

DEPENDENCE OF THE URBACH ENERGY ON THE FERMI LEVEL IN A-Si:H FILMS

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As is known, there exist a lot of experimental results indicating the relation between the Urbach parameter (energy) and the Fermi level. But no analytical expression determining these dependences is available in the literature up to now. In the given work, we have obtained new formulas that determine the relationship between the Urbach energy and the Fermi level for pseudodoped amorphous semiconductors, in which the electron state densities in the tails of the allowed bands depend exponentially on the energy. It is shown that the results obtained by these formulas can explain experimental data quite well.

The Urbach energy represents one of the parameters that determine the efficiency of a working layer (*i*-layer, i.e. a layer with intrinsic conduction) of optical devices prepared on the basis of amorphous semiconductors. At present, the Urbach energy is evaluated from the exponential region of experimentally obtained spectral characteristic curves of the absorption coefficient, by using the Urbach rule [1,2]. As is known, variations of the density of electron states lying in the tails of the allowed bands result in a change of this parameter and the corresponding shifts of the Fermi level [3]. Works [4,5] present the results obtained from experimental investigations of the dependence of the Urbach energy on the Fermi level for pseudo-doped a-Si:H films. However, the formulas explaining these dependences are not obtained till now. That is why the given work considers the conditions determining these dependences with the help of the Kubo–Greenwood formula. The spectra of the absorption coefficient were calculated using the Davis–Mott approximation [6]. We established three types of optical electron transitions that determine the values of the absorption coefficient in the spectral region where the Urbach rule is met. That is why the integral in the Kubo–Greenwood formula is divided into the corresponding components that determine the above-mentioned optical electron transitions.

When growing the films of amorphous hydrogenated silicon (a-Si:H) used for the preparation of the active region of photoelectric devices, it is worth paying

attention to the requirement that the concentration of dangling bonds (defects) in them must not influence the electric and photoelectric properties of the sample. That is why the energy position of the Fermi level (ε_F) in this material is mainly determined by the density of localized electron states lying in the “tails” of the allowed bands. These states in amorphous semiconductors exponentially depend on the energy [7,8]

$$g(\varepsilon) = N(\varepsilon_V) \exp(-\beta_1(\varepsilon - \varepsilon_V)), \quad \text{at } \varepsilon_V < \varepsilon < \varepsilon_F, \quad (1)$$

$$g(\varepsilon) = N(\varepsilon_C) \exp(\beta_2(\varepsilon - \varepsilon_C)), \quad \text{at } \varepsilon_F < \varepsilon < \varepsilon_C, \quad (2)$$

where β_1 and β_2 denote the parameters that determine the curvature of the exponential “tails” of the valence and conduction bands, respectively (for a-Si:H, their values lie in the range (16–30) eV⁻¹ [9]), ε_V and ε_C are the edges of the valence band and the conduction one, $N(\varepsilon_V)$ and $N(\varepsilon_C)$ denote the effective densities of electron states in the valence and conduction bands. In pseudodoped a-Si:H films, the shifts of the Fermi level are realized at the expense of the variation of the technological conditions of growth (pseudodoping effect [3]). In these samples, the Fermi level determines only the densities of electron states lying in the “tails” of the allowed bands, and it is located at the point of the intersection of the exponential tails of the valence band and the conduction one. That is why it is easy to prove the validity of the following expressions:

$$\varepsilon_C - \varepsilon_F \approx \left(\beta_1 E_g + \ln \frac{N(\varepsilon_C)}{N(\varepsilon_V)} \right) / (\beta_1 + \beta_2), \quad (3)$$

$$\varepsilon_F - \varepsilon_V \approx \left(\beta_2 E_g + \ln \frac{N(\varepsilon_V)}{N(\varepsilon_C)} \right) / (\beta_1 + \beta_2), \quad (4)$$

where E_g stands for the width of the mobility gap (forbidden band). If $N(\varepsilon_V) = N(\varepsilon_C)$, one can see that,

at $\beta_1 > \beta_2$, the Fermi level is located above the middle of the mobility gap, and these samples have conduction of the n type. In the case where $\beta_1 < \beta_2$, it lies lower and the samples have conduction of the p type. For intrinsic pseudodoped a-Si:H samples, the condition $\beta_1 = \beta_2$ is realized. At first, we consider samples with the n -type conduction. If the energy of absorbed photons is lower than the mobility gap width, the spectral characteristic of the optical absorption coefficient obeys the Urbach rule that is empirically described in the following way [1, 2]:

$$\alpha(\hbar\omega) = \alpha_0 \exp\left(\frac{\hbar\omega}{E_U}\right). \tag{5}$$

Whence we obtain the Urbach energy

$$E_U = \alpha(\hbar\omega) \left(\frac{d(\alpha(\hbar\omega))}{d(\hbar\omega)}\right)^{-1}. \tag{6}$$

In the region of the spectral characteristic of the optical absorption coefficient in the a-Si:H films, where the Urbach rule is met (i.e. $\hbar\omega < E_g$), one can observe three kinds of optical electron transitions:

1. From the valence band to the “tail” of the conduction band,
2. From the “tail” of the valence band to the “tail” of the conduction band,
3. From the “tail” of the valence band to the conduction band.

