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DANGEROUS BONDS INDIVIDUAL OF HYDROGENATED AMORPHOUS SILICON AND DEFECT ABSORPTION SPECTRA

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In this work, defect absorption spectra for defects characteristic of hydrogenated amorphous silicon are theoretically studied. It is shown that in order to determine defect absorption spectra using the Kubo-Greenwood formula, the indefinite integral in this formula must be written in a certain form. It was discovered that electronic transitions involving defect states are divided into two parts depending on the energy of absorbed photons. The values of the partial defect absorption spectrum at low energies of absorbed photons have almost no effect on the overall defect absorption spectrum. It has been established that the main role in determining the defect absorption spectrum is played by partial spectra determined by optical transitions of electrons between allowed bands and defects. It is shown that with a power-law distribution of the density of electronic states in allowed bands, the spectra of optical transitions between them and defects do not depend on the value of this power.

Keywords: *Amorphous semiconductors; Optical transitions of electrons with the participation of defects; Defect absorption spectra; Partial spectra*
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INTRODUCTION

It is known that hydrogenated amorphous silicon (*α-Si:H*), forming dangling bonds in the mobility gap, is divided into three types depending on their charge state. D^0-neutral defect having one electron and one hole, D^--defect with negative charge having two electrons and D^+-defect with positive charge having two holes. All these defects act as traps for electrons.

It was shown in [1] that, regardless of the charge state, defects are involved in all optical transitions of electrons. Therefore, the experiment gives the total sum of the values of all partial spectra corresponding to optical transitions, including all defect states.

In [2,3], for the energy positions and concentrations of these defects in *α-Si:H* obtained in a glow gas discharge, the following are given: $\varepsilon_D{}^0-\varepsilon_V\approx 0{,}78\ eV$, $\varepsilon_D{}^--\varepsilon_V\approx 0{,}5\ eV$, $\varepsilon_D{}^+-\varepsilon_V\approx 1{,}28\ eV$ *and* $N_D{}^0 = 4.5\cdot10^{15}$ cm^{-3}, $N_D{}^- = 3\cdot10^{15}$ cm^{-3}, $N_D{}^+ = 3\cdot10^{15}$ sm^{-3}.

It is known that during the absorption of photons, electronic transitions occur with the participation of defect states and the valence band and its tail, as well as with the conduction band and its tail. Depending on the energy of absorbed photons, these optical transitions of electrons are shown in Figure 1.

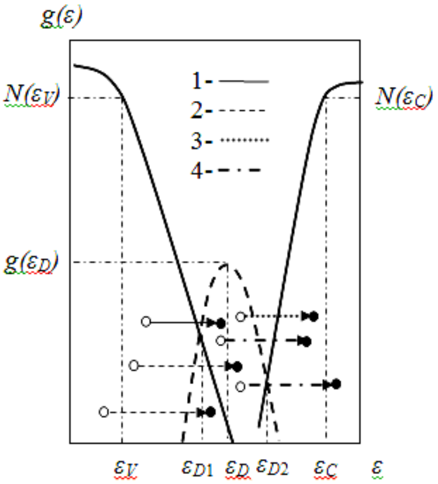

Figure 1. Types of optical electronic transitions involving defect states occurring in amorphous semiconductors at the energy of absorbed photons. 1 - $\varepsilon_{D1}-\varepsilon_V<\hbar\omega$ and 2-$\varepsilon_{D1}-\varepsilon_V<\hbar\omega$, 3 - $\varepsilon_C-\varepsilon_{D2}>\hbar\omega$ and 4 - $\varepsilon_C-\varepsilon_{D2}<\hbar\omega$

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When the condition 1-ε_{D1}-ε_V>ħω for the energy of absorbed photons is fulfilled, the electrons participating in the optical transition pass only from the tail of the valence band to the defect, and when the condition 2 –ε_{D1}-ε_V<ħω is fulfilled, the electrons simultaneously pass from the valence band and from tail for a defect. Where ε_{D1} is the energy position of the intersection point of the distribution of electronic states, the tail of the valence band and defects (Fig. 1.), ε_V is the upper boundary of the valence band.

