TEMPERATURE EFFECT IN ABSORPTION SPECTRA OF AMORPHOUS SEMICONDUCTORS

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The absorption spectra of amorphous semiconductors become shifted toward lower energies at elevated temperatures (the temperature effect). To explain this phenomenon, we, making use of the Kubo–Greenwood formula and following the Mott–Davis method, have derived new relations for the absorption coefficient which contain only one temperature-dependent parameter, the width of the mobility gap. The formulas obtained have well described the temperature effect in amorphous semiconductors observed in experiment.

The absorption coefficient is known to be the key parameter which governs the optical properties of amorphous semiconductors. The absorption spectra of the latter become shifted as a whole, when the temperature changes. Accordingly, the absorption coefficient of such semiconductors and the optical parameters of devices fabricated on their basis also change. This phenomenon is called the temperature effect in absorption spectra. However, any formula, which could describe it, has not been derived yet. In this work, we have derived, making use of the Kubo–Greenwood formula and following the Mott–Davis approximation method [1, 2], new formulas which describe the spectral characteristics of the photon absorption coefficient, provided that the energy of an absorbed photon is lower than the width of the mobility gap (the energy gap) E_g, and explain the temperature effect.

In the range, where the Urbach rule is obeyed, the spectrum of absorption coefficient can be written down in the form

$$\alpha = \alpha_0 \exp\left(\frac{\hbar\omega}{E_{\mathrm{U}}}\right), \qquad (1)$$

where E_{U} is the parameter called the Urbach energy. At temperatures $T < 550$ K, the value of E_{U} does not depend on the temperature [1, 3]. Making use of formula (1), one cannot even evaluate the temperature dependence of the absorption coefficient. Hence, it is evident that formula (1) cannot explain

the temperature effect in absorption spectra. In works [1,2], taking advantage of the Kubo–Greenwood formula and following the Mott–Davis approximation method, expressions for the exponential section in the spectral dependence of the optical absorption coefficient were obtained. However, they also turned out incapable of describing the experimental results for the temperature dependence of the absorption coefficient in amorphous semiconductors (in Fig. 1, an example for amorphous As_2Se_3 [1] is demonstrated). Therefore, we consider the continuation of researches in this direction to be expedient.

The Kubo–Greenwood formula for the Mott–Davis approximation method can be written down in the form

$$\alpha = A \int\limits_{\varepsilon_0-\hbar\omega}^{\varepsilon_0} g(\varepsilon)\, g(\varepsilon+\hbar\omega)\left[f(\varepsilon) - f(\varepsilon+\hbar\omega)\right]\frac{d\varepsilon}{\hbar\omega}, \qquad (2)$$

where A is the proportionality factor that is independent of the absorbed photon frequency, $g(\varepsilon)$ is the initial and
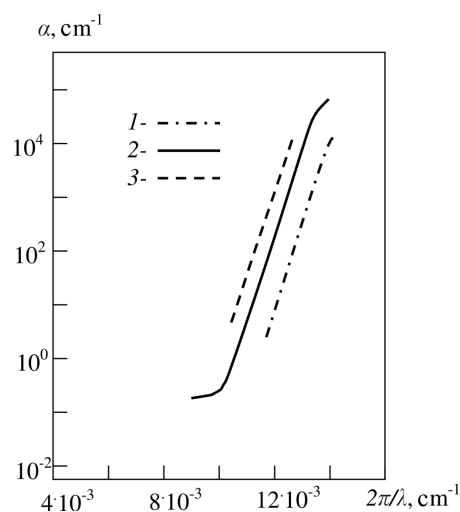

Fig. 1. Optical absorption spectra of amorphous As_2Se_3 at various temperatures $T = -196$ (*1*), 24 (*2*), and 80 °C (*3*) [1]

$g(\varepsilon + \hbar\omega)$ the final state of electrons participating in transitions with the absorption of a photon with the energy $\hbar\omega$, ε_0 is the highest energy of electrons that participate in optical transitions, and $f(\varepsilon)$ and $f(\varepsilon + \hbar\omega)$ are the Fermi–Dirac distributions. Numerical calculations showed, that formula (2) can be rewritten in the form

$$\alpha = A \int\limits_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} g(\varepsilon) g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega}. \tag{3}$$

Calculations carried out for the quantity α by those formulas give identical results, if the absorbed photon energy is more than 0.2 eV.