Based on the data obtained in [6,9] and considering that the density distributions of non-localized electron states in the allowed bands have a power dependence on the energy, we choose them in the following form: for the valence band,

$$g(\varepsilon) = N(\varepsilon_V) \left(\frac{\varepsilon_C - \varepsilon}{E_g}\right)^m, \tag{7}$$

whereas for the conduction band,

$$g(\varepsilon) = N(\varepsilon_C) \left(\frac{\varepsilon - \varepsilon_V}{E_g}\right)^m, \tag{8}$$

where $m = 0, \frac{1}{2}, 1$.

In amorphous semiconductors, the spectral characteristic of the optical absorption coefficient can be determined from the Kubo–Greenwood formula using the Davis–Mott approximation [6]

$$\alpha \sim \int_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega}, \tag{9}$$

where $g(\varepsilon)$ and $g(\varepsilon + \hbar\omega)$ denote the initial and final states of the electrons taking part in transitions in the case of the absorption of a photon with energy $\hbar\omega$, ε_0 is the highest energy position of the electrons participating in optical transitions. At $T = 0$ K, this energy corresponds to the point of intersection of the tails of the allowed bands (i.e. with the Fermi level $\varepsilon_0 = \varepsilon_F$).

As is known, the optical absorption coefficient represents an additive parameter [10]. That is why, in order to calculate the spectra of the absorption coefficient based on formula (9), one should divide the integral into components corresponding to the above-mentioned electron transitions:

$$\begin{aligned} \alpha \sim & \int_{\varepsilon_F - \hbar\omega}^{\varepsilon_F} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} = \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_F} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} + \\ & + \int_{\varepsilon_V}^{\varepsilon_C - \hbar\omega} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} + \\ & + \int_{\varepsilon_F - \hbar\omega}^{\varepsilon_V} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} = \alpha_1 + \alpha_2 + \alpha_3 \end{aligned} \tag{10}$$

where α_1 , α_2 , and α_3 are the spectra of the absorption coefficient corresponding to the electron transitions 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, respectively. Thus, the performed numerical calculations of the spectra of the optical absorption coefficient, determined by electron transitions with participation of the electron states located in the allowed bands and in the “tails” of these bands, demonstrate that the obtained spectral characteristics practically do not differ at different m . That’s why we present here the analytical expressions obtained only for $m = 0$ in the following forms:

$$\alpha_1 \sim \frac{1}{\beta_1 \hbar\omega} \exp(\beta_1(\hbar\omega - E_g)) [1 - \exp(\beta_1(\varepsilon_C - \varepsilon_F - \hbar\omega))], \tag{11}$$

$$\begin{aligned} \alpha_2 \sim & \frac{1}{(\beta_2 - \beta_1) \hbar\omega} \exp(\beta_1(\hbar\omega - E_g)) \times \\ & \times [1 - \exp((\beta_2 - \beta_1)(\hbar\omega - E_g))], \end{aligned} \tag{12}$$

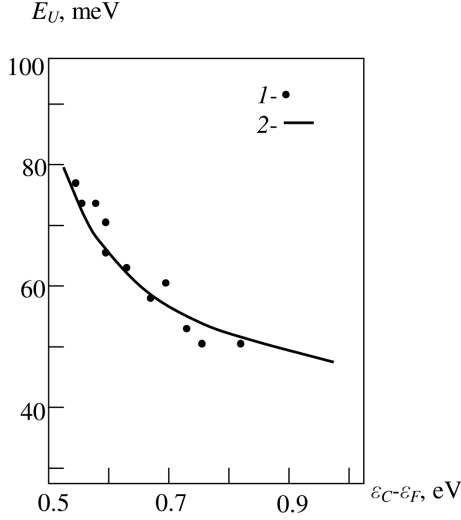


Fig. 1. Dependence of the Urbach energy on the position of the Fermi level for pseudodoped a-Si:H samples with n -type conduction. 1 – experimental results [4,5], 2 – results of calculations of this work

$$\alpha_3 \sim \frac{1}{\beta_2 \hbar \omega} \exp(\beta_2(\hbar \omega - E_g)) [1 - \exp(\beta_2(\varepsilon_F - \varepsilon_V - \hbar \omega))]. \quad (13)$$

In view of these expressions and formula (6), the Urbach energy can be determined as

$$E_U = (\alpha_1 + \alpha_2 + \alpha_3) / \left(\frac{d\alpha_1}{d(\hbar \omega)} + \frac{d\alpha_2}{d(\hbar \omega)} + \frac{d\alpha_3}{d(\hbar \omega)} \right). \quad (14)$$

