

<https://doi.org/10.15407/ujpe64.4.315>

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## DENSITY OF DEFECT STATES AND SPECTRA OF DEFECT ABSORPTION IN a-Si:H

*Spectral characteristics of the coefficient of defect absorption in amorphous hydrogenated silicon have been studied. The characteristics are determined, by analyzing the electron transitions occurring with the participation of the energy states of dangling bonds. It is shown that the principal role in the formation of the defect absorption coefficient value is played by the electron transitions between defect and non-localized states. It is also shown that the spectral characteristics are mainly determined by the distribution function of the electron density of states in the valence or conduction band. It is found that the maxima in the spectrum of the defect absorption coefficient are observed only if there are pronounced maxima in the density of states at the edges of allowed bands.*

*Keywords:* amorphous semiconductors, distribution of electron density of states, Kubo–Greenwood formula, Davis–Mott approximation, optical electron transitions, spectral characteristics, defect absorption coefficient.

### 1. Introduction

It is well known that the spectral characteristic of the coefficient of optical absorption in the films of pseudodoped amorphous hydrogenated silicon (a-Si:H) includes a defect absorption region, where electron transitions take place with the participation of states located in dangling bonds (defects or impurity centers) [1]. It should be noted that pseudodoped a-Si:H has no doping impurities. Therefore, the spectra of the defect absorption coefficient are governed exactly by defect states.

But those spectra differ from one another not only quantitatively, but also qualitatively. It seems to be interesting to study the origin of this difference. Therefore, this work was devoted to the spectral characteristics of the defect absorption coefficient. The corresponding parameters are determined, by analyzing the electron transitions, in which the energy states of dangling bonds in pseudodoped a-Si:H participated.

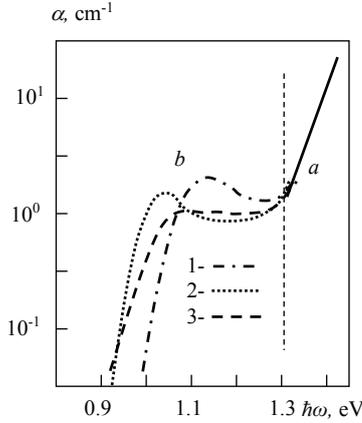
Conditions responsible for the types of defect absorption coefficient spectra are considered, and conditions for the maxima to appear in those spectra are determined.

### 2. Calculations and Discussion of Results

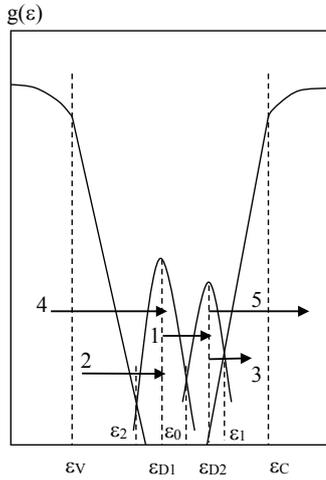
In Fig. 1, the experimental spectra of defect absorption in pseudodoped a-Si:H specimens are depicted. The corresponding results were obtained at room temperature using the constant photocurrent method (CPM). The parameters of experimental specimens are quoted in Table. The notations used in Table are as follows:  $E_g$  is the energy gap width,  $\varepsilon_C - \varepsilon_F$  the activation energy,  $\sigma_t$  the electrical conductivity, and  $\sigma_f$  the photoconductivity at room temperature.

Every experimental specimen was obtained under the same technological conditions, i.e. by decomposing silane ( $\text{SiH}_4$ ) in a glow discharge [2]. Therefore, we may assume that the distribution functions of defect states should have the same form in all specimens. However, as one can see from Fig. 1, the defect absorption spectra turned out very different: each of spectra 1 and 2 has a well-pronounced maximum, whereas spectrum 3 has no such maximum.