One can see that, in order to obtain analytical expressions, one has to know the densities of electrons participating in optical transitions in the initial and final states. Therefore, basing on the results of works [4–6], we assume that the distributions of the electron density of states in the valence and conduction bands are linear, parabolic, or constant. At the same time, the dependences of the localized electron states in the "tails" of those bands are supposed exponential. Therefore, the distribution of the electron density of states looks like

$$g(\varepsilon) = N(\varepsilon_V) \left(\frac{\varepsilon_C - \varepsilon}{E_g} \right)^n \tag{4}$$

in the valence band ($\varepsilon_V > \varepsilon$) and

$$g(\varepsilon) = N(\varepsilon_C) \left(\frac{\varepsilon - \varepsilon_V}{E_g} \right)^n \tag{5}$$

in the conduction one ($\varepsilon > \varepsilon_C$). Here, $N(\varepsilon_V)$ and $N(\varepsilon_C)$ are the effective values for the electron density of states in the valence and conduction bands, respectively; ε_V and ε_C are the edges of the valence and conduction bands, respectively; and the power exponent $n = 0, 1/2$, or 1, depending on the distribution model. In the valence band tail, i.e. at $\varepsilon_V < \varepsilon < \varepsilon_0$,

$$g(\varepsilon) = N(\varepsilon_V) \exp\left(-\beta_1(\varepsilon - \varepsilon_V)\right), \tag{6}$$

and, in the conduction band tail, i.e. at $\varepsilon_0 < \varepsilon < \varepsilon_C$,

$$g(\varepsilon) = N(\varepsilon_C) \exp\left(\beta_2(\varepsilon - \varepsilon_C)\right). \tag{7}$$

Here, ε_0 is the energy coordinate of the intersection point of the valence and conduction band tails; and β_1 and β_2 are the parameters that determine the slopes of the electron distribution tails in the valence and conduction bands, respectively.

Basing on the results of work [7] and accounting the independence of partial values of the absorption coefficient for different electron transitions, we did not take into consideration those electron transitions which involve the electron states associated with defects or impurity centers. Therefore, if the effective values of the electron density of states in the allowed bands are equal, i.e. $N(\varepsilon_V) = N(\varepsilon_C)$, the following expressions can be obtained for ε_0:

$$\varepsilon_C - \varepsilon_0 = \frac{\beta_1 E_g}{\beta_1 + \beta_2}, \quad \varepsilon_0 - \varepsilon_V = \frac{\beta_2 E_g}{\beta_1 + \beta_2}. \tag{8}$$

It is known that, in amorphous semiconductors, $\beta_1 < \beta_2$ [8], and the type of electron transitions induced by optical absorption depends on the energy of photons. Therefore, let us consider the following ranges of the absorbed photon energy and the corresponding electron transitions:

– Range 1: $0 < \hbar\omega < \varepsilon_C - \varepsilon_0$. The transitions occur only between the localized states in the tails of the allowed bands.

– Range 2: $\varepsilon_C - \varepsilon_0 \leq \hbar\omega < \varepsilon_0 - \varepsilon_V$. The transitions occur between the localized states in the valence band tail and the conduction band states.

