

Temperature Dependence of Urbach Energy in Non-Crystalline Semiconductors

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Abstract

Until now, no analytical relationships have been derived for the temperature dependence of the Urbach energy in non-crystalline semiconductors. Consequently, the problem associated with the theoretical study of the temperature dependence of this energy has not been solved. This paper presents the results of theoretical calculations and attempts to establish the temperature dependence of the Urbach energy in non-crystalline semiconductors. A linear increase in the Urbach energy with increasing temperature is shown.

Keywords

Non-Crystalline Semiconductors, Urbach Rules, Urbach Energy, Optical Transitions

1. Introduction

Exponential frequency dependence of the light absorption coefficient in non-crystalline semiconductors near the optical absorption edge, *i.e.* in the frequency range $\hbar\omega < E_g$ has the form [1]:

$$\alpha(\hbar\omega) = \text{const} \cdot \exp\left(\frac{\hbar\omega}{E_U}\right) \quad (1)$$

where E_U is the Urbach energy, which for noncrystalline semiconductors can take on a value of 30 - 100 meV. In this case, optical transitions can occur, both forming photoconductivity and not forming photoconductivity. The absorption coefficient spectra of both optical transitions will be exponential [2].

In [3], the types of distributions of the density of electronic states are provided, at the edges of the allowed bands in the following forms: for the valence band

$$g(\varepsilon) = N(\varepsilon_V) \left(\frac{\varepsilon_C - \varepsilon}{E_g} \right)^{n_1}, \text{ when } \varepsilon \leq \varepsilon_V \quad (2)$$

for the conduction band

$$g(\varepsilon) = N(\varepsilon_C) \left(\frac{\varepsilon - \varepsilon_V}{E_g} \right)^{n_2}, \text{ when } \varepsilon_C \leq \varepsilon \quad (3)$$

where the powers n_1 and n_2 can take on the values 0, 1/2 or 1, *i.e.* distributions of the density of electronic states, in the edges of the expanded zones can be constant, parabolic or linear. And the distributions of the density of electronic states located on the tails of the allowed bands: for the tail of the valence band

$$g(\varepsilon) = N(\varepsilon_V) \exp(-\beta_1(\varepsilon - \varepsilon_V)), \text{ when } \varepsilon_V < \varepsilon < \varepsilon_0 \quad (4)$$

for the tail of the conduction band

$$g(\varepsilon) = N(\varepsilon_C) \exp(\beta_2(\varepsilon - \varepsilon_C)), \text{ when } \varepsilon_0 < \varepsilon < \varepsilon_C \quad (5)$$

where β_1 and β_2 are parameters determining the slopes of the tails of the allowed zones.

In general terms, the Kubo-Greenwood formula is written as follows:

$$\alpha(\hbar\omega) = \frac{8\pi^2 e^2 \hbar^3 \Omega}{(m^*)^2 n_0 c} \int_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} \frac{g(\varepsilon) g(\varepsilon + \hbar\omega)}{\hbar\omega} (f(\varepsilon) - f(\varepsilon + \hbar\omega)) |D|^2 d\varepsilon \quad (6)$$

where e is the electron charge, \hbar is Planck's constant, Ω is the normalized volume for the eigenfunction of an electron with energy ε , m^* is the effective mass of charge carriers, n_0 is the refractive index among, $f(\varepsilon)$ and $g(\varepsilon + \hbar\omega)$ are the initial and final densities of electronic states of the involved optical transitions, $f(\varepsilon)$ and $f(\varepsilon + \hbar\omega)$ are the Fermi-Dirac distributions, $|D|^2$ is the dispersion of the matrix element of the optical transition. If for the energy of the absorbed photon, the conditions $\hbar\omega \gg kT$ are satisfied, then we can assume that $f(\varepsilon) = 1$ and $f(\varepsilon + \hbar) = 0$. According to the Davis-Mott approximation for one type of optical transition, the dispersion of the matrix element is considered constant and the Kubo-Greenwood formula is written as follows:

$$\begin{aligned} \alpha(\hbar\omega) &= \frac{8\pi^2 e^2 \hbar^3 \Omega}{(m^*)^2 n_0 c} |D|^2 \int_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} \frac{g(\varepsilon) g(\varepsilon + \hbar\omega)}{\hbar\omega} d\varepsilon \\ &= B \int_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} \frac{g(\varepsilon) g(\varepsilon + \hbar\omega)}{\hbar\omega} d\varepsilon \end{aligned} \quad (7)$$