Optical transitions of electrons with the participation of electron states in defects are known to be classified into three types: between defect states, between defect states and localized states in the tails of allowed bands, and between defect states and non-localized states in the allowed bands (Fig. 2). In



**Fig. 1.** Experimental spectral characteristics of the absorption coefficient obtained for pseudodoped a-Si:H specimens: interval of exponential absorption (a), interval of defect absorption (b)



**Fig. 2.** Optical electron transitions and involved defect states: between defect states (1), from the valence band tail into defect states (2), from defect states into the conduction band tail (3), from the valence band into defect states (4), from defect states into the conduction band (5)

**Parameters of pseudodoped a-Si:H specimens (Fig. 1)**

No.	$E_g$ , eV	$\epsilon_v - \epsilon_F$ , eV	$\sigma_t$ , $\Omega^{-1}\text{cm}^{-1}$	$\sigma_f$ , $\Omega^{-1}\text{cm}^{-1}$
1	1.8	0.95	$1 \times 10^{-11}$	$1.5 \times 10^{-6}$
2	1.78	0.95	$6 \times 10^{-10}$	$6.6 \times 10^{-6}$
3	1.77	0.72	$1.12 \times 10^{-10}$	$1.65 \times 10^{-7}$

works [1, 3], it was shown that the density of electron states in defects in amorphous semiconductors is well described by the Gaussian distribution

$$g(\epsilon) = g(\epsilon_D) \exp(-a(\epsilon - \epsilon_D)^2), \quad (1)$$

where  $g(\epsilon_D)$  is the maximum value of defect state density, and  $\epsilon_D$  is the energy position of this maximum.

The dependence of the spectral characteristic of the absorption coefficient on the distribution of the electron density of states that are engaged in optical transitions is determined, by using the Kubo–Greenwood formula [4–6]. In the Davis–Mott approximation, when  $\hbar\omega \gg kT$ , the Kubo–Greenwood formula can be written in the form

$$\alpha(\hbar\omega) = B \int_{\epsilon_0 - \hbar\omega}^{\epsilon_0} g(\epsilon)g(\epsilon + \hbar\omega) \frac{d\epsilon}{\hbar\omega}, \quad (2)$$

where  $\epsilon_0$  is the highest energy of electrons participating in optical transitions, and  $g(\epsilon)$  and  $g(\epsilon + \hbar\omega)$  are the initial and final, respectively, densities of electron states participating in optical transitions. The proportionality coefficient  $B$  does not depend of the absorbed photon frequency and is determined by the formula

$$B = \frac{8\pi^2 e^2 \hbar^3 a}{(m^*)^2 n_0 c},$$

where  $a$  is the average interatomic distance,  $n_0$  the light refractive index,  $c$  the velocity of light in vacuum,  $m^*$  the effective electron mass,  $e$  the elementary charge, and  $\hbar$  Planck’s constant [7].

One can see that, if using the Gaussian distribution, it is impossible to obtain an analytical solution of Eq. (2). On the other hand, numerical calculations make further researches in this area more complicated. Therefore, in work [9], an integrable function in the form of hyperbolic secant was proposed, which slightly differs from the Gaussian distribution:

$$g(\epsilon) = \frac{g(\epsilon_D)}{\cosh b(\epsilon - \epsilon_D)}, \quad (3)$$

where the value of the parameter  $b$  falls within an interval of 10–30 eV for a-Si:H [10]. In work [9], it was shown that the correspondence between distributions (1) and (3) is obtained at  $b = \sqrt{\pi a}$ .

On the basis of the results of works [4, 5, 10], the following exponential dependences were chosen to approximate the energy dependence of the density of localized states located in the tails of allowed bands:

- in the valence band tail (at  $\epsilon_V < \epsilon$ ),

$$g(\epsilon) = N(\epsilon_V) \exp(-\beta_1(\epsilon - \epsilon_V)); \quad (4)$$

- in the conduction band tail (at  $\varepsilon < \varepsilon_C$ ),

$$g(\varepsilon) = N(\varepsilon_C) \exp(\beta_2(\varepsilon - \varepsilon_C)). \quad (5)$$

In Eqs. (4) and (5),  $N(\varepsilon_V)$  and  $N(\varepsilon_C)$  are the effective densities of electron states in the valence and conduction, respectively, bands; and the parameters  $\beta_1$  and  $\beta_2$  determine the slope of the exponential tails of the allowed bands. The  $\beta_1$ - and  $\beta_2$ -values lie within an interval of 15–30 eV<sup>-1</sup> for pseudodoped a-Si:H [10]. At the same time, it is known that the distribution of the electron state density in the allowed bands has a power-law dependence [3, 8, 11]. It can be written down in the form:

- for the valence band (at  $\varepsilon < \varepsilon_V$ ),

$$g(\varepsilon) = N(\varepsilon_V) \left( -\frac{\varepsilon - \varepsilon_V}{E_g} \right)^{n_1}; \quad (6)$$

- for the conduction band (at  $\varepsilon_C < \varepsilon$ ),

$$g(\varepsilon) = N(\varepsilon_C) \left( \frac{\varepsilon - \varepsilon_C}{E_g} \right)^{n_2}; \quad (7)$$

where  $E_g$  is the mobility gap width, and the power exponents  $n_1$  and  $n_2$  can acquire such values as 1/2 or 1, i.e. those distributions can be parabolic or linear [8, 11].

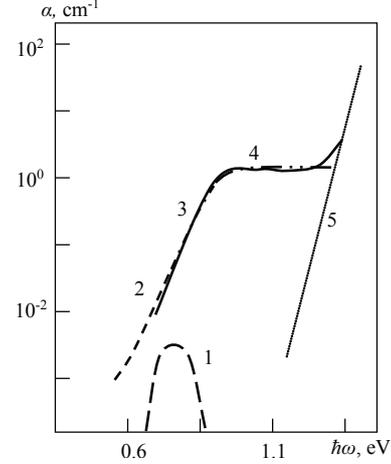
Note that the absorption coefficient has an additive structure [12, 13], i.e.

$$\alpha(\hbar\omega) = \sum_i \alpha_i(\hbar\omega), \quad (8)$$

where  $\alpha_i(\hbar\omega)$  is the partial absorption coefficient associated with the optical electron transition of the  $i$ -th type. Formula (8) means that the absorption spectrum can be calculated separately for each of the electron transitions indicated above. Accordingly, the calculation procedure by formula (8) includes a few stages.

1. First of all, in order to calculate the spectral characteristics of the electron transitions between defect states, it is necessary to determine the limits of the integral in Eq. (2), i.e. the parameter  $\varepsilon_0$ . In particular, as the value of this parameter, we may take the energy position of the intersection point of the defect state density distributions (Fig. 2). For instance, if both those distributions are described by the hyperbolic secant, then

$$\varepsilon_0 = \frac{b_2 \varepsilon_{D_2} + b_1 \varepsilon_{D_1} + \ln \frac{g(\varepsilon_{D_2})}{g(\varepsilon_{D_1})}}{b_1 + b_2}. \quad (9)$$



**Fig. 3.** Calculated spectral characteristics of defect absorption coefficients in amorphous hydrogenated silicon: between defect states (1), between defect states and the conduction band tail (interval  $\varepsilon_C - \varepsilon_1 > \hbar\omega$ ) (2), between defect states and the conduction band tail (interval  $\varepsilon_C - \varepsilon_1 \leq \hbar\omega$ ) (3), between defect states and the conduction band (4), interval of exponential absorption (5), the solid line corresponds to experimental results (see Fig. 1)

At  $b_1 \neq b_2$ , it is impossible to obtain the spectra in the analytical form. However, numerical calculations showed that if  $10 \text{ eV}^{-1} < (b_1, b_2) < 30 \text{ eV}^{-1}$ , the resulting spectral characteristics for  $b_1 \neq b_2$  do not differ much from those calculated for  $b_1^{\text{new}} = b_2^{\text{new}} = (b_1 + b_2)/2 = b^{\text{new}}$ . Taking all that into account and using formulas (2) and (3), we can obtain an analytical approximation for the spectra of the electron transitions between defect states:

$$\begin{aligned} \alpha(\hbar\omega) &= \frac{Ag(\varepsilon_{D_1})g(\varepsilon_{D_2})}{b^{\text{new}}\hbar\omega N(\varepsilon_C)N(\varepsilon_V)} \times \\ &\times \frac{1}{\sinh[b^{\text{new}}(\varepsilon_{D_2} - \varepsilon_{D_1} - \hbar\omega)]} \times \\ &\times \ln \left\{ \frac{1 + \exp[2b^{\text{new}}(\varepsilon_{D_1} - \varepsilon_0)]}{1 + \exp[2b^{\text{new}}(\varepsilon_{D_2} - \varepsilon_0)]} \right\} \times \\ &\times \frac{1 + \exp[2b^{\text{new}}(\varepsilon_{D_1} - \varepsilon_0 + \hbar\omega)]}{1 + \exp[2b^{\text{new}}(\varepsilon_{D_2} - \varepsilon_0 - \hbar\omega)]}. \end{aligned} \quad (10)$$

As was shown in work [7], the value of the coefficient  $A = BN(\varepsilon_C)N(\varepsilon_V)$  approximately equals  $2.5 \times 10^5 \text{ cm}^{-1}$ .

Figure 3 demonstrates the results of calculations of this spectral characteristic (curve 1). The calculations were made for the parameter values  $b = 18 \text{ eV}^{-1}$ ,

$\varepsilon_{D_1} - \varepsilon_{D_2} = 0.7$  eV,  $g(\varepsilon_{D_1}) = 8 \times 10^{16}$  eV<sup>-1</sup>cm<sup>-3</sup>, and  $g(\varepsilon_{D_2}) = 8 \times 10^{17}$  eV<sup>-1</sup>cm<sup>-3</sup>.

2. Now, let us proceed to the calculation of the spectra of the optical transitions between defect states and the tails of allowed bands. If the energy of absorbed photons does not exceed  $\varepsilon_C - \varepsilon_1$ , i.e.  $\varepsilon_C - \varepsilon_1 > \hbar\omega$ , electrons transit from defect states into states in the conduction band tail. Therefore, substituting distributions (3) and (5) into the Kubo–Greenwood formula, we obtain

$$\alpha(\hbar\omega) = A \frac{g(\varepsilon_{D_1})}{N(\varepsilon_V)} \int_{\varepsilon_1 - \hbar\omega}^{\varepsilon_1} \frac{\exp[\beta_2(\varepsilon - \varepsilon_C + \hbar\omega)]}{\cosh[b(\varepsilon - \varepsilon_{D_1})]} \frac{d\varepsilon}{\hbar\omega}. \quad (11)$$

At the energies of absorbed photons  $\hbar\omega < \varepsilon_2 - \varepsilon_V$ , the electrons will transit from the states in the valence band tail into defect states. Therefore, using now distributions (3) and (4), we obtain

$$\alpha(\hbar\omega) = A \frac{g(\varepsilon_{D_2})}{N(\varepsilon_C)} \int_{\varepsilon_2 - \hbar\omega}^{\varepsilon_2} \frac{\exp[-\beta_1(\varepsilon - \varepsilon_V)]}{\cosh[b(\varepsilon - \varepsilon_{D_2} + \hbar\omega)]} \frac{d\varepsilon}{\hbar\omega}. \quad (12)$$

The corresponding calculations showed that these spectra strongly depend on the integral limits in Eqs. (11) and (12), i.e. on the parameters  $\varepsilon_1$  and  $\varepsilon_2$ . The values of the latter can be taken as the energy positions of the intersection point of the defect state distribution with the state distributions either in the conduction band tail (the parameter  $\varepsilon_1$ ) or in the valence band tail (the parameter  $\varepsilon_2$ ) (see Fig. 2). Then, analogously to formula (9), we can obtain the expressions

$$\varepsilon_1 = \frac{\beta_2 \varepsilon_C + b \varepsilon_{D_2} + \ln \frac{2g(\varepsilon_{D_2})}{N(\varepsilon_C)}}{\beta_2 + b} \quad (13)$$

and

$$\varepsilon_2 = \frac{\beta_1 \varepsilon_V + b \varepsilon_{D_1} + \ln \frac{N(\varepsilon_V)}{2g(\varepsilon_{D_1})}}{\beta_1 + b}. \quad (14)$$