To obtain an analytical expression, the integral in formula (3) should be decomposed into components corresponding to the electron transitions specified above. As a result, we obtain

$$\alpha = A \int\limits_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} g(\varepsilon) g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} =$$

$$= A \int\limits_{\varepsilon_C - \hbar\omega}^{\varepsilon_0} g(\varepsilon) g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} +$$

$$+ A \int\limits_{\varepsilon_0 - \hbar\omega}^{\varepsilon_C - \hbar\omega} g(\varepsilon) g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} = = \alpha_1 + \alpha_2 \tag{9}$$

– Range 3: $\varepsilon_0 - \varepsilon_C \leq \hbar\omega < \varepsilon_C - \varepsilon_V = E_g$. The transitions occur between the localized states in the valence band tail and the conduction band states, and between the valence band states and the states in the conduction band tail. In this range, integral (3) has three components, in accordance with the aforesaid. We can write down

$$\alpha = A \int\limits_{\varepsilon_0 - \hbar\omega}^{\varepsilon_0} g(\varepsilon) g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} =$$

$$A \int\limits_{\varepsilon_C - \hbar\omega}^{\varepsilon_0} g(\varepsilon)g(\varepsilon + \hbar\omega)\frac{d\varepsilon}{\hbar\omega} + A \int\limits_{\varepsilon_V}^{\varepsilon_C - \hbar\omega} g(\varepsilon)g(\varepsilon + \hbar\omega)\frac{d\varepsilon}{\hbar\omega} +$$

$$+A \int\limits_{\varepsilon_F - \hbar\omega}^{\varepsilon_0} g(\varepsilon)g(\varepsilon + \hbar\omega)\frac{d\varepsilon}{\hbar\omega} = \alpha_1 + \alpha_2 + \alpha_3. \quad (10)$$

Using these formulas, we obtained analytical solutions in the cases where the electron densities of states in the allowed bands are described by the power-law dependences with the exponents $n = 1$ and 0. A comparison of the spectra obtained by those formulas and the data of numerical calculations of the spectrum in the case of the parabolic dependence of the density of states in the allowed bands, i.e. for $n = 1/2$, showed, that the results do not differ in effect. Therefore, we present only the formulas for the spectral dependence of the optical absorption coefficient obtained in the case $n = 1$:
In range 1:

$$\alpha = A\frac{\exp\left(\left(\beta_1 - \beta_2\right)\left(\varepsilon_C - \varepsilon_0\right)\right)}{\beta_2 - \beta_1}\frac{\exp\left(\beta_1\left(\hbar\omega - E_g\right)\right)}{\hbar\omega} \times$$

$$\times \left(\exp\left(\left(\beta_2 - \beta_1\right)\hbar\omega\right) - 1\right). \quad (11)$$

In range 2:

$$\alpha_1 = \frac{A}{\hbar\omega}\frac{1 - \exp\left(\left(\beta_1 - \beta_2\right)\left(\varepsilon_C - \varepsilon_0\right)\right)}{\beta_2 - \beta_1}\exp\left(\beta_1\left(\hbar\omega - E_g\right)\right), \quad (12)$$

$$\alpha_2 = \frac{A}{\beta_1 E_g \hbar\omega}\left(\left(E_g + \frac{1}{\beta_1}\right) - \left(\left(\varepsilon_0 - \varepsilon_V\right) + \frac{1}{\beta_1} + \hbar\omega\right) \times \right.$$

$$\left. \times \exp\left(\beta_1\left(\varepsilon_C - \varepsilon_0 - \hbar\omega\right)\right)\right) \times$$

$$\times \exp(\beta_1(\hbar\omega - E_g)). \quad (13)$$

And, in range 3, we have

$$\alpha_1 = A\frac{\exp\left(\beta_1\left(\hbar\omega - E_g\right)\right)}{\left(\beta_2 - \beta_1\right)\hbar\omega} \times$$

$$\times \left(1 - \exp\left(\left(\beta_2 - \beta_1\right)\left(\hbar\omega - E_g\right)\right)\right), \quad (14)$$

$$\alpha_2 = A\frac{\exp(\beta_1(\hbar\omega - E_g))}{E_g \beta_1 \hbar\omega}\left(\left(E_g + \frac{1}{\beta_1}\right) - \right.$$

$$\left. - \left(\varepsilon_0 - \varepsilon_V + \frac{1}{\beta_1} + \hbar\omega\right)\exp(\beta_1(\varepsilon_C - \varepsilon_0 - \hbar\omega))\right), \quad (15)$$

