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RG Ikramov
Namangan Engineering and
Technology Institute,
Namangan, Uzbekistan

MA Nuriddinova
Namangan Engineering and
Technology Institute,
Namangan, Uzbekistan

Kh. A Muminov
Namangan Engineering and
Technology Institute,
Namangan, Uzbekistan

Spectra of the coefficient of defect absorption and the energy position of defects in amorphous hydrogenated silicon

RG Ikramov, MA Nuriddinova and Kh. A Muminov

Abstract

In the present work, the influence of light on defects of pseudo-doped amorphous hydrogenated silicon is theoretically investigated using the Davis-Mott approximation using the Kubo-Greenwood formula. It is showing that the shape of the spectra of the defective absorption coefficient is determining by the distribution of the density of states in the allowed zones. It was determined that the defect absorption spectra have maxima, where the maxima of the distribution of the energy position of defective states are located. It is shown that from the experimental data obtained for the defect absorption spectra one can determine the energy position of the defects.

Keywords: Amorphous hydrogenated silicon, the density distribution of electron states of defects, Kubo-greenwood formula, Davis-Mott approximation, optical transitions, absorption coefficient

Introduction

As is known, pseudo-doped hydrogenated amorphous silicon (*a-Si:H*) has no dopants. In this material, the Fermi level is shifted by changing the technological conditions of cultivation. Therefore, it is in *a-Si:H* that the term defective absorption spectra belong. In ^[1, 2], it was shown that the energy position of the main defects (D^0 is a neutral defect, D^- is a negatively charged defect, D^+ is a positively charged defect) of *a-Si:H* samples located in the interval $\varepsilon_C - \varepsilon_{D^0} = 0.95-1.05$ eV, $\varepsilon_C - \varepsilon_{D^-} = 0.65-0.75$ eV, $\varepsilon_C - \varepsilon_{D^+} = 0.35-0.45$ eV. Because the energy positions of defects also depend on the technological conditions of cultivation. The experimental results of the spectral characteristics of the defect absorption coefficient in *a-Si:H* films are shown in Figure 1 ^[3]. It can be seen that some spectra have clear maxima, and some do not. In the present work, the interaction of light to defects of pseudo-doped *a-Si:H* is theoretically investigated using the spectral characteristic of the defect absorption. A method for determining the energy positions of defects and conditions for the appearance of maxima in the spectrum of defective absorption is proposed.

As is known, optical transitions of electrons, the participation of defective states, are of three types: between defects, between defects and tails of allowed bands, between defects and allowed bands. It was shown in ^[1] that the main role of these optical transitions is played by passing between defects and allowed bands. The spectral characteristics of the defect absorption coefficient depend on the energy position of the defects and the distribution of the density of states in the defects and allowed bands. The spectral characteristics of the defect absorption coefficient of amorphous semiconductors are calculated by the Davis-Mott approximation method from the Kubo-Greenwood formula as follows ^[4, 6].

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

where ε_0 - is the highest energy position of electrons participating in optical transitions, $g(\varepsilon)$ - and $g(\varepsilon + \hbar\omega)$ are the initial and final density of electronic states involved in optical transitions.

$B = \frac{8\pi^2 e^2 \hbar^3 a}{(m^*)^2 n_0 c}$ is a proportionality coefficient that does not depend on the frequency of the absorbed photon, where a - is the average inter-atomic distance, n_0 - is the refractive index

Corresponding Author:
RG Ikramov
Namangan Engineering and
Technology Institute,
Namangan, Uzbekistan

of light, c - is the speed of light in vacuum, m^* - is the effective mass of the electron, e - is the charge of the electron, \hbar - is the Planck constant. In [7, 8] it was shown that when calculating the spectra of the defect absorption coefficient in amorphous semiconductors, the density of states in defects can be chosen in the form of Gaussian distributions or hyperbolic secant, and for state density distributions at the boundaries of the allowed bands in the form of power or hyperbolic secant [8].

The energy dependence of the densities of defective states in the Gaussian distribution is as follows

$$g(\varepsilon) = g(\varepsilon_D) \exp(-a(\varepsilon - \varepsilon_D)^2) \quad (2)$$

where $g(\varepsilon_D)$ is the maximum value of the density distribution of electronic states in defects and ε_D is the energy position of this maximum; a - is the parameter that determines the effective half width Gaussian distribution [1, 5].