The absorption coefficient is an additive parameter, *i.e.* [3]:

$$\alpha = \sum_i \alpha_i \quad (8)$$

This means that if the energy of the absorbed photon lies in the range $\varepsilon_0 - \varepsilon_V < \hbar\omega < \varepsilon_C - \varepsilon_V = E_g$ in non-crystalline semiconductors, electrons simultaneously participate in the following optical 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, from the valence band to the tail of the conduction band

[4]. Therefore, the values of the absorption coefficient are determined by the sum of the partial absorption coefficients of the corresponding above optical transitions:

$$\alpha(\hbar\omega) = \alpha_1 + \alpha_2 + \alpha_3 \quad (9)$$

where α_1 —corresponds to the spectrum of the optical transition of electrons from the tail of the valence band to the conduction band of the generating electron photoconductivity; α_2 —from the tail of the valence band, to the tail of the conduction band that does not generate photoconductivity; α_3 —from the valence band to the tail of the conduction band generating hole photoconductivity.

Let us calculate the Urbach energy for the spectra of the coefficient of optical transitions with the participation of localized electronic states at the exponential tails of the allowed bands. For this, we take the derivative of formula (1) with respect to the energy of absorbed photons $\hbar\omega$

$$\frac{d(\alpha(\hbar\omega))}{d(\hbar\omega)} = \frac{1}{E_U} \text{const} \cdot \exp\left(\frac{\hbar\omega}{E_U}\right), \quad (10)$$

or

$$\frac{d(\alpha(\hbar\omega))}{d(\hbar\omega)} = \frac{\alpha(\hbar\omega)}{E_U}, \quad (11)$$

therefore, we get for the Urbach energy

$$E_U = \alpha(\hbar\omega) \Big/ \frac{d(\alpha(\hbar\omega))}{d(\hbar\omega)}. \quad (12)$$

This formula for the section $\varepsilon_0 - \varepsilon_V < \hbar\omega < \varepsilon_C - \varepsilon_V = E_g$ can be written in the form

$$E_U = (\alpha_1 + \alpha_2 + \alpha_3) \left(\frac{d\alpha_1}{d(\hbar\omega)} + \frac{d\alpha_2}{d(\hbar\omega)} + \frac{d\alpha_3}{d(\hbar\omega)} \right)^{-1}. \quad (13)$$

In [3], the calculation of the spectra of the optical absorption coefficient for all optical transitions was carried out according to the Kubo-Greenwood formula using the Davis-Mott approximation method. Calculations of expressions for determining the exponential absorption spectra were carried out in the cases of constant, parabolic, and linear distributions of the densities of electronic states at the boundaries of the allowed bands. An insignificant difference in the values of the spectral absorption coefficients of optical transitions with the participation of the above states was shown. Based on these considerations, in order to simplify the analytical form of the expressions for these spectra, we consider the case of constant nonlocalized electronic states. The following results were obtained for these spectra:

$$\alpha_1 = \frac{A}{\beta_1 \hbar\omega} \exp(-\beta_1(E_g - \hbar\omega)) \left[1 - \exp(\beta_1(\varepsilon_C - \varepsilon_0 - \hbar\omega)) \right] \quad (14)$$

$$\alpha_2 = \frac{A}{(\beta_2 - \beta_1) \hbar\omega} \exp(\beta_1(\hbar\omega - E_g)) \left[1 - \exp((\beta_2 - \beta_1)(\hbar\omega - E_g)) \right] \quad (15)$$

$$\alpha_3 = \frac{A}{\beta_2 \hbar \omega} \exp(\beta_2 (\hbar \omega - E_g)) [1 - \exp(\beta_2 (\varepsilon_0 - \varepsilon_v - \hbar \omega))] \quad (16)$$

where $A = BN(\varepsilon_v)N(\varepsilon_c)$ is the proportionality coefficient independent of temperature and the frequency of absorbed photons, the numerical value of which is given in [3] $A \approx 2.5 \times 10^5 \text{ cm}^{-1}$; ε_c is the lower edge of the conduction band; ε_v is the upper edge of the valence band; ε_0 is the energy position of the point of intersection of the tails of the allowed zones.