When condition 3 - ε_C-ε_{D2}>ħω is met, electrons pass only from defects to the tail of the conduction band, and when condition 4 - $\varepsilon_C-\varepsilon_{D2}<\hbar\omega$ is met, optical transitions of electrons simultaneously occur from defect states to the tail of the conduction band, as well as to the conduction band. Where ε_{D2} is the energy position of the intersection point of the distribution, electronic states of the tail of the conduction band and defect states (Fig. 1), ε_C is the lower boundary of the conduction band.

It follows from this that eighteen optical transitions involving defect states occur simultaneously in *α-Si:H*. Therefore, the theoretical calculation of the defect absorption of *α-Si:H* is a very difficult problem in the physics of amorphous semiconductors.

The disorder in the structural lattice of amorphous semiconductors leads to the fact that the wave vector of electrons involved in optical transitions is not a good quantum number. Therefore, the spectra of all types of optical transitions of electrons in noncrystalline semiconductors are calculated using the Kubo-Greenwood formula using the Davis-Mott approximation method

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

In this equation A is a proportionality coefficient independent of the energy of absorbed photons, g(ε) is the density of initial and $g(\varepsilon+\hbar\omega)$ final states of electrons participating in optical transitions. It was shown in [4] that the integral in equation (1) should be written in the form of a definite integral to determine the Eigen solutions of the absorption coefficient spectra.

It can be seen from this equation that, in order to determine the analytical solutions of partial defect absorption spectra, it is necessary to know the distribution of electronic states in allowed bands and their tails, as well as in defects; for this, different models are usually used [5, 6]. In all these models, the distribution of electronic states in the allowed bands is parabolic, while the distribution of electronic states in the tails of the allowed bands is exponential. Taking this into account, the following model of the distribution of the density of electronic states in allowed bands and their tails was proposed in [7] in the following forms:

$$g(\varepsilon) = N(\varepsilon_V)\left(\frac{\varepsilon_C-\varepsilon}{E_g}\right)^{n_1}, \quad n_1 = 0, 1/2, 1 \quad \text{and} \quad g(\varepsilon) = N(\varepsilon_V)\exp\left(-\beta_1(\varepsilon-\varepsilon_V)\right), \tag{2}$$

$$g(\varepsilon) = N(\varepsilon_C)\left(\frac{\varepsilon-\varepsilon_V}{E_g}\right)^{n_2}, \quad n_2 = 0, 1/2, 1 \quad \text{and} \quad g(\varepsilon) = N(\varepsilon_C)\exp\left(\beta_2(\varepsilon-\varepsilon_C)\right), \tag{3}$$

where $N(\varepsilon_V)$ are the effective values of the density of electronic states in the valence band and $N(\varepsilon_C)$ in the conduction band, E_g is the energy width of the mobility gap, β_1 and β_2 are the parameters that determine the curvature of the exponential tails of the valence band and the conduction band. n_1 - and n_2 - degree of the distribution function of electronic states in the valence band and in the conduction band.

As shown in [8], the distribution of defect states in amorphous semiconductors obeys the distribution of the hyperbolic secant:

$$g(\varepsilon) = \frac{g(\varepsilon_D)}{ch\left(b(\varepsilon-\varepsilon_D)\right)} = \frac{2g(\varepsilon_D)}{\exp\left(b(\varepsilon-\varepsilon_D)\right)+\exp\left(-b(\varepsilon-\varepsilon_D)\right)}, \tag{4}$$

or Gaussian distribution:

$$g(\varepsilon) = g(\varepsilon_D)\exp\left(-a(\varepsilon-\varepsilon_D)^2\right), \tag{5}$$

where *b* and *a* are the parameters that determine the effective half-width of the distribution of the density of electronic states in defects, ε_D is the energy position of the maximum of defect states, and $g(\varepsilon_D)$ is the maximum value of the distribution of the density of electronic states in defects.

In the same work, it was shown that the defect concentrations determined by equation (4) and (5) will be equal to each other when the condition $a = b^2/\pi$ is satisfied.

