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States Density Distribution for Determination of a-Si:H Photoconductivity

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The paper presents an empirical model of the spectral dependence of the distribution of densities of electron states, which covers the main features of hydrogenated amorphous silicon. The effect of the degree of disorder the amorphous structure on the shape and size of tails in electronic states valence band and conduction band. These tails in the forbidden area affect many of the unique properties of amorphous semiconductors. The results can be applied for optimization of technology and modeling of many devices based on amorphous silicon (solar cells, transistors, etc.).

Keywords: Solar element, Amorphous silicon, Photo absorption, Energy zones.

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1. INTRODUCTION

Currently, the introduction of alternative sources of energy, autonomous and decentralized, is more advantageous both from the economic and environmental points of view. The basis of the current photovoltaics is a battery based on silicon and its compounds. The choice of silicon as a raw material for manufacturing photovoltaic converters (PVC) is conditioned by several factors. Si is the most abundant element after oxygen on the Earth and its industrial production in quartz raw materials processing is well developed. The solar spectrum provides the highest output electric power obtained from solar cells made of semiconductors, the band gap of which lies in the range of 1-1.5 eV. Efficiency of conversion of light into electricity, exhibited by a silicon battery, reaches 30 %, efficiency of the nearest analogue, namely, organic solar panels, is at the level of 5-7 %.

Combining of electrical and optical properties in nanostructures of amorphous silicon is crucial to creating devices of the light re-emission. Chemical vapor deposition from the gas phase creates a hydrogenated amorphous thin film with microcrystalline structure, resulting in dense hydrogen plasma or in a high temperature reactor. The problem of increasing efficiency of solar cells (c-Si) consists of two parts: short-wave re-emission of short wave photons in the region of the edge of the visible spectrum through the mechanism of direct optical transitions the area-the zone in monohydride silicon, and an effective generation charge carriers across the entire spectrum of solar radiation. The difficulty is that the drift mobility of the charge is very low in the amorphous silicon structures.

Porous silicon, produced by electrochemical etching of silicon wafers (c-Si) in solutions of hydrofluoric acid, is an interconnected ensemble of silicon nanocrystals. Depending on the pore on the pores size the porous silicon is divided into microporous (< 2 nm), mesoporous (2-50 nm) and macroporous (> 50 nm). Porous silicon has a large effective surface area (200 m^2/cm^3), so the influence of external factors, such as light radiation, can lead to a significant change in the concentration of charge carriers and photoconductivity [1-2].

In this regard, the study of the properties of a-Si:H, control of structural inhomogeneity in the films and the fundamental possibility of stabilization of their properties are of particular importance. The solution to the problem requires in-depth study of the mechanism of recombination in a-Si:H and its relation to the microstructure of the material. In the study of electronic properties of a-Si:H great emphasis should be made on the study of photoconductivity.

2. PHOTOCONDUCTIVITY OF A-SI:H AND A FUNCTION OF STATES DENSITY

Stationary photoconductivity can be determined using the density of free carriers and their mobility, such as:

$$\sigma_{ph} = (n - n_0) \cdot \mu_n \cdot e + (p - p_0) \cdot \mu_p \cdot e \,, \qquad (1)$$

The problem consists in finding the number of free electrons and holes, what is the equation of electro neutrality and the condition of equality of the generation rate and recombination rate in a stationary state.

$$\begin{cases} \sum Q = 0 \\ \dfrac{d\sum Q}{dt} = 0 \end{cases}, \qquad (2)$$

where Q – is the charge in the bulk semiconductor.

Dark, equilibrium concentrations n_0 and p_0 are determined, respectively, as:

$$n_0 = N_c \cdot \exp\left(-\frac{E_c - E_F}{k \cdot T}\right), \qquad (3)$$

$$p_0 = N_v \cdot \exp\left(-\frac{E_F - E_v}{k \cdot T}\right). \qquad (4)$$

View the density of localized states in a-Si:H is shown in Fig. 1. There are the following groups of states that have the same function of employment:

1. The tail state of the valence band and the

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conduction band (CT and VT). The density of states and the ratio of the capture cross section R are reduced exponentially by the middle of the forbidden zone:

$$N_{CT}(E) = N_C^0 \cdot \exp\left(-\frac{E_C - E}{k \cdot T_c}\right), \quad (5)$$

$$N_{VT}(E) = N_V^0 \cdot \exp\left(-\frac{E - E_V}{k \cdot T_V}\right), \quad (6)$$

where $k \cdot T_c$ and $k \cdot T_V$ are the characteristic energies for conduction band and valence band, respectively.