If either  $b \neq \beta_1$  or  $b \neq \beta_2$ , it is impossible to obtain the spectra in the analytical form. However, numerical calculations showed that if  $15$  eV<sup>-1</sup>  $< (\beta_1, \beta_2) < 30$  eV<sup>-1</sup> and  $10$  eV<sup>-1</sup>  $< b < 30$  eV<sup>-1</sup>, the resulting spectral characteristics do not differ strongly from those calculated for  $b^{\text{new}} = \beta_1^{\text{new}} = \beta_2^{\text{new}} = (\beta_1 + \beta_2)/2$ . Taking all that into account,

we obtain analytical approximations for the spectra of the electron transitions between defect states and the tails of allowed bands. For the optical transitions from defect states into the states in the conduction band tail, the spectrum calculated with the use of formula (11) looks like

$$\alpha(\hbar\omega) = \frac{Ag(\varepsilon_{D_1}) \exp(b^{\text{new}}(\varepsilon_{D_1} - \varepsilon_C + \hbar\omega))}{b^{\text{new}} \hbar\omega N(\varepsilon_V)} \times \ln \left[ \frac{\frac{2g(\varepsilon_{D_1})}{N(\varepsilon_C)} \exp(b^{\text{new}}(\varepsilon_C - \varepsilon_{D_1})) + 1}{\frac{2g(\varepsilon_{D_1})}{N(\varepsilon_C)} \exp(b^{\text{new}}(\varepsilon_C - \varepsilon_{D_1} - 2\hbar\omega)) + 1} \right]. \quad (15)$$

At the same time, according to formula (12), for optical transitions from the states in the valence band tail into defect states, we obtain

$$\alpha(\hbar\omega) = \frac{Ag(\varepsilon_{D_2}) \exp(b^{\text{new}}(\varepsilon_V - \varepsilon_{D_2} + \hbar\omega))}{b^{\text{new}} \hbar\omega N(\varepsilon_C)} \times \ln \left[ \exp(2b^{\text{new}} \hbar\omega) \times \frac{\frac{N(\varepsilon_V)}{g(\varepsilon_{D_2})} \exp(b^{\text{new}}(\varepsilon_V - \varepsilon_{D_2})) + 1}{\frac{N(\varepsilon_V)}{g(\varepsilon_{D_2})} \exp(b^{\text{new}}(\varepsilon_V - \varepsilon_{D_2} + 2\hbar\omega)) + 1} \right]. \quad (16)$$

The plot of spectrum (15) (at  $\hbar\omega < \varepsilon_C - \varepsilon_1$ ) is shown in Fig. 3 (curve 2). The corresponding calculations were made for the parameter values  $b = 18$  eV<sup>-1</sup>,  $\varepsilon_C - \varepsilon_D = 0.8$  eV, and  $g(\varepsilon_D) = 2 \times 10^{16}$  eV<sup>-1</sup>cm<sup>-3</sup>. It is evident that the spectrum has an exponential behavior.

It should be noted that, on the basis of the data of work [11], we assume hereafter that, irrespective of their charge state, the defects simultaneously participate in all electron transitions.

3. If photons with energies  $\hbar\omega \geq \max(\varepsilon_C - \varepsilon_1, \varepsilon_2 - \varepsilon_V)$  are absorbed, the electron transitions take place between defect and localized states and, simultaneously, between defect and nonlocalized states. Therefore, the Kubo–Greenwood formula must be divided into two parts [8] as follows:

$$\alpha = B \int_{\varepsilon_1 - \hbar\omega}^{\varepsilon_1} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} = \alpha_1 + \alpha_2, \quad (17)$$

where

$$\alpha_1 = B \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_1} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} \quad (18)$$

is the spectrum of the electron transitions from defect states into the conduction band, and

$$\alpha_2 = B \int_{\varepsilon_1 - \hbar\omega}^{\varepsilon_C - \hbar\omega} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega}. \quad (19)$$