RESULTS AND DISCUSSION

We write the integral in the Kubo-Greenwood equation as a definite integral for the condition ε_{D1}-ε_V> ħω as follows:

$$\alpha = A\int\limits_{\varepsilon_{D1}-\hbar\omega}^{\varepsilon_{D1}} g(\varepsilon)g(\varepsilon+\hbar\omega)\frac{d\varepsilon}{\hbar\omega}. \tag{6}$$

Substituting the densities of states (2), (3), and (4) into equation (6), we obtain the following expression:

$$\begin{gathered}\alpha = A\int\limits_{\varepsilon_{D1}-\hbar\omega}^{\varepsilon_{D1}} N(\varepsilon_V)\exp\left(-\beta_1(\varepsilon-\varepsilon_V)\right)\frac{g(\varepsilon_D)}{ch\left(b\left(\varepsilon-\varepsilon_D+\hbar\omega\right)\right)}\frac{d\varepsilon}{\hbar\omega} = \frac{Bg(\varepsilon_D)}{bN(\varepsilon_C)}\times \\ \times\exp(b(\varepsilon_V-\varepsilon_D+\hbar\omega))(2b\hbar\omega+\ln\frac{(\exp(2b(\varepsilon_{D1}-\varepsilon_D))+1)}{(\exp(2b(\varepsilon_{D1}-\varepsilon_D+\hbar\omega))+1)})\end{gathered}, \tag{7}$$

where *B=AN(ε_V)N(ε_C)*. To obtain an analytical solution to equation (7), the condition must be satisfied. It will be shown below that the value of b has almost no effect on the defect absorption spectra. Equation (6) is adapted to the optical transitions of electrons, under the condition *ε_{D1}-ε_V<ħω*:

$$\begin{gathered}\alpha = A\int\limits_{\varepsilon_{D1-\hbar\omega}}^{\varepsilon_{D1}} g(\varepsilon)g(\varepsilon+\hbar\omega)\frac{d\varepsilon}{\hbar\omega} = A\int\limits_{\varepsilon_V}^{\varepsilon_{D1}} g(\varepsilon)g(\varepsilon+\hbar\omega)\frac{d\varepsilon}{\hbar\omega} + A\int\limits_{\varepsilon_{D1}-\hbar\omega}^{\varepsilon_V} g(\varepsilon)g(\varepsilon+\hbar\omega)\frac{d\varepsilon}{\hbar\omega} = \\ = \alpha_1+\alpha_2\end{gathered}, \tag{8}$$

where is the partial spectrum of electronic transitions from the tail of the valence band to the defect, and is the partial spectrum of optical transitions from the valence band to the defect. For optical transitions of electrons from the tail of the valence band to defects, we obtain the expression:

$$\begin{gathered}\alpha_1 = A\int\limits_{\varepsilon_V}^{\varepsilon_{D1}} N(\varepsilon_V)\exp\left(-\beta_1(\varepsilon-\varepsilon_V)\right)\frac{g(\varepsilon_D)}{ch\left(b\left(\varepsilon-\varepsilon_D+\hbar\omega\right)\right)}\frac{d\varepsilon}{\hbar\omega} = \\ = \frac{Bg(\varepsilon_D)}{bN(\varepsilon_C)\hbar\omega}\exp(b(\varepsilon_V-\varepsilon_D+\hbar\omega))(2b(\varepsilon_{D1}-\varepsilon_V))+\ln\frac{(\exp(2b(\varepsilon_V-\varepsilon_D+\hbar\omega))+1)}{(\exp(2b(\varepsilon_{D1}+\varepsilon_D+\hbar\omega))+1)})\end{gathered}. \tag{9}$$

To obtain equation (9), the condition $\beta_1 = \mathrm{b}$ was also required. The partial spectra of optical transitions of electrons from the valence band to defects are calculated. For the case when *n_1=0* we get the expression:

$$\begin{gathered}\alpha_2 = A\int\limits_{\varepsilon_{D1}-\hbar\omega}^{\varepsilon_V} N(\varepsilon_V)\frac{g(\varepsilon_D)}{ch\left(b\left(\varepsilon-\varepsilon_D+\hbar\omega\right)\right)}\frac{d\varepsilon}{\hbar\omega} = \frac{2Bg(\varepsilon_D)}{bN(\varepsilon_C)\hbar\omega}\times \\ \times(arctg\exp(b(\varepsilon_V-\varepsilon_D+\hbar\omega)) - arctg\exp(b(\varepsilon_{D1}-\varepsilon_D)))\end{gathered}. \tag{10}$$