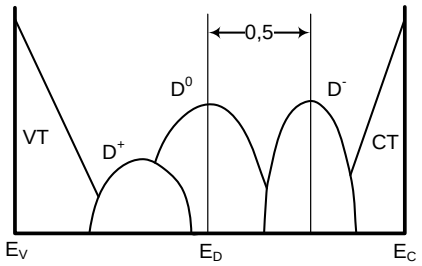

Fig. 1 - Schematic representation of density of localized states in the mobility gap of a-Si:H

2. Condition caused by defects in a type of "dangling bonds" D^0, D^- and D^+, where D^0 – neutral defect, D^- and D^+ – positively and negatively ionized dangling bonds, respectively. The density of states has Gaussian distribution with a peak within the forbidden zone, the energy correlations between states of the D^0 and D^- of the order of 0.4 eV:

$$N_{DB}(E) = \frac{N_t}{\sqrt{2 \cdot \pi \cdot W_1}} \cdot \exp\left(-\frac{(E - E_t)^2}{2 \cdot W_1^2}\right). \quad (7)$$

The D^0 state, the capture of an electron goes into D^- and the capture of a hole – in D^+, and back, respectively.

The electronic states density functions and the amorphous silicon optical absorption functions associated with them, being used in calculations, describe the experimental data insufficiently accurately. That is why the analytical description of the given functions is still current.

The absorption spectrum terminates with a jump in the forbidden zone in a defect of less crystalline semiconductor. The absorption spectrum tail exists in the amorphous semiconductor. The tail presence in the absorption spectrum creates difficulties in the experimental definition of the amorphous semiconductor absorption edge. As a result various empirical methods for estimating the optical spectrum and the tail absorption width were developed. Though these methods facilitate the quantitative analysis of the absorption edge their correspondence to the real physical processes are open to question.

The tails states distribution advances into the forbidden zone in the amorphous semiconductor though distribution of the crystalline semiconductors defects states sharply terminates at the zones edges. The analysis shows that the tails electronic states distributions are localized on the boundaries and there is some critical energy termed as the mobility threshold, which separates the localized states from their extended analogues. These localized states act on numerous unique properties inherent in the amorphous semiconductors [3].

An empirical model for description of the electronic states distribution and definition of the corresponding optical absorption spectrum in the frameworks of this model is used in this work. Establishment of the clear interrelation between the form of the optical absorption spectrum and the form of electronic states distribution based on the presented models is sufficiently urgent.

Distribution of electronic states for the amorphous semiconductors remains true as well as for the crystalline ones. The question about the "states in the forbidden zone" is particularly important both for the extrinsic and own characteristic nature. Absence of the long-range order inherent in the amorphous semiconductors results in the emergence of tails of electronic states of the valence band and conduction band, as this takes place the tails value depends on the degree of disorder. It is rather difficult to derive the expression for the states density due to the lack of data for the atoms equilibrium state (i.e., atom structure), photon spectrum and causes for electronic subsystem excitation. For the amorphous semiconductors it is complicated by their fabrication technology.

At present, a number of theories and models, making it possible to carry out theoretical analysis of the electronic states distribution on the amorphous semiconductors, have been created. Models of Cohen-Fricher-Ovchinkovskyi and Mott-Device [4, 5] are used the most frequently of them. The first one assumes that the tails of the states' density overlap the completely forbidden zone and the states density dependence on the energy is an uninterrupted one. According to the Mott- Device model, the tails of the local states are narrow and they propagate into the forbidden zone for several tenths of electron volt. Moreover, in the proximity to the forbidden zone the presence of the compensated levels zone is supposed, which owes its existence to the defects in the random atomic lattice. These states can manifest themselves both as donors and as acceptors, in this case the conditions of a single-valued or double filling of these states results in formation of two zones divided by the corresponding Hubbard energy. At present, the formation mechanism of the tails electronic states distribution remains unqualified.

To avoid this uncertainty an empirical model of electronic states distribution is advanced, which embraces the main particularities of the material. It is commonly known that the states distribution exhibits the quadratic dependence in the field of the conduction (valent) zone and the exponential dependence in the tail area though the exact form of the tail still causes substantial contradictions. It is also known that the states density function transition between the zone and the field at the tail is smooth. The zones of the tails formation are characterized by the tail width of the conduction zone γ_c and by the tails width of the valent zone γ_v. These parameters of the tails width are the measure of the amorphous silicon disorder. Under conditions of isolation of separate sections of the tails elec-

tronic states distribution and stretching of all zonal states, it is possible to assume that the levels with the energies $E_c+\gamma_c/2$ and $E_t-\gamma_v/2$ represent the thre shold of the conduction zone and valent zone mobility, respectively. Thus, the states' density function for the conduction zone has the form