2. Calculation and Discussion of Results

If we differentiate these formulas by $\hbar \omega$, then we get the following expressions:

$$\frac{d\alpha_1}{d(\hbar \omega)} = \frac{A}{\beta_1 (\hbar \omega)^2} \exp(\beta_1 (\hbar \omega - E_g)) [\beta_1 \hbar \omega - 1 + \exp(\beta_1 ((\varepsilon_c - \varepsilon_0) - \hbar \omega))] \quad (17)$$

$$\frac{d\alpha_2}{d(\hbar \omega)} = \frac{A}{(\beta_2 - \beta_1) (\hbar \omega)^2} \left((\beta_1 \hbar \omega - 1) \exp(\beta_1 (\hbar \omega - E_g)) - (\beta_2 \hbar \omega - 1) \exp(\beta_2 (\hbar \omega - E_g)) \right) \quad (18)$$

$$\frac{d\alpha_3}{d(\hbar \omega)} = \frac{A}{\beta_2 (\hbar \omega)^2} \exp(\beta_2 (\hbar \omega - E_g)) [\beta_2 \hbar \omega - 1 + \exp(\beta_2 ((\varepsilon_0 - \varepsilon_v) - \hbar \omega))] \quad (19)$$

Substituting into these expressions the dependences of the intersection points of the exponential tails of the allowed zones [4]

$$\varepsilon_c - \varepsilon_0 = \frac{\beta_1 E_g}{\beta_1 + \beta_2}, \quad (20)$$

$$\varepsilon_0 - \varepsilon_v = \frac{\beta_2 E_g}{\beta_1 + \beta_2}, \quad (21)$$

then it is possible to obtain new the dependence for the Urbach energy on the parameters β_1 , β_2 and E_g .

Calculations show that the main role in the exponential region of the absorption coefficient spectra is played by optical transitions that do not form photoconductivity (Figure 1) [5]. Therefore, the expression for the Urbach energy can be written in the form:

$$E_U = \alpha_2 (\hbar \omega) \left(\frac{d(\alpha_2 (\hbar \omega))}{d(\hbar \omega)} \right)^{-1}. \quad (22)$$

Substituting (15) and (18) into (22), we can obtain a formula for determining the Urbach energy:

$$E_U = \frac{A}{(\beta_2 - \beta_1) \hbar \omega} \exp(\beta_1 (\hbar \omega - E_g)) (1 - \exp((\beta_2 - \beta_1) (\hbar \omega - E_g))) \times \left[\frac{A}{(\beta_2 - \beta_1) (\hbar \omega)^2} \left((\beta_1 \hbar \omega - 1) \exp(\beta_1 (\hbar \omega - E_g)) - (\beta_2 \hbar \omega - 1) \exp(\beta_2 (\hbar \omega - E_g)) \right) \right]^{-1} \quad (23)$$

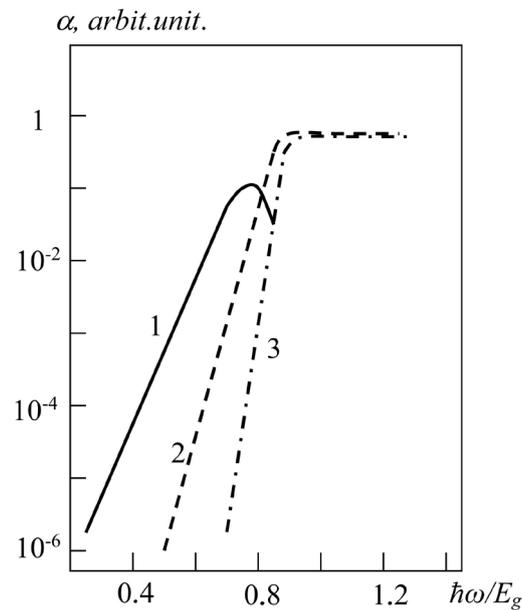


Figure 1. Absorption coefficient in hydrogenated amorphous semiconductors with n -type conductivity for electronic transitions: where 1—photoconductivity is not created; 2—electronic photoconductivity is formed; 3—hole photoconductivity is formed.