And for the case when *n_1=1*:

$$\begin{gathered}\alpha_2 = A\int\limits_{\varepsilon_{D1}-\hbar\omega}^{\varepsilon_V} N(\varepsilon_V)\left(\frac{\varepsilon_C-\varepsilon}{E_g}\right)\frac{g(\varepsilon_D)}{ch\left(b\left(\varepsilon-\varepsilon_D+\hbar\omega\right)\right)}\frac{d\varepsilon}{\hbar\omega} = \frac{2Bg(\varepsilon_D)}{bN(\varepsilon_C)E_g\hbar\omega}(\varepsilon_C-\varepsilon_D+\hbar\omega)\times \\ \times(arctg\exp(b(\varepsilon_V-\varepsilon_D+\hbar\omega)) - arctg\exp(b(\varepsilon_{D1}-\varepsilon_D))) - \\ -\frac{Bg(\varepsilon_D)}{2aN(\varepsilon_C)E_g\hbar\omega}(\exp(-a(\varepsilon_V-\varepsilon_D+\hbar\omega)^2 - \exp(-a(\varepsilon_{D1}-\varepsilon_D)^2)\end{gathered}. \tag{11}$$

In expressions (10) and (11), the quantity b can take arbitrary values. An analytical solution for the case when *n_1=1/2* could not be obtained, so it was calculated using approximate calculation methods. When *ε_C-ε_{D2}>ħω* to calculate the spectra of optical transitions of electrons from the defect to the tail of the conduction band, we write the Kubo-Greenwood formula as follows:

$$\alpha = A\int_{\varepsilon_{D2}-\hbar\omega}^{\varepsilon_{D2}} g(\varepsilon)g(\varepsilon+\hbar\omega)\frac{d\varepsilon}{\hbar\omega}. \tag{12}$$

Let's carry out calculations by substituting the distribution functions given by equations (2)-(4) into equation (12):

$$\begin{aligned}\alpha &= A\int_{\varepsilon_{D2}-\hbar\omega}^{\varepsilon_{D2}} \frac{g(\varepsilon_D)}{ch(b(\varepsilon-\varepsilon_D))}N(\varepsilon_C)\exp(\beta_2(\varepsilon-\varepsilon_C+\hbar\omega))\frac{d\varepsilon}{\hbar\omega} = \\ &= \frac{Bg(\varepsilon_D)}{N(\varepsilon_V)b\hbar\omega}\exp(b(\varepsilon_D-\varepsilon_C+\hbar\omega))\ln\frac{(1+\exp(2b(\varepsilon_{D2}-\varepsilon_D)))}{(1+\exp(2b(\varepsilon_{D2}-\varepsilon_D-\hbar\omega)))}\end{aligned} \tag{13}$$

Equation (13) was calculated for $\beta_2 = \mathrm{b}$.

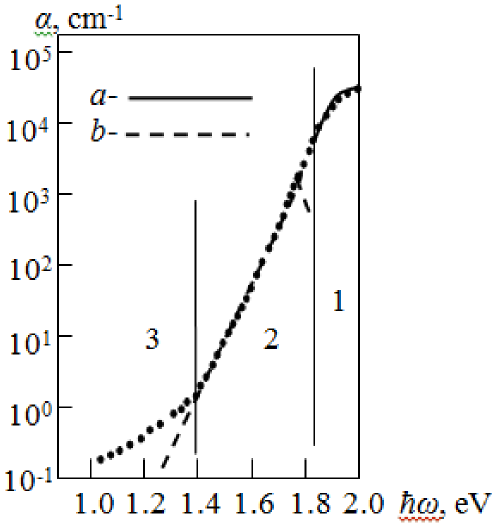

Figure 2. Experimentally determined optical absorption spectrum of amorphous hydrogenated silicon
1 – region of interband absorption, 2 – region of exponential absorption, 3 – region of defective absorption.