The density distribution of states in the form of a hyperbolic secant is recorded as follows:

$$g(\varepsilon) = \frac{g(\varepsilon_D)}{\operatorname{ch}(b(\varepsilon - \varepsilon_D))} = \frac{2g(\varepsilon_D)}{\exp(b(\varepsilon - \varepsilon_D)) + \exp(-b(\varepsilon - \varepsilon_D))} \quad (3)$$

where b is the parameter that determines the effective half width and for a -Si:H lies in the interval 10 - 30 eV^{-1} . The correspondence between the distributions (2) and (3) is obtained when $b = \sqrt{\pi a}$ [8].

In [7, 9] it was shown that in the case when the density distribution of electronic states at the boundaries of the valence and conduction bands has power dependence, they can be written as follows:

$$g(\varepsilon) = N(\varepsilon_V) \left(\frac{\varepsilon_C - \varepsilon}{E_g} \right)^{n_1}, \text{ When } \varepsilon \leq \varepsilon_V \quad (4)$$

$$g(\varepsilon) = N(\varepsilon_C) \left(\frac{\varepsilon - \varepsilon_V}{E_g} \right)^{n_2}, \text{ when } \varepsilon_C \leq \varepsilon \quad (5)$$

where $N(\varepsilon_V)$ and $N(\varepsilon_C)$ are effective values of the density of states in the valence and conduction band, ε_V is the highest border of the valence band, and ε_C is the lower boundary of the conduction band. E_g is the energy width of the mobility gap (bandgap). Considering that the density distribution of states at the boundaries of the allowed bands can be parabolic or linear [4, 10] that is, $n_1 = n_2 = 1/2$ and $n_1 = n_2 = 1$. When the densities of electronic states of the allowed bands correspond, the Gaussian distribution can be written as follows way [1, 10]: for the valence band

$$g(\varepsilon) = N(\varepsilon_V) \exp(-a(\varepsilon - \varepsilon_V)^2), \quad (6)$$

for conduction band

$$g(\varepsilon) = N(\varepsilon_C) \exp(-a(\varepsilon - \varepsilon_C)^2), \quad (7)$$

As is known the integral of the Gaussian distribution does not have an analytical solution; therefore, to obtain analytical solutions of the defect absorption spectra, one can apply the distributions in the form of a hyperbolic secant: for the valence bands

$$g(\varepsilon) = \frac{2N(\varepsilon_V)}{\exp(b(\varepsilon - \varepsilon_V)) + \exp(-b(\varepsilon - \varepsilon_V))}, \quad (8)$$

for conduction band

$$g(\varepsilon) = \frac{2N(\varepsilon_C)}{\exp(b(\varepsilon - \varepsilon_C)) + \exp(-b(\varepsilon - \varepsilon_C))}, \quad (9)$$

As shown in [10, 11], the distribution of the density of states in the tails of the allowed bands is exponential and is described by the following expressions: for the tail of the valence band

$$g(\varepsilon) = N(\varepsilon_V) \exp(-\beta_1(\varepsilon - \varepsilon_V)), \text{ when } \varepsilon_V < \varepsilon; \quad (10)$$

and for the tail of the conduction band

$$g(\varepsilon) = N(\varepsilon_C) \exp(\beta_2(\varepsilon - \varepsilon_C)), \text{ when } \varepsilon < \varepsilon_C; \quad (11)$$

where β_1 and β_2 are the parameters that determine the slope of the tails of the valence band and conduction band,