We also have

$$\alpha = B \int_{\varepsilon_2 - \hbar\omega}^{\varepsilon_2} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} = \bar{\alpha}_1 + \bar{\alpha}_2, \quad (20)$$

where

$$\bar{\alpha}_1 = B \int_{\varepsilon_V}^{\varepsilon_2} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} \quad (21)$$

is the spectrum of the electron transitions from valence band into defect states, and

$$\bar{\alpha}_2 = B \int_{\varepsilon_2 - \hbar\omega}^{\varepsilon_V} g(\varepsilon)g(\varepsilon + \hbar\omega) \frac{d\varepsilon}{\hbar\omega} \quad (22)$$

is the spectrum of the electron transitions from valence band tail into defect states. By substituting distributions (3) and (5) into Eq. (19), we obtain an analytical expression for the spectrum of the optical transitions from defect states into the conduction band tail:

$$\begin{aligned} \alpha_2(\hbar\omega) &= \frac{Ag(\varepsilon_{D_1})}{b\hbar\omega N(\varepsilon_V)} \exp(b(\varepsilon_{D_1} - \varepsilon_C + \hbar\omega)) \times \\ &\times \left\{ 2b(\varepsilon_C - \varepsilon_1) - \right. \\ &\left. - \ln \left[ \frac{1 + \exp(-2b(\varepsilon_C - \varepsilon_{D_1} - \hbar\omega))}{1 + \exp(-2b(\varepsilon_1 - \varepsilon_{D_1} - \hbar\omega))} \right] \right\}. \quad (23) \end{aligned}$$

Analogously, substituting distributions (3) and (4) into Eq. (21), we obtain an analytical approximation for the spectrum of the optical transitions from the valence band tail into defect states:

$$\begin{aligned} \bar{\alpha}_1(\hbar\omega) &= \frac{Ag(\varepsilon_{D_2})}{b\hbar\omega N(\varepsilon_C)} \exp(b(\varepsilon_V - \varepsilon_{D_2} + \hbar\omega)) \times \\ &\times \left\{ 2b(\varepsilon_V - \varepsilon_2 + \hbar\omega) + \right. \\ &\left. + \ln \left[ \frac{1 + \exp(2b(\varepsilon_2 - \varepsilon_{D_2}))}{1 + \exp(2b(\varepsilon_V - \varepsilon_{D_2} + \hbar\omega))} \right] \right\}. \quad (24) \end{aligned}$$

Spectrum (24) is shown in Fig. 3 by curve 3. It is evident that this spectrum also has an exponential character.

Numerical calculations of the spectra of electron transitions between defect and nonlocalized states showed that the spectral characteristics obtained at  $n_1 = n_2 = 1/2$  and  $n_1 = n_2 = 1$  [see Eqs. (6) and (7)] are the same. They testify that if the density of electron states in the allowed bands has a power-law dependence, then the defect absorption spectra do not depend on this power exponent. Taking this fact into account, we present here the absorption coefficient spectra calculated for  $n_1 = n_2 = 1$ , i.e. for the linear dependence of the density of electron states in the allowed bands.

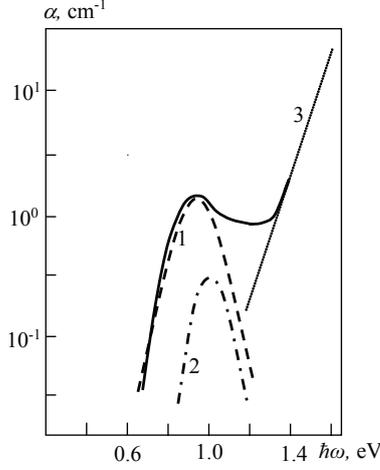
Substituting distributions (1), (3), and (7) into Eq. (18), we obtain the analytical expression for the spectra of the optical transitions from defect states into the conduction band for  $n_2 = 1$ :

$$\begin{aligned} \alpha_1(\hbar\omega) &= \frac{Ag(\varepsilon_{D_1})}{E_g \hbar\omega N(\varepsilon_V)} \frac{\varepsilon_{D_1} - \varepsilon_V + \hbar\omega}{b} \times \\ &\times \arctan \left\{ \frac{\exp[b(\varepsilon_0 - \varepsilon_{D_1} + \hbar\omega)] - \exp[b(\varepsilon_C - \varepsilon_{D_1} - \hbar\omega)]}{1 + \exp[b(\varepsilon_C - \varepsilon_0 - 2\varepsilon_{D_1} + \hbar\omega)]} \right\} - \\ &- \frac{1}{2a} \left\{ \exp[-a(\varepsilon_0 - \varepsilon_{D_1})^2] - \exp[-a(\varepsilon_C - \varepsilon_{D_1} - \hbar\omega)^2] \right\}. \quad (25) \end{aligned}$$