Now we agree on equation (12) for the condition ε_C-ε_{D2}<ħω to optical transitions of electrons:

$$\alpha = A\int_{\varepsilon_{D2}-\hbar\omega}^{\varepsilon_{D2}} g(\varepsilon)g(\varepsilon+\hbar\omega)\frac{d\varepsilon}{\hbar\omega} = A\int_{\varepsilon_C-\hbar\omega}^{\varepsilon_{D2}} g(\varepsilon)g(\varepsilon+\hbar\omega)\frac{d\varepsilon}{\hbar\omega} + A\int_{\varepsilon_{D2}-\hbar\omega}^{\varepsilon_C-\hbar\omega} g(\varepsilon)g(\varepsilon+\hbar\omega)\frac{d\varepsilon}{\hbar\omega} = \alpha_1+\alpha_2. \tag{14}$$

where α_1 are the partial spectra of optical transitions of electrons from defect states to the conduction band, and α_2 are from the defect to the tail of the conduction band. Let us calculate partial spectra for electron transitions from a defect to conduction bands by substituting distribution functions (2)–(5) into equation (14). For the case *n_2=0:*

$$\alpha_1 = A\int_{\varepsilon_C-\hbar\omega}^{\varepsilon_{D2}} \frac{g(\varepsilon_D)}{ch(b(\varepsilon-\varepsilon_D))}N(\varepsilon_C)\frac{d\varepsilon}{\hbar\omega} = \frac{2Bg(\varepsilon_D)}{b\hbar\omega N(\varepsilon_V)}(arctg(\exp(b(\varepsilon_{D2}-\varepsilon_D)) - arctg(\exp(b(\varepsilon_C-\varepsilon_D-\hbar\omega))). \tag{15}$$

in the case of *n_2=1*, we obtain the expressions:

$$\begin{aligned}\alpha_1 &= A\int_{\varepsilon_C-\hbar\omega}^{\varepsilon_{D2}} \frac{g(\varepsilon_D)}{ch(b(\varepsilon-\varepsilon_D))}N(\varepsilon_C\left(\frac{\varepsilon-\varepsilon_V+\hbar\omega}{E_g}\right)\frac{d\varepsilon}{\hbar\omega} = \\ &= \frac{2Bg(\varepsilon_D)}{b\hbar\omega E_g N(\varepsilon_V)}(arctg(\exp(b(\varepsilon_{D2}-\varepsilon_D)) - arctg(\exp(b(\varepsilon_C-\varepsilon_D-\hbar\omega))) - \\ &- \frac{Bg(\varepsilon_D)}{2a\hbar\omega E_g N(\varepsilon_V)}(\exp(-a(\varepsilon_{D2}-\varepsilon_D)^2) - \exp(-a(\varepsilon_C-\varepsilon_D-\hbar\omega)^2))\end{aligned} \tag{16}$$

For *n_2=1/2*, it was not possible to obtain an analytical solution, so it was calculated using approximate calculation methods. In equation s (15) and (16), *b* can take arbitrary values.

Let us now calculate the partial spectrum of optical transitions of electrons from the defect to the tail of the conduction bands:

$$\alpha_2 = A\int_{\varepsilon_{D2}-\hbar\omega}^{\varepsilon_C-\hbar\omega}\frac{g(\varepsilon_D)}{ch\left(b(\varepsilon-\varepsilon_D)\right)}N(\varepsilon_C)\exp\left(\beta_2(\varepsilon-\varepsilon_C+\hbar\omega)\right)\frac{d\varepsilon}{\hbar\omega}=\frac{Bg(\varepsilon_D)}{b\hbar\omega N(\varepsilon_C)}\times$$
$$\times\exp(b(\varepsilon_D-\varepsilon_C+\hbar\omega))Ln\frac{(1+\exp(2b(\varepsilon_C-\varepsilon_D-\hbar\omega)))}{(1+\exp(2b(\varepsilon_{D2}-\varepsilon_D-\hbar\omega)))} \qquad (17)$$

In equation (17), calculations were made for $\beta_2 = \mathrm{b}$. In equations (15) and (16), the quantity b can take arbitrary values. To calculate the values of the above partial spectra, it is necessary to determine the parameters B, E_g, β_1, β_2, for which we will use the experimentally determined values of the optical absorption spectrum of the absorption coefficient. The work [9] presents the absorption coefficient spectrum determined from the experiment of amorphous hydrogenated silicon grown in a high-frequency glow gas discharge (Fig. 2).