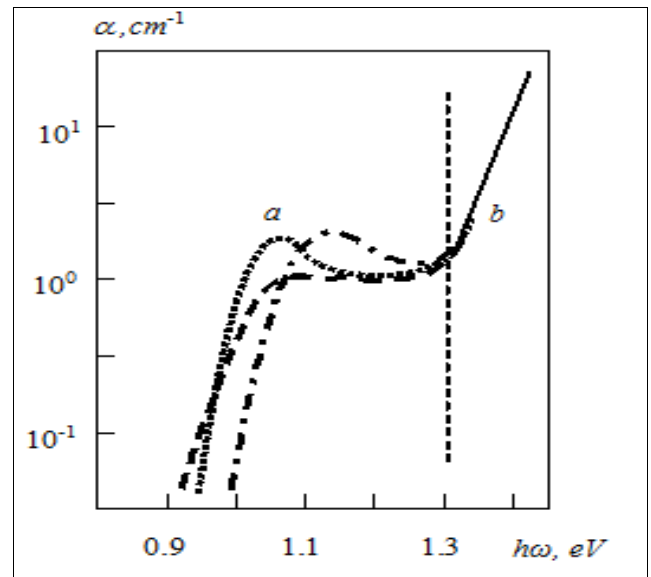


Fig 1: Experimental results of the spectral characteristics. A – Defective absorption section of pseudo-doped samples a-Si:H, B – exponential absorption section.

Calculation and discussion: When the energy of absorbed photons is $\varepsilon_{01} - \varepsilon_V < \hbar\omega$ and $\varepsilon_C - \varepsilon_{02} < \hbar\omega$, where ε_{01} - and ε_{02} are the energy positions of the point of intersection of the tails of the expanded bands and defects (see Figure 2), then optical transitions are formed between the defects and expanded bands.

In the case when the density distribution of states in the allowed bands is parabolic ($n_1 = n_2 = 1/2$), the spectra of the defect absorption coefficient are written in the following forms: for optical transitions from a defect to the conduction band

$$\alpha(\hbar\omega) = B \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_C} \frac{g(\varepsilon_D)}{ch(b(\varepsilon - \varepsilon_D + \hbar\omega))} N(\varepsilon_C) \sqrt{\frac{\varepsilon - \varepsilon_V + \hbar\omega}{E_g}} \frac{d\varepsilon}{\hbar\omega}, \quad (12)$$

from valence to defect

$$\alpha(\hbar\omega) = B \int_{\varepsilon_V - \hbar\omega}^{\varepsilon_V} N(\varepsilon_V) \sqrt{\frac{\varepsilon_C - \varepsilon}{E_g}} \frac{g(\varepsilon_D)}{ch(b(\varepsilon - \varepsilon_D + \hbar\omega))} \frac{d\varepsilon}{\hbar\omega}, \quad (13)$$

As is known, these integrals have no analytical solution. Therefore, these spectra were obtained using numerical methods. The results of the calculations are shown in Figure 3-a.

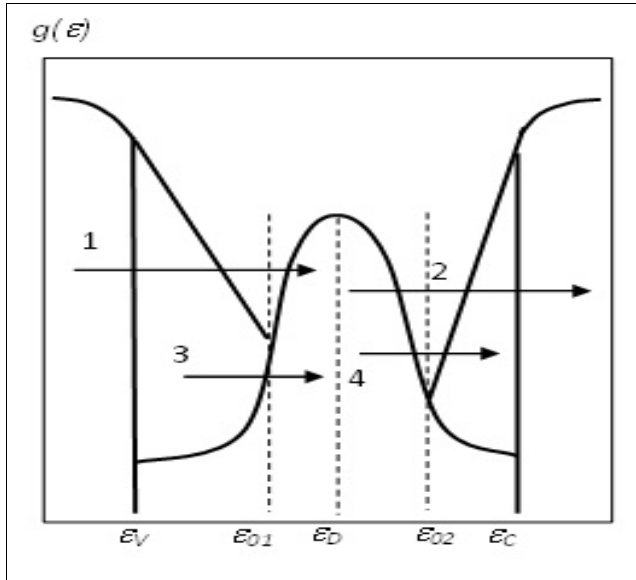


Fig 2: Types of optical transitions in amorphous semiconductors where defective states are involved: 1 - from the valence band to the defect, 2 - from the defective states to the conduction band, 3 - from the valence band tails to the defect, 4 - from the defective.

