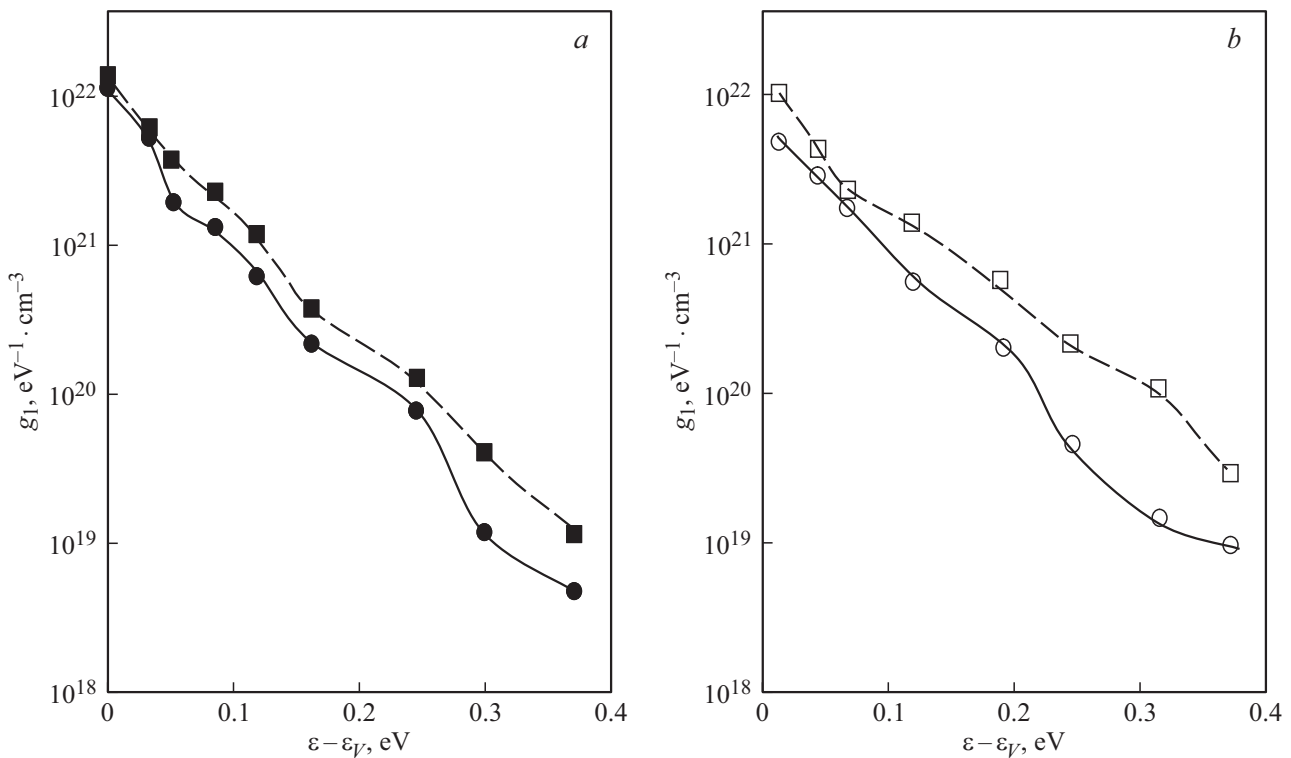


Figure 4. Density distributions of electronic states in the tail of the valence band for amorphous $\text{Se}_{0.5}\text{S}_{0.5}$ (a) and $\text{Se}_{0.7}\text{S}_{0.3}$ (b) calculated by formulas (15) and (16) — solid (circles) and dashed curves (squares) respectively.

and the energy of absorbed photons, we write formula (14) in the form

$$g_1(\varepsilon_i) = \frac{(\hbar\omega_{i+1} + \hbar\omega_i)N(\varepsilon_V) \times \left(\frac{2B\beta_2}{(\hbar\omega_{i+1} + \hbar\omega_i)(\beta_2 - \beta_1)} \exp\left(\beta_2 \left(\frac{\hbar\omega_{i+1} + \hbar\omega_i}{2} - E_g \right)\right) \right)}{2B \left(\frac{\beta_2}{(\beta_2 - \beta_1)} + 1 \right)} - \frac{(\hbar\omega_{i+1} + \hbar\omega_i)N(\varepsilon_V) \left(\frac{\alpha(\hbar\omega_{i+1}) - \alpha_i(\hbar\omega_i)}{\hbar\omega_{i+1} - \hbar\omega_i} + \frac{\alpha(\hbar\omega_{i+1}) + \alpha_i(\hbar\omega_i)}{\hbar\omega_{i+1} + \hbar\omega_i} \right)}{2B \left(\frac{\beta_2}{(\beta_2 - \beta_1)} + 1 \right)}, \quad (15)$$

$$g_1(\varepsilon_i) = N(\varepsilon_V) \exp\left(-\beta_1 \left(\frac{\hbar\omega_i + \hbar\omega_{i+1}}{2} \right)\right). \quad (16)$$

Here $\alpha(\hbar\omega_i)$ and $\hbar\omega_i$ are the absorption coefficient and the energy of absorbed photons, respectively, determined experimentally.

Substituting in (15) and (16) the measurement results of the exponential absorption spectrum, we calculate the density distributions of electronic states in the tail of the valence band calculated for $a\text{-Se}_{0.5}\text{S}_{0.5}$ (Fig. 4, a) and $a\text{-Se}_{0.7}\text{S}_{0.3}$ (Fig. 4, b) by the formulas (15) and (16). They practically repeat each other. It can be seen that the density values of the electronic states in the tail of the valence band increase with increasing of selenium content in the solid solution $a\text{-Se}_x\text{S}_{1-x}$.

Thus, in this paper, by comparing the experimental results with those calculated from the analytical expression for the exponential absorption spectrum, we show the possibility of determining the parameters that determine the curvature of the exponential tails of the valence and conduction bands. Using the Kubo-Greenwood formula in the Davis-Mott approximation for the region of exponential absorption, a new formula is derived that determines the density distributions of electronic states in the tail of the valence band. Using the experimental results obtained for the exponential absorption spectrum, the possibility of determining the density distribution of the electronic states in the tail of the valence band is shown. It is shown that the values of density distribution of the electronic states in the tail of the valence band increase with increasing of selenium content in the solid solution $a\text{-Se}_x\text{S}_{1-x}$.

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