Let us divide this spectrum into the regions of interband, exponential, and defect absorption. Considering B and E_g in the analytically calculated equation as fitting parameters, we determine by comparing the values of the interband absorption spectra obtained from the experiment. Precisely, in the same way we determine β_1, and β_2 from the region of exponential absorption. In [10], an analytical expression was obtained for the interband absorption spectrum when:

$$n_1 = n_2 = 1/2: \quad \alpha(\hbar\omega)=\frac{\mathrm{B}}{4\hbar\omega E_g}\left[2(\hbar\omega-E_g)\sqrt{E_g\hbar\omega}-(E_g-\hbar\omega)^2 arctg\left(\frac{E_g-\hbar\omega}{2\sqrt{E_g\hbar\omega}}\right)\right]. \qquad (18)$$

It was determined that when, $B = 1.71*10^5\ sm^{-1}$ and $E_g = 1.78\ eV$ corresponds to the experimentally determined and calculated results obtained from formula (18) for the interband absorption spectrum (Fig. 2 - curve a).

In [11] studied the spectra of exponential absorption and for the analytical solution of exponential absorption, the following expressions were obtained:

$$\alpha(\hbar\omega)=\frac{\mathrm{B}}{(\beta_2-\beta_1)\hbar\omega}\exp(\beta_1(\hbar\omega-E_g))\exp((\beta_1-\beta_2)(\varepsilon_C-\varepsilon_0))[\exp((\beta_2-\beta_1)\hbar\omega)-1]. \qquad (19)$$

It is also shown there that B and E_g have equal values for the entire region of the optical absorption coefficient.

It was found that the results calculated by the equation (19) of the exponential absorption determined from the experiment are consistent with each other, then $\beta_1 = 24.2\ eV^{-1}$ and $\beta_2 = 31.7\ eV^{-1}$ (Fig. 2, curve b). Since ε_{D1} and ε_{D2} are the intersection points of the exponential tails of allowed bands and the distribution of electronic states in defects, we calculate them using the following equations:

$$N(\varepsilon_C)\exp\left(\beta_2(\varepsilon_{D2}-\varepsilon_C)\right)=2g(\varepsilon_D)\exp(b(\varepsilon_{D2}-\varepsilon_D)), \qquad (20)$$

$$N(\varepsilon_V)\exp\left(-\beta_1(\varepsilon_{D1}-\varepsilon_V)\right)=2g(\varepsilon_D)\exp(-b(\varepsilon_{D1}-\varepsilon_D)). \qquad (21)$$

From this we obtain the following expressions:

$$\varepsilon_{D1}=(\ln(\frac{N(\varepsilon_V)}{2g(\varepsilon_D)})+b\varepsilon_D+\beta_1\varepsilon_V)/(b+\beta_1), \qquad (22)$$

$$\varepsilon_{D2}=(\ln(\frac{2g(\varepsilon_D)}{N(\varepsilon_C)})+b\varepsilon_D+\beta_2\varepsilon_C)/(b+\beta_2). \qquad (23)$$

Calculations using equations (22) and (23) showed that when the value of $\beta_1 = \mathrm{b}$ and $\beta_2 = \mathrm{b}$ changes in the range (12–35) eV^{-1}, the values of ε_{D1} and ε_{D2} change within $\Delta\varepsilon\approx 0.1\ eV$. Calculations of the partial spectra of the absorption coefficient in defects showed that these changes in ε_{D1} and ε_{D2} do not significantly affect the shape of the defect absorption spectra.

Calculated equations (7), (13) for the conditions $\varepsilon_{D1}-\varepsilon_V<\hbar\omega$ and $\varepsilon_C-\varepsilon_{D2}<\hbar\omega$. Calculated equations (9), (17), (15) and (10), (11) and (16) and for the conditions $\varepsilon_{D1}-\varepsilon_V<\hbar\omega$ and $\varepsilon_C-\varepsilon_{D2}>\hbar\omega$.