$$\alpha_3 = A\frac{\exp\left(\left(\beta_2 - \beta_1\right)\left(\hbar\omega - E_g\right)\right)\exp\left(\beta_1\left(\hbar\omega - E_g\right)\right)}{E_g \beta_1 \hbar\omega} \times$$

$$\times \left(\left(E_g + \frac{1}{\beta_1}\right) - \left(\varepsilon_C - \varepsilon_0 + \frac{1}{\beta_1} + \hbar\omega\right) \times \right.$$

$$\left. \times \exp\left(\beta_1\left(\varepsilon_0 - \varepsilon_V - \hbar\omega\right)\right)\right). \quad (16)$$

The calculations by those expressions demonstrated that the Urbach rule is satisfied for all the ranges of the absorption spectrum indicated above (Fig. 2).

One can see that the proportionality factor A is constant and does not influence the spectrum shape. Therefore, by confronting the spectral absorption characteristics in formulas (11)–(16) with expression (8), it is evident that only two fitting parameters governing the spectral shape remain in them. These are the parameters β_1 and β_2, and, as was shown in work [9], they do not depend on the temperature at $T < 600$ K. Moreover, since calculations are carried out for a specific amorphous semiconductor, the quantity E_g has a specific value. Then, the formulas concerned include only a single parameter depending on the temperature: it is the width of the mobility gap. This dependence can be written down in the form

$$E_g(T) = E_g(0) - \delta T, \quad (17)$$

where δ is the temperature coefficient of the mobility gap width.

Figure 3 demonstrates the variations occurring in the absorption coefficient spectra with increasing temperature, which were calculated in this work. One can see that the temperature growth gives rise to a parallel shift of the spectral dependence of the absorption coefficient toward the range of low-energy photons. However, this effect is observed only for specimens, for which $\beta_1 < \beta_2$. If the condition $\beta_1 \geq \beta_2$ is fulfilled for amorphous semiconductors under investigation, the types of electron transitions in spectral range 2 change,
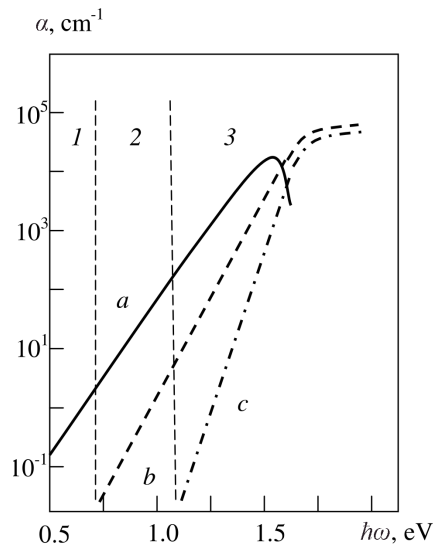
Fig. 2. Partial spectral characteristics of amorphous semiconductors calculated for different types of electron transitions: (*a*) between the conduction band tails, (*b*) from the valence band tail into the conduction band, and (*c*) from the valence band into the conduction band tail. The calculation parameters are $\varepsilon_C - \varepsilon_0 = 0.7$ eV, $E_g = 1.8$ eV, $\beta_1 = 16$ eV^{-1}, and $\beta_2 = 25$ eV^{-1}. Spectral ranges: (*1*) $0 < \hbar\omega < \varepsilon_C - \varepsilon_0$, (*2*) $\varepsilon_C - \varepsilon_0 \leq \hbar\omega < \varepsilon_0 - \varepsilon_V$, and (*3*) $\varepsilon_0 - \varepsilon_C \leq \hbar\omega < \varepsilon_C - \varepsilon_V = E_g$
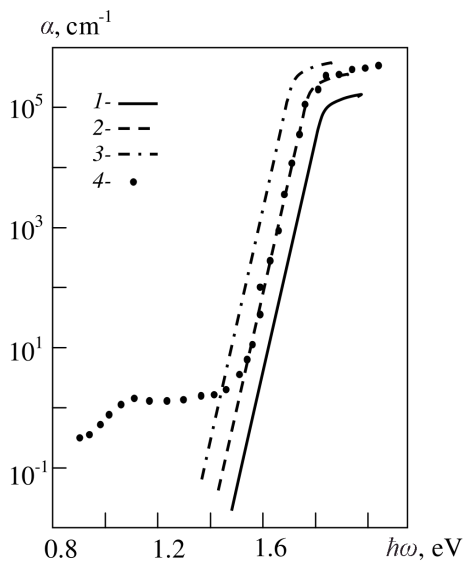