As shown in [5], the value of the densities of states at the tails of the allowed bands in the temperature range $T < 550$ K does not change. Taking into account the above, in formula (23) there remains the only parameter E_g which depends on the temperature

$$E_g(T) = E_g(0) - \gamma T. \quad (24)$$

It was shown in [6] [7] that Urbach's rule can be written as follows:

$$\alpha = \alpha_0 \cdot \exp\left(\frac{\sigma \cdot (E - E_0)}{kT}\right), \quad (25)$$

where $E = \hbar\omega$ is the radiation photon energy; α_0 is the absorption coefficient at the energy value $E = E_0$; k is the Boltzmann constant; T is the operating temperature; σ is a coefficient that characterizes the degree of steepness of the dependence of the absorption coefficient, that is, the Urbach slope, depending on the parameters of the material. Comparing both expressions (1) and (25), we find the Urbach energy as follows:

$$E_U = \frac{kT}{\sigma} \quad (26)$$

From this formula it can be seen that the temperature dependence of the Urbach energies is linear. The slope of these lines is $\text{tg}\varphi = \frac{k}{\sigma}$. To establish the temperature dependence of the Urbach energy, it is necessary to determine the σ coefficient depending on the parameters of the material

$$\sigma = \frac{k}{\text{tg}\varphi} \quad (27)$$

The experimental results of the dependence of the Urbach energy on temperature on films of amorphous semiconductors are presented in [8]. This shows that this relationship is linear. The slope of this line will be close to the slope of the temperature dependence of the width of the mobility gap in amorphous semiconductors

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Figure 2 shows the results of theoretical calculations after substitution of expressions (24) in (23), taking into account the value of ($\gamma \approx 10^{-5} - 10^{-4} \text{ eV}\cdot\text{K}^{-1}$) from [9] for amorphous semiconductors.

The calculations were performed for hydrogenated amorphous silicon (a-Si:H) with $E_g = 1.8 \text{ eV}$. In this material, the slope of the tail of the valence band is somewhat larger than the slope of the tail of the conduction band [5]. Therefore, when calculating the Urbach energy for the slope of the exponential tails of the valence and conduction bands, the following values were chosen $\beta_1 = 14 \text{ eV}^{-1}$ and $\beta_2 = 25 \text{ eV}^{-1}$ (line-1, **Figure 2**), $\beta_1 = 19 \text{ eV}^{-1}$ and $\beta_2 = 25 \text{ eV}^{-1}$ (line-2, **Figure 2**). It can be seen from the figure that the calculated values of the Urbach energy obtained from formula (16) increase linearly with increasing temperature. The slope of the 1-straight line is equal to $\text{tg}\varphi_1 = 4 \times 10^{-5} \text{ eV}\cdot\text{K}^{-1}$, and the slope of the 2-line is equal to $\text{tg}\varphi_2 = 6.5 \times 10^{-5} \text{ eV}\cdot\text{K}^{-1}$. These values show that they are close to the slope of the temperature dependence of the width of the mobility gap in amorphous semiconductors.