The forms of these equations are close to each other; it can be considered that the partial spectra of defect absorption calculated by these equations almost do not differ from each other. Therefore, we calculate the partial spectra of defective absorption only for the defect $\varepsilon_D-\varepsilon_V=0.5\ eV$ and $g(\varepsilon_D^+)=3\times10^{15}\ eV^{-1}cm^{-3}$ for optical transitions of electrons from the defect to the tail of the conduction band.

It can be seen from the above equations that as the value of $g(\varepsilon_D)$ increases or decreases, these spectra move in parallel up or down, respectively. Calculations were obtained using equations (10) and (11) for $n_1=1$, $n_1=0$, and numerical calculations obtained for $n_l=1/2$ showed that these spectra do not differ from each other at all (Fig. 3). To establish the value of $g(\varepsilon_D)$, we use the equation for determining the concentration of defective states and obtain:

$$N_D = \int_{-\infty}^{\infty} \frac{g(\varepsilon_D)}{ch(b(\varepsilon-\varepsilon_D))} d(\varepsilon) = \frac{2}{b} g(\varepsilon_D) arctg \exp(b(\varepsilon-\varepsilon_D))\Big|_{-\infty}^{\infty} = \frac{2\pi}{b} g(\varepsilon_D), \;\; g(\varepsilon_D) = \frac{bN_D}{2\pi} \; . \tag{24}$$

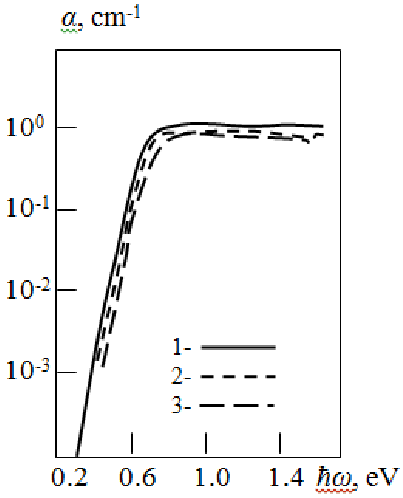

Figure 3. Partial spectra of optical transitions of electrons between allowed zones and defects 1-$n_l=1$, 2-$n_l=1/2$, 3-$n_l=0$. Calculations are made for defect D_0.

The calculation results obtained by equation (24) are shown in Table 1.

Table 1. Calculated data for $g(\varepsilon_D)$ obtained using equation (24).

	b, eV^{-1}	$g(\varepsilon_D)$, $eV^{-1} sm^{-3}$	b, eV^{-1}	$g(\varepsilon_D)$, $eV^{-1} sm^{-3}$	b, eV^{-1}	$g(\varepsilon_D)$, $eV^{-1} sm^{-3}$
D^0	12	8.6×10^{15}	24	1.72×10^{16}	32	2.29×10^{16}
D^-	12	5.73×10^{15}	24	1.15×10^{16}	32	1.53×10^{16}
D^+	12	5.73×10^{15}	24	1.15×10^{16}	32	1.53×10^{16}

The results of calculations obtained by equations (7) and (9) for various values of b at ε_D-$\varepsilon_V=0.5$ eV and $g(\varepsilon_D^-)$ are shown in Figure 4. This figure also shows the spectrum for comparison optical transitions of electrons from a defect to the conduction band, calculated by equation (11). It can be seen from this figure that the partial spectra determined by the optical transitions of electrons between defects, the tails of allowed bands, at different values of b have practically no effect on the value of the defect absorption spectrum.

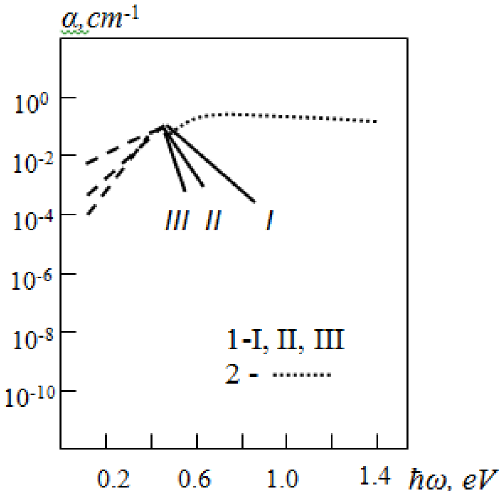

Figure 4. Partial spectra of optical transitions of an electron 1-from a D^-defect to the tail of the conduction band I - $b=12$ eV^{-1}, II - $b=24$ eV^{-1}, III - $b=32$ eV^{-1}, -when ε_{D1}-$\varepsilon_V>\hbar\omega$, - when ε_{D1}-$\varepsilon_V<\hbar\omega$. 2-partial spectrum of optical transitions of an electron from a D^- defect to the conduction band