Analogously, substituting distributions (1), (3), and (6) into Eq. (22), we obtain the analytical expression for the spectra for the optical transitions from the valence band into defect states for  $n_1 = 1$ :

$$\begin{aligned} \bar{\alpha}_2(\hbar\omega) &= \frac{Ag(\varepsilon_{D_2})}{E_g \hbar\omega N(\varepsilon_C)} \frac{\varepsilon_C - \varepsilon_{D_2} + \hbar\omega}{b} \times \\ &\times \arctan \left\{ \frac{\exp[b(\varepsilon_V - \varepsilon_{D_2} + \hbar\omega)] - \exp[b(\varepsilon_0 - \varepsilon_{D_2})]}{1 + \exp[b(\varepsilon_V - \varepsilon_0 - 2\varepsilon_{D_2} + \hbar\omega)]} \right\} - \\ &- \frac{1}{2a} \left\{ \exp[-a(\varepsilon_V - \varepsilon_{D_2} + \hbar\omega)^2] - \right. \\ &\left. - \exp[-a(\varepsilon_0 - \varepsilon_{D_2})^2] \right\}. \quad (26) \end{aligned}$$

The plots of those spectra are shown in Fig. 3 (curve 4). The calculations were made for the parameter values  $b = 18 \text{ eV}^{-1}$  and  $a = 103 \text{ eV}^{-2}$ . Figure 3 also exhibits experimental data (curve 6). One can see that the calculated and experimental results are in good agreement.



**Fig. 4.** Calculated spectral characteristics of absorption coefficients: defect states into the conduction band (1), from the valence band into defect states ( $E_g = 1.8$  eV,  $\varepsilon_C - \varepsilon_D = 0.8$  eV) (2), exponential absorption spectrum (3), the solid line corresponds to experimental results (see Fig. 1)

The calculations of the spectral characteristics of absorption coefficients carried out separately for the electron transitions indicated above showed that changes in the values of  $g(\varepsilon_D)$  and  $\varepsilon_D$  do not affect the form of the defect absorption coefficient spectra. So, we may assert that if the energy distributions of the electron state densities in the allowed bands have a power-low dependence, then the spectral characteristics do not demonstrate apparent maxima, which are observed experimentally.

The spectral characteristics of the absorption coefficient for crystalline semiconductors are known to possess several pronounced maxima. They are a consequence of the anisotropy of a lattice structure in crystalline semiconductors. Each direction in the crystal lattice structure forms a subband of electron states, i.e. there arise Brillouin zones. As a result, in the extended zones, there appear maxima corresponding to those subbands. Proceeding from this scenario and in order to obtain maxima in the defect absorption spectra, we assume that the edges of extended zones have clearly pronounced maxima.

The calculations carried out to determine the formation of maxima in the defect absorption spectra showed that the explicit maxima are only formed in the spectra, if the allowed zones also have pronounced maxima at their edges. We assumed that the distribution of those maxima is also expressed by formula

(3). Numerical calculations carried out for  $b \neq b_1$  and  $b \neq b_2$  showed that the results of integration are almost identical to those obtained for  $b_1^{\text{new}} = b_2^{\text{new}} = (b_1 + b_2)/2 = b^{\text{new}}$  if  $10 \text{ eV}^{-1} < (b_1, b_2) < 30 \text{ eV}^{-1}$ . Therefore, in order to obtain an analytical expression for the absorption coefficient spectra, we put  $b_1 = b_2 = b^{\text{new}}$  and, using Eqs. (1) and (3), get the formula