Differentiating the absorption coefficients in (11), (12), and (13), we obtain

$$\frac{d\alpha_1}{d(\hbar \omega)} \sim \frac{1}{\beta_1 (\hbar \omega)^2} \exp(\beta_1(\hbar \omega - E_g)) \times [\hbar \omega \beta_1 - 1 + \exp(\beta_1(\varepsilon_C - \varepsilon_F - \hbar \omega))], \quad (15)$$

$$\frac{d\alpha_2}{d(\hbar \omega)} \sim \frac{1}{(\beta_2 - \beta_1)(\hbar \omega)^2} \exp(\beta_1(\hbar \omega - E_g)) \times [\beta_1 \hbar \omega - 1 - (\beta_2 \hbar \omega - 1) \exp((\beta_2 - \beta_1)(\hbar \omega - E_g))], \quad (16)$$

$$\frac{d\alpha_3}{d(\hbar \omega)} \sim \frac{1}{\beta_2 (\hbar \omega)^2} \exp(\beta_2(\hbar \omega - E_g)) \times [\hbar \omega \beta_2 - 1 + \exp(\beta_2(\varepsilon_F - \varepsilon_V - \hbar \omega))]. \quad (17)$$

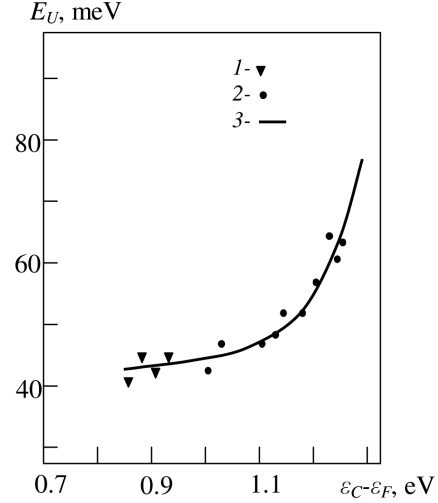


Fig. 2. Experimental dependences of the Urbach energy on the position of the Fermi level for pseudodoped a-Si:H samples with intrinsic (1) and p -type conduction (2) obtained in [4,5] and the results of calculations of this work (3)

One can see that formulas (11), (13) and (15), (17) depend on the Fermi level; therefore, the dependence of the Urbach energy on the Fermi level can be determined from (14).

The results of calculations with the use of formula (14) and the experimental data [4,5] for pseudodoped a-Si:H films are presented in Fig. 1. One can see that these data are in good agreement. In addition, the calculations have demonstrated that, with increasing β_1 and β_2 , the curves determining the dependence of the Urbach energy on the Fermi level shift upward.

If a sample has intrinsic or hole conduction, then the types of optical electron transitions do not change. That is why the formulas corresponding to these transitions have the same form. As was said above, for samples with p -type conduction, the condition $\beta_1 < \beta_2$ holds true, that is why the curve $E_U(\varepsilon_F)$ rises with increasing $\varepsilon_C - \varepsilon_F$ (Fig. 2). For samples with intrinsic conduction, the conditions $\beta_1 \approx \beta_2 \approx \beta$ and $\varepsilon_C - \varepsilon_F \approx \varepsilon_F - \varepsilon_V \approx \frac{E_g}{2}$ are met. Therefore, the formulas for the absorption coefficient spectra have the form

$$\alpha_1 \approx \alpha_3 \sim \frac{1}{\beta \hbar \omega} \exp(\beta(\hbar \omega - E_g)) \left[1 - \exp\left(\beta\left(\frac{E_g}{2} - \hbar \omega\right)\right) \right], \quad (18)$$

$$\alpha_2 \sim \frac{E_g - \hbar \omega}{\hbar \omega} \exp(\beta(\hbar \omega - E_g)). \quad (19)$$

The correspondence between the experimental results obtained in [4,5] for these samples and the results of this work is shown in Fig. 2.

Thus, we have investigated the dependences of the Urbach energy on the Fermi level for pseudodoped a-Si:H films. The formulas of the spectral characteristic of the optical absorption coefficient are obtained for the case where the condition $\hbar\omega < E_g$ is met (the Urbach edge). The formulas expressing the dependences of the Urbach energy on the Fermi level are derived as well. It is shown that these formulas can well explain the experimental data obtained in [4,5]. The results of the given work favor the improvement of optical properties of devices based on amorphous semiconductors. These results can be also used for other semiconductors, in which the absorption coefficient spectra obey the Urbach rule.

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ЗАЛЕЖНІСТЬ ЕНЕРГІЇ УРБАХА ВІД РІВНЯ ФЕРМІ В ПЛІВКАХ a-Si:H

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Резюме

Як відомо, існує багато експериментальних результатів, які вказують на зв'язок між параметром (енергія) Урбаха та рівнем Фермі. Але до цього часу в літературі немає аналітичного виразу, що визначає ці залежності. В цій роботі одержано нові формули, що визначають зв'язок між енергією Урбаха та рівнем Фермі для псевдолегованих аморфних напівпровідників, у яких щільності електронних станів, що знаходяться у хвостах дозволених зон, мають експоненціальну залежність від енергії. Показано, що результати, одержані за цими формулами, цілком можуть пояснити експериментальні дані.