From the slopes of these lines using formula (27), one can determine σ —the coefficient depending on the parameters of the material, that is, on β_1 and β_2 :

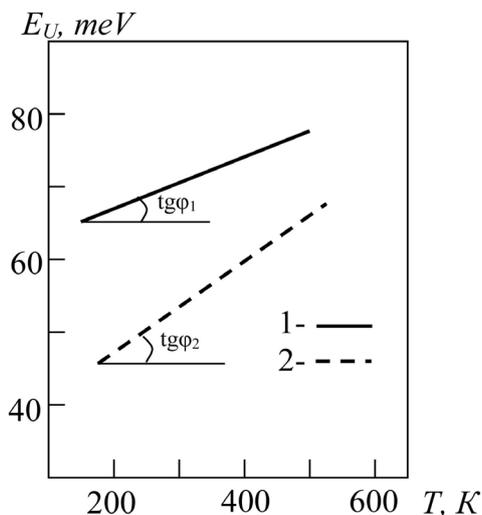


Figure 2. Temperature dependence of the Urbach energy on films of hydrogenated amorphous silicon at $E_g = 1.8 \text{ eV}$. 1— $\beta_1 = 14 \text{ eV}^{-1}$ and $\beta_2 = 25 \text{ eV}^{-1}$; 2— $\beta_1 = 19 \text{ eV}^{-1}$ and $\beta_2 = 25 \text{ eV}^{-1}$.

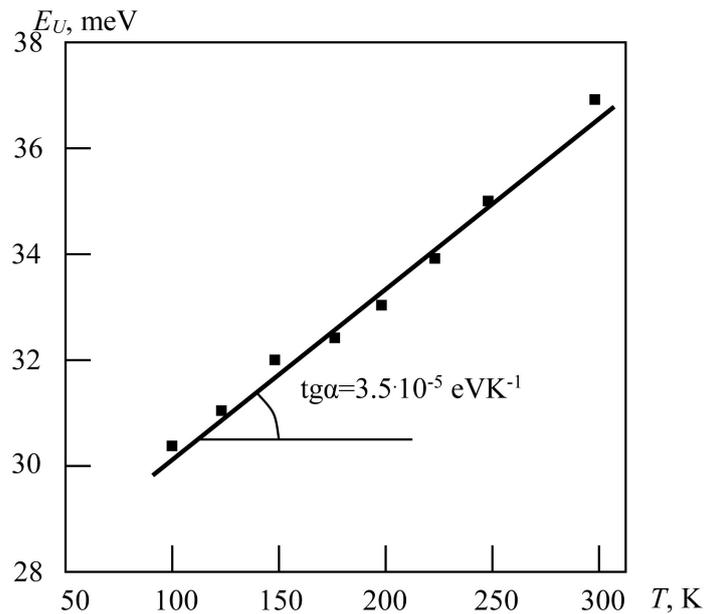


Figure 3. Experimental results of the temperature dependence of the Urbach energy on temperature for CuIn_3Te_5 [10].

when $\beta_1 = 14 \text{ eV}^{-1}$ and $\beta_2 = 25 \text{ eV}^{-1}$ then $\sigma_1 = 2.156$, when $\beta_1 = 19 \text{ eV}^{-1}$ and $\beta_2 = 25 \text{ eV}^{-1}$ then $\sigma_2 = 1.327$. As is known, when the values of the parameters that determine the slope of the exponential tails of the allowed bands decrease, the quality of hydrogenated amorphous silicon deteriorates. Since in these samples, the shift of the Fermi level is complicated due to doping. This means that increasing the value of σ degrades the quality of the material.

Figure 3 shows the experimental results obtained for the temperature dependence of the Urbach energy of a noncrystalline semiconductor CuIn_3Te_5 . It is seen that this dependence is linear and the slope of this line is equal at

$$\text{tg}\alpha = 3.5 \times 10^{-5} \text{ eV}\cdot\text{K}^{-1}.$$

3. Conclusions

Thus, in this work:

- 1) Theoretically, a new formula for the Urbach energy of non-crystalline semiconductors has been obtained. The temperature dependence of the Urbach energy is investigated on the basis of the obtained new formula.
- 2) Shown is the linear growth of Urbach energy with increasing temperature. It is determined that the slopes of these lines are close to the slope of the temperature dependence of the width of the mobility gap of noncrystalline semiconductors.
- 3) The dependence of the coefficient determining the Urbach slope on the parameters determining the slope of the tails of the valence and conduction bands is obtained. It is known that an increase in the value of the coefficient of the degree of spectral slope degrades the quality of semiconductor materials (complicates the preparation of semiconductor devices).

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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