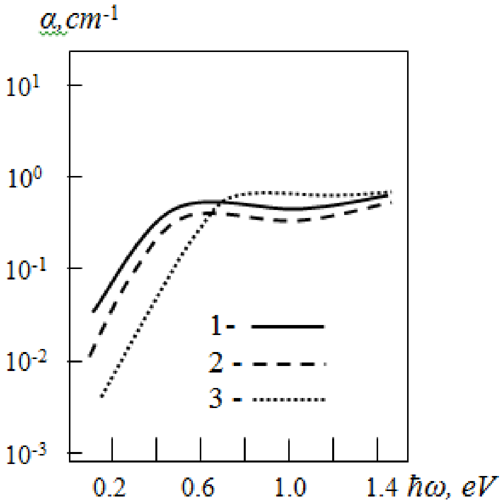

Figure 5. Total values of partial spectra of the defect absorption coefficient obtained using equations (7), (9), (11), (13), (16), (17). For 1-D^+, 2-D^- and 3-D^0, forming optical transitions between defect states and allowed bands and their tails. Calculations were carried out for $b=12$ eV^{-1}

It is known that the total sum of partial absorption spectra corresponding to all optical transitions of electrons with the participation of defect states is determined in the experimental spectra of defective absorption. Therefore, for each defect ε_{D0}-$\varepsilon_V=0.78$ eV, ε_D-$\varepsilon_V=0.5$ eV, $\varepsilon_{D+}\varepsilon_V=1.28$ eV calculated by equations (7), (9), (10) (11) and (13), (15), (16), (17) sums of partial absorption spectra are shown in Fig. 5. It should be noted that the experiment gives the total value of these spectra. It can be seen that when the energy of absorbed photons is greater than 0.6 eV, these spectra have almost the same form. But, none of them can explain the defective absorption spectrum of the representations in Fig. 2. Probably, this sample has the values of the energy position, or the concentration of these defects does not correspond to the above values.

CONCLUSIONS

Thus, in the present work, we carried out a theoretical study of the defect absorption spectra of hydrogenated amorphous silicon. It was found that partial spectra determined by optical transitions of electrons between allowed bands and defects play a key role in determining the defect absorption spectrum. It was found that the spectrum of defective absorption in the case of a power-law distribution of the density of electronic states in allowed bands does not depend on the value of the exponent.

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НЕБЕЗПЕЧНІ ЗВ'ЯЗКИ МІЖ ГІДРОГЕНІЗОВАНИМ АМОРФНИМ КРЕМНІЄМ ТА СПЕКТРАМИ ПОГЛИНАННЯ ДЕФЕКТІВ

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У даній роботі теоретично досліджено спектри дефектного поглинання дефектів, характерних для гідрогенізованого аморфного кремнію. Показано, що для визначення спектрів поглинання дефектів за формулою Кубо-Грінвуда необхідно записати невизначений інтеграл у цій формулі в певному вигляді. Було виявлено, що електронні переходи за участю дефектних станів поділяються на дві частини в залежності від енергії поглинених фотонів. Значення парціального дефектного спектра поглинання при малих енергіях поглинених фотонів майже не впливають на загальний спектр поглинання дефектів. Встановлено, що основну роль у визначенні спектра поглинання дефектів відіграють парціальні спектри, які визначаються оптичними переходами електронів між дозволеними зонами та дефектами. Показано, що при степеневому розподілі щільності електронних станів у дозволених зонах спектри оптичних переходів між ними та дефектами не залежать від величини цієї потужності.

Ключові слова: *аморфні напівпровідники; оптичні переходи електронів за участю дефектів; спектри поглинання дефектів; часткові спектри*