Fig. 3. Spectral dependences of the optical absorption coefficient calculated for amorphous hydrogenated silicon (a-Si:H). The calculation parameters are $\delta \approx 5 \times 10^{-4}$ eV/K, $E_g(T = 300K) = 1.8$ eV, $\beta_1 = 16$ eV^{-1}, and $\beta_2 = 25$ eV^{-1}. The temperature $T = 200$ (*1*), 300 (*2*), and 400 K (*3*). Points *4* correspond to experimental data

but the analytical solutions obtained for them following the method described above do not differ from Eqs. (11)–(16).

To summarize, we have studied the spectral dependences of the absorption coefficient in amorphous semiconductors, the spectra of which satisfy the Urbach rule. Three ranges were distinguished in the spectrum, each of the ranges being related to the absorbed photon energy and characterized by the corresponding types of optical electron transitions. New formulas for the spectral dependence of the absorption coefficient have been obtained. The Urbach rule was shown to be obeyed in those ranges by all partial absorption coefficients associated with different types of electron transitions. It was also demonstrated that the spectra of the total absorption coefficient, which were obtained in this work, can explain the experimentally observed parallel shift of the spectra with temperature variation, i.e. the temperature effect, in amorphous semiconductors [1, 3]. The results of this work can be used for other semiconductors, the absorption coefficient spectra of which satisfy the Urbach rule.

1. N.F. Mott and E.A. Davies, *Electronic Processes in Non-Crystalline Materials* (Oxford University Press, Oxford, 1979).

2. S. Tamasaki, S. Kuroda, and K. Tanaka, J. Non-Cryst. Solids **59-60**, 141 (1983).

3. A. Feltz, *Amorphous Inorganic Materials and Glasses* (VCH, Weinheim, 1993).

4. A.V. Kolobov and O.V. Konstantinov, Philos. Mag. **40**, 475 (1979).

5. V.L. Bonch-Bruevich, R. Enderlein, B. Esser, R. Keiper, A.G. Mironov, and I.P. Zvyagin, *Elektronentheorie Ungeordneter Halbleiter* (Deutscher Verlag der Wissenschaften, Berlin, 1984).

6. V.L. Bonch-Bruevich, Usp. Fiz. Nauk **140**, 583 (1983).

7. P.S. Kireev, *Physics of Semiconductors* (Vysshaya Shkola, Moscow, 1969) (in Russian).

8. O.A. Golikova, Fiz. Tekh. Poluprovodn. **25**, 1517 (1991).

9. *Amorphous Semiconductors,* edited by M.H. Brodsky (Springer, Berlin, 1979).

ТЕМПЕРАТУРНИЙ ЕФЕКТ У СПЕКТРАХ ПОГЛИНАННЯ АМОРФНИХ НАПІВПРОВІДНИКІВ

С. Зайнобідінов, Р.Г. Ікрамов, М.А. Нурітдінова, Р.М. Жалалов

Р е з ю м е

В аморфних напівпровідниках з підвищенням температури спектри поглинання паралельно зсуваються в бік малих енергій (температурний ефект). Для пояснення цього явища за допомогою формули Кубо–Грінвуда методом Девіса–Мотта було отримано нові співвідношення для коефіцієнта поглинання, в яких тільки один параметр – ширина щілини рухливості – залежить від температури. Показано, що ці формули можуть пояснити температурний ефект в аморфних напівпровідниках, який спостерігається в експерименті.