$$N_c(E)=\frac{\sqrt{2}\cdot m_c^{*3/2}}{\pi^2\cdot\hbar^3}\times\begin{cases}\sqrt{E-E_c}, E\ge E_c+\dfrac{\gamma_c}{2},\\ \sqrt{\dfrac{\gamma_c}{2}}\cdot\exp\left(-\dfrac{1}{2}\right)\cdot\exp\left(\dfrac{E-E_c}{\gamma_c}\right), E<E_c+\dfrac{\gamma_c}{2},\end{cases} \quad (8)$$

where m_c^* – is the effective mass of the electron in the conduction band; E_c – is the energy of the disordered bottom of the conduction band; $E_c+\gamma_c/2$ – is the transaction point between the square and exponential distribution of the states' density of the conduction zone. The states density function for the valent zone has the similar form

$$N_v(E)=\frac{\sqrt{2}\cdot m_v^{*3/2}}{\pi^2\cdot\hbar^3}\times\begin{cases}\sqrt{\dfrac{\gamma_v}{2}}\cdot\exp\left(-\dfrac{1}{2}\right)\cdot\exp\left(\dfrac{E_v-E}{\gamma_v}\right), E\ge V_v-\dfrac{\gamma_v}{2},\\ \sqrt{E_v-E}, E<E_v-\dfrac{\gamma_v}{2},\end{cases} \quad (9)$$

where m_v^* – is the hole effective mass in the valent zone; E_v – is the tail of the valence zone; γ_v – the width

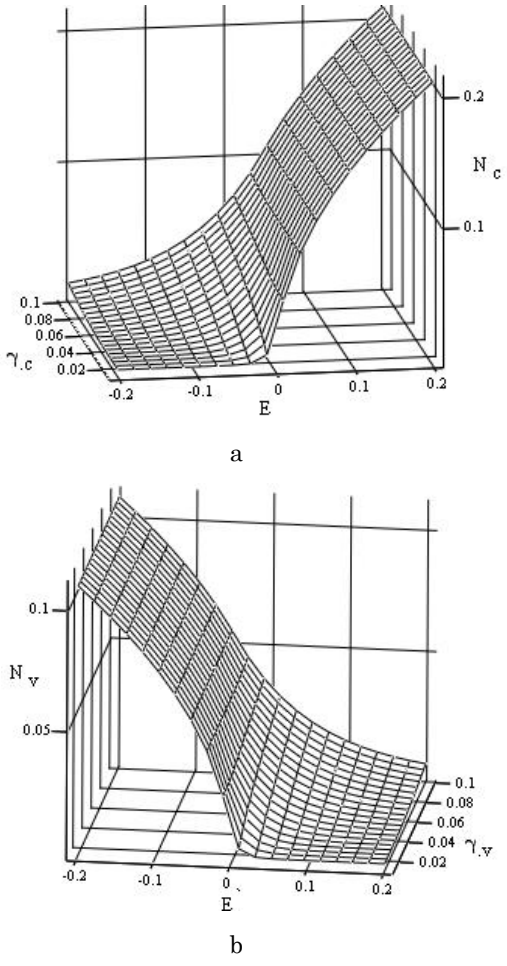

Fig. 2 - Dependence of the density of states for: (a) conduction zone and (b) valence zone

of the tail of the valence zone; $E_t-\gamma_v/2$ – the transition point between the square and the exponential distribution, the density of states of the valence zone.

To study the action of disordering we investigate a sensitivity of the functions of the states' density of the conduction zone and valent zone to variations in γ_c and γ_v. Fig. 2 demonstrates the calculation results. For the specified values of γ_c the distribution of the tails electronic states reveals itself lower than the mobility threshold. With the increase in γ_v, the general number of the chosen tails of electronic states increases and the tails distribution extends to the considerable distance into the forbidden zone.

3. DISTRIBUTION OF ELECTRONIC STATES

The generalized function of states density distribution at low temperatures in the undoped or low-doped amorphous semiconductors can be written as:

$$J(\hbar\cdot\omega)=\int_{-\infty}^{\infty}N_c(E)\cdot N_v(E-\hbar\cdot\omega)dE, \quad (10)$$

In an effort to simplify the calculations a normalized function of the states' density distribution $\xi(\hbar\cdot\omega)$ is introduced

$$\xi(\hbar\cdot\omega)\equiv\frac{\pi^2\cdot\hbar^3}{\sqrt{2}\cdot m_c^{*3/2}}\cdot\frac{\pi^2\cdot\hbar^3}{\sqrt{2}\cdot m_v^{*3/2}}\cdot J(\hbar\cdot\omega), \quad (11)$$