If the density distribution in the allowed bands has a linear ($n_1 = n_2 = 1$) dependence:

$$\alpha(\hbar\omega) = B \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_C} \frac{g(\varepsilon_D)}{ch(b(\varepsilon - \varepsilon_D))} N(\varepsilon_C) \frac{\varepsilon - \varepsilon_V + \hbar\omega}{E_g} \frac{d\varepsilon}{\hbar\omega}. \quad (14)$$

$$\alpha(\hbar\omega) = B \int_{\varepsilon_V - \hbar\omega}^{\varepsilon_V} N(\varepsilon_V) \frac{\varepsilon_C - \varepsilon}{E_g} \frac{g(\varepsilon_D)}{ch(b(\varepsilon - \varepsilon_D + \hbar\omega))} \frac{d\varepsilon}{\hbar\omega}, \quad (15)$$

To obtain an analytical solution of these integrals, they must be divided into two components: for the distribution of the hyperbolic secant and Gaussian.

In the case of such a replacement, the error of error does not exceed the error of the experiment [18].

$$\alpha(\hbar\omega) = \frac{Ag(\varepsilon_D)}{N(\varepsilon_V)E_g\hbar\omega} \left[\int_{\varepsilon_C - \hbar\omega}^{\varepsilon_C} \frac{1}{ch(b(\varepsilon - \varepsilon_D))} d\varepsilon + \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_C} \varepsilon \exp(-a(\varepsilon - \varepsilon_D)^2) d\varepsilon \right]. \quad (16)$$

$$\alpha(\hbar\omega) = \frac{Ag(\varepsilon_D)}{N(\varepsilon_C)E_g\hbar\omega} \left[\int_{\varepsilon_V - \hbar\omega}^{\varepsilon_C} \frac{1}{ch(b(\varepsilon - \varepsilon_D + \hbar\omega))} d\varepsilon - \int_{\varepsilon_V - \hbar\omega}^{\varepsilon_C} \varepsilon \exp(-a(\varepsilon - \varepsilon_D + \hbar\omega)^2) d\varepsilon \right], \quad (17)$$

where $A = BN(\varepsilon_C)N(\varepsilon_V)$, when the $a=b^2/\pi$ relationship holds, the concentration of defects, determined by the distribution of the hyperbolic secant and gauss, will be equal to [18].

The analytical solutions of these integrals are written as follows:

$$\alpha(\hbar\omega) = \frac{Ag(\varepsilon_D)}{N(\varepsilon_C)E_g\hbar\omega} \left\{ \frac{2}{b}(\varepsilon_D - \varepsilon_V + \hbar\omega) \operatorname{arctg}(\exp(b(\varepsilon_C - \varepsilon_D))) - \operatorname{arctg}(\exp(b(\varepsilon_C - \varepsilon_D - \hbar\omega))) - \frac{1}{2a} [\exp(-a(\varepsilon_C - \varepsilon_D)^2) - \exp(-a(\varepsilon_C - \varepsilon_D - \hbar\omega)^2)] \right\}. \quad (18)$$

$$\alpha(\hbar\omega) = \frac{Ag(\varepsilon_D)}{N(\varepsilon_V)E_g\hbar\omega} \left\{ \frac{2}{b}(\varepsilon_C - \varepsilon_D + \hbar\omega) \operatorname{arctg}(\exp(b(\varepsilon_V - \varepsilon_D + \hbar\omega))) - \operatorname{arctg}(\exp(b(\varepsilon_V - \varepsilon_D))) + \frac{1}{2a} [\exp(-a(\varepsilon_V - \varepsilon_D + \hbar\omega)^2) - \exp(-a(\varepsilon_V - \varepsilon_D)^2)] \right\}. \quad (19)$$

The results obtained from the calculation of formulas (18) and (19) are shown in Figure 3b. It can be seen that these curves in figures 3a and 3b are the same. These results show that the spectra of the defect absorption coefficient do not depend on the degree of distribution of the density of states in the allowed bands. In these spectra, the weak maxima are in the energy position, where the energy of the absorbed photon is equal to $\hbar\omega = \varepsilon_C - \varepsilon_D$ and $\hbar\omega = \varepsilon_D - \varepsilon_V$.