$$\alpha(\hbar\omega) = \frac{A}{b^{\text{new}}\hbar\omega N(\varepsilon_V)} \frac{g(\varepsilon_{D_1})}{\sinh(b^{\text{new}}(\varepsilon_C - \varepsilon_{D_1} - \hbar\omega))} \times \ln \left( 1 + \frac{g(\varepsilon_{D_1})^2}{N(\varepsilon_C)} + 2 \frac{g(\varepsilon_{D_1})}{N(\varepsilon_C)} \cosh(b^{\text{new}}(\varepsilon_C - \varepsilon_{D_1})) \right) / \left( 1 + \frac{g(\varepsilon_{D_1})^2}{N(\varepsilon_C)} + 2 \frac{g(\varepsilon_{D_1})}{N(\varepsilon_C)} \times \cosh(b^{\text{new}}(2\hbar\omega - \varepsilon_C - \varepsilon_{D_1})) \right) \quad (27)$$

for the electron transitions from defect states into the conduction band and the formula

$$\alpha(\hbar\omega) = \frac{A}{b^{\text{new}}\hbar\omega N(\varepsilon_C)} \frac{g(\varepsilon_{D_2})}{\sinh(b^{\text{new}}(\varepsilon_{D_2} - \varepsilon_V - \hbar\omega))} \times \ln \left( 1 + \frac{N(\varepsilon_V)^2}{g(\varepsilon_{D_2})} + 2 \frac{N(\varepsilon_V)}{g(\varepsilon_{D_2})} \cosh(b^{\text{new}}(\varepsilon_{D_2} - \varepsilon_V)) \right) / \left( 1 + \frac{N(\varepsilon_V)^2}{g(\varepsilon_{D_2})} + 2 \frac{N(\varepsilon_V)}{g(\varepsilon_{D_2})} \times \cosh(b^{\text{new}}(2\hbar\omega - \varepsilon_{D_2} - \varepsilon_V)) \right) \quad (28)$$

for the electron transitions from the valence band into the defect electron states. The spectra calculated by these formulas are shown in Fig. 4. Figure 4 also exhibits the corresponding experimental data (curve 3). One can see that the theoretical and experimental results are in good agreement. The results of calculations by formulas (27) and (28) showed that if  $N(\varepsilon_V) = N(\varepsilon_C)$ , dominating are the electron transitions from defect states into that allowed band, to which the energy position of defect states is closer.

The calculations also showed that the maxima appearing owing to the transitions from the valence band into defect states and from defect states into the conduction band always occupy an energy interval equal to  $|(\varepsilon_D - \varepsilon_V) - (\varepsilon_C - \varepsilon_D)| = \varepsilon_C - \varepsilon_V$ . Therefore, only one maximum can be observed experimentally. By comparing Figs. 3 and 4, we may assume that the type of the defect absorption spectra is mainly determined by the distribution of the density of electronic states located in the allowed bands.

### 3. Conclusions

To summarize, the spectral characteristics of the defect absorption coefficient, which are determined by electron transitions with the participation of the energy states of dangling bonds in amorphous hydrogenated silicon, have been studied. Analytical approximations are obtained for the absorption coefficient spectra, where defect states are engaged in optical transitions. It is shown that the defect absorption intensity strongly depends on the density of electronic states located at the edges of the valence and conduction bands. This fact makes it possible to change the photosensitivity of photovoltaic devices fabricated on the basis of amorphous semiconductors. The results obtained can also be applied to doping impurities, i.e. donor and acceptor states in crystalline semiconductors.

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Received 13.12.18.

Translated from Russian by O.I. Voitenko

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ЩІЛЬНІСТЬ ДЕФЕКТНИХ СТАНІВ  
І СПЕКТРИ ДЕФЕКТНОГО ПОГЛИНАННЯ a-Si:H

Р е з ю м е

Досліджено спектральні характеристики коефіцієнта дефектного поглинання аморфного гідрогенізованого кремнію, які визначаються з електронних переходів, в яких беруть участь енергетичні стани обірваних зв'язків (дефекти). Показано, що в значеннях коефіцієнта дефектного поглинання основну роль відіграють електронні переходи між дефектними і нелокалізованими станами. Також показано, що спектральна характеристика в основному визначається функцією розподілу щільності електронних станів, що знаходяться в валентній зоні або в зоні провідності. Визначено, що максимуми в спектральній характеристиці коефіцієнта дефектного поглинання з'являються у тому випадку, коли в межах дозволених зон є яскраво виражені максимуми.