Then the functional dependence for the normalized generalized function of the states' density distribution $\xi(\hbar\cdot\omega)$:

$$\xi(\hbar\cdot\omega)\to\begin{cases}\dfrac{\pi}{8}\cdot(\hbar\cdot\omega-E_c+E_v)^2, \hbar\cdot\omega\ge E_c-E_v,\\ 0, \hbar\cdot\omega<E_c-E_v,\end{cases} \quad (12)$$

where $E_c-E_v=E_{g0}$ – is a bandgap, defined for amorphous semiconductors from the Taus law (Chausovsky bandgap). Analysis of dependences of the normalized generalized function of states density distribution on the photons energy is carried out in two energy bands.

$\hbar\cdot\omega \le E_{g0}+\frac{\gamma_c}{2}+\frac{\gamma_v}{2}$ in addition $\hbar\cdot\omega \ge E_{g0}+\frac{\gamma_c}{2}+\frac{\gamma_v}{2}$. From the equations (1), (2), (5) and (6) are functional

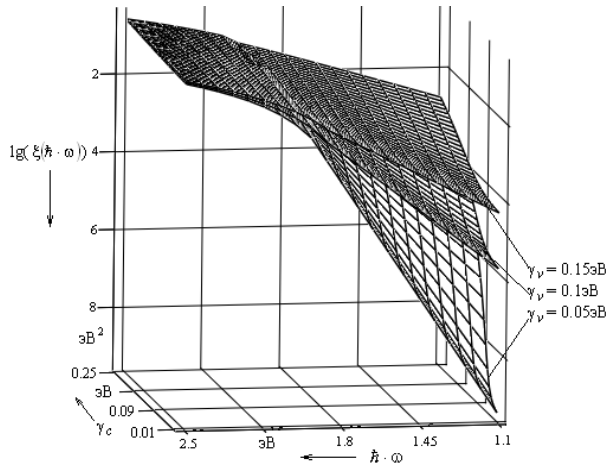

Fig. 3 - Spectral dependences of the normalized generalized function of the states density distribution

dependencies are found for the random values of disorder degrees. Fig. 3 shows the results of calculation of the dependence $\xi(\hbar\cdot\omega)$ for the case γ_c and γ_v. As it follows from the analysis of dependences, the tail of absorption tail of the spectral dependence of the normalized generalized function of the states' density distribution intrudes into the forbidden zone domain and the width of this tail increases with the increase in the disorder degree.

4. CONCLUSION

Therefore, the photoconductivity is provided by the transfer of non-equilibrium charge carriers, the concentration of which is determined by the recombination mechanisms. Interpretation of the results on photoconductivity is reduced to the understanding of recombination processes, which are largely determined by the type and density distribution of these states in the gap of mobility. The presence of a continuous distribution of density of States in the gap of mobility leads to a complex picture of recombination. Thus, the empirical model of the spectral dependence of the normalized generalized function of the states' density distribution for the amorphous silicon taking into account the degree of disorder of its structure is presented in this work. The given model can be used for definition of the electronic states density distribution when describing the optical absorption spectrum of a-Si:H.

Распределение плотности состояний для определения фотопроводимости a-Si:H

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В работе приведена эмпирическая модель спектральной зависимости распределения плотностей электронных состояний, которая охватывает основные особенности аморфного кремния. Показано влияние степени разупорядоченности аморфной структуры на форму и величину хвостов электронных состояний валентной зоны и зоны проводимости. Данные хвосты в запрещенной зоне влияют на многие уникальные свойства аморфных полупроводников. Результаты могут быть применены для оптимизации технологии и моделировании работы многих приборов на основе аморфного кремния (солнечных элементов, транзисторов и др.).

Ключевые слова: Солнечный элемент, Аморфный кремний, Фотопроводимость, Энергетические зоны.

Розподіл щільності станів для визначення фотопровідності a-Si:H

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В роботі наведена емпірична модель спектральної залежності розподілу щільності електронних станів, яка охоплює основні особливості аморфного кремнію. Показано вплив ступеня розупорядкованості аморфної структури на форму і величину хвостів електронних станів валентної зони та зони провідності. Ці хвости в забороненій зоні впливають на багато унікальних властивостей аморфних напівпровідників. Результати можуть бути застосовані для оптимізації технології та моделюванні роботи багатьох приладів на основі аморфного кремнію (сонячних елементів, транзисторів та ін).

Ключові слова: Сонячний елемент, Аморфний кремній, Фотопровідність, Енергетичні зони.

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