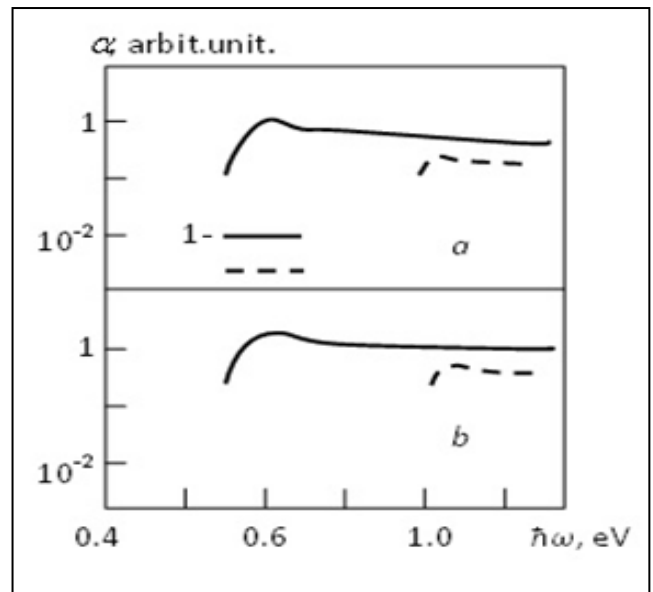


Fig 3: Spectra of optical transitions between allowed bands and defective states. 1- from defect to conduction band, 2- from valence band to defect: a- $n_1=n_2=1/2$, b- $n_1=n_2=1$.

It is determined from the calculations that the change in the maximum (ε_D) of the states of electrons in defects will only change the value of the absorption coefficient.

Experiments show that the appearance of the spectra can vary for different samples as the technology of their growth changes. For example, Figure 1 shows the spectral characteristics of the defect absorption coefficients; all of these samples were grown using the same technology (according to the method of decomposition of silane in a gas discharge). It is seen that some spectral characteristics have obvious maxima and minima. It is known that the energy dependence of the density of states in the valence band and conduction band is very complex and may have several maxima and minima [4]. Taking this into account, we assume that the density of non-localized electronic states at the boundaries of the allowed bands obeys the distribution of a gauss or hyperbolic secant, i.e. boundary of the conduction band

$$g(\varepsilon) = N(\varepsilon_C) \exp(-a_1(\varepsilon - \varepsilon_C)^2) \approx N(\varepsilon_C) / \text{ch}(b_1(\varepsilon - \varepsilon_C)), \quad (20)$$

and the border of the valence band

$$g(\varepsilon) = N(\varepsilon_V) \exp(-a_2(\varepsilon - \varepsilon_V)^2) \approx N(\varepsilon_V) / \text{ch}(b_2(\varepsilon - \varepsilon_V)). \quad (21)$$

If b_1 and b_2 have different values, it is impossible to obtain the analytical form of the defect absorption spectra. The method of numerical calculations shows that if the values of b_1 and b_2 in formulas (20) and (21) do not differ much from each other, then instead of them you can use the expressions $b = (b_1 + b_2) / 2$, then the permissible error does not exceed 9%

given this, you can write them as follows

$$\alpha = \frac{Ag(\varepsilon_D)}{N(\varepsilon_V)} \int_{\varepsilon_V}^{\varepsilon_0} \frac{1}{\text{ch}(b(\varepsilon - \varepsilon_D))\text{ch}(b(\varepsilon - \varepsilon_C + \hbar\omega))} \frac{d\varepsilon}{\hbar\omega}, \quad (22)$$

$$\alpha = \frac{Ag(\varepsilon_D)}{N(\varepsilon_C)} \int_{\varepsilon_C - \hbar\omega}^{\varepsilon_0} \frac{1}{\text{ch}(b(\varepsilon - \varepsilon_V))\text{ch}(b(\varepsilon - \varepsilon_D + \hbar\omega))} \frac{d\varepsilon}{\hbar\omega}. \quad (23)$$

From here we obtain the following result for the defect absorption spectra: for optical transitions from a defect to the conduction band:

$$\alpha = \frac{A}{b\hbar\omega} \frac{g(\varepsilon_D)}{N(\varepsilon_C) \text{sh}(b(\varepsilon_C - \varepsilon_D - \hbar\omega))} \ln \left[\frac{1 + \left(\frac{g(\varepsilon_D)}{N(\varepsilon_C)}\right)^2 + 2\left(\frac{g(\varepsilon_D)}{N(\varepsilon_C)}\right) \text{ch}(b(\varepsilon_C - \varepsilon_D))}{1 + \left(\frac{g(\varepsilon_D)}{N(\varepsilon_C)}\right)^2 + 2\left(\frac{g(\varepsilon_D)}{N(\varepsilon_C)}\right) \text{ch}(b(2\hbar\omega - \varepsilon_C - \varepsilon_D))} \right]. \quad (24)$$

and for optical transitions from the valence band to defects:

$$\alpha = \frac{Ag(\varepsilon_D)}{N(\varepsilon_C) b\hbar\omega} \frac{1}{\text{sh}(b(\varepsilon_D - \varepsilon_V - \hbar\omega))} \ln \left[\frac{1 + \left(\frac{N(\varepsilon_V)}{g(\varepsilon_D)}\right)^2 + 2\left(\frac{N(\varepsilon_V)}{g(\varepsilon_D)}\right) \text{ch}(b(\varepsilon_D - \varepsilon_V))}{1 + \left(\frac{N(\varepsilon_V)}{g(\varepsilon_D)}\right)^2 + 2\left(\frac{N(\varepsilon_V)}{g(\varepsilon_D)}\right) \text{ch}(b(2\hbar\omega - \varepsilon_D - \varepsilon_V))} \right]. \quad (25)$$

The calculation results obtained from these formulas are shown in Figure 4 (it can be compared with Figure 1). As can be seen from the figure, the defect absorption spectra have obvious maxima and the energy positions of these maxima are located at $\hbar\omega = \varepsilon_C - \varepsilon_D$ or $\hbar\omega = \varepsilon_D - \varepsilon_V$. These results show that the spectra of defective absorption can differ greatly from each other, due to the difference in the distribution of the density of states in the allowed bands.

Conclusion

From the results obtained, the following conclusions can be made in this study:

- The form of the spectral characteristics of the defect absorption coefficients is determined by the distribution of the density of states in the allowed bands.
- The defect absorption spectra have weak maxima when the distribution of the density of states, at the boundaries of the allowed bands, has a power dependence on the energy at the points where the photon energy is $\hbar\omega = \varepsilon_C - \varepsilon_D$ and $\hbar\omega = \varepsilon_D - \varepsilon_V$.
- The apparent maxima in the spectral characteristics of the defect absorption coefficient corresponding to the experimental results are formed when the distribution of the density of states at the boundaries of the allowed bands has obvious maxima. These maximums are located in the energy position $\hbar\omega = \varepsilon_C - \varepsilon_D$ or $\hbar\omega = \varepsilon_D - \varepsilon_V$.

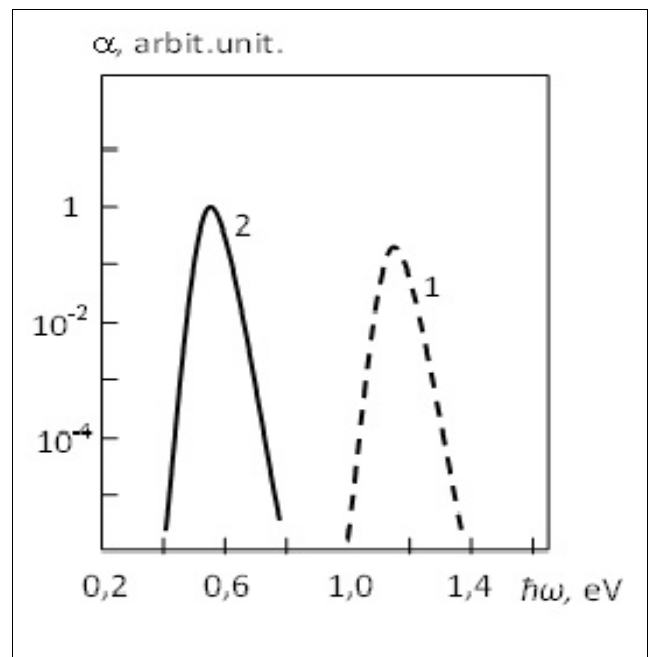


Fig 4: The spectra of the defect absorption coefficient, when the boundary of the allowed bands has clear maxima. 1- $\varepsilon_C - \varepsilon_D = 0,6$ eV, 2- $\varepsilon_C - \varepsilon_D = 1,2$ eV.

This suggests that using the defect absorption spectra in *a-Si:H*, it is possible to reveal the energy position of the defects.

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