The process of charge carrier generation in photosensitive elements based on heterojunction of monocrystalline and amorphous silicon

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Abstract. In this article, to describe the process of charge carrier generation and current transfer, we consider a model for calculating the characteristics of photovoltaic cells based on heterojunctions of amorphous - monocrystalline silicon in the kinetic approximation. Developed the main provisions of a numerical model for the study, based on the statistics of the broken bonds, and physics of photogeneration and sign conclusion nonequilibrium carriers, and the experimental verification of the obtained simulation results. The use of a simplified model of the density of states in the mobility gap of hydrogenated amorphous silicon is substantiated. This model allows to carry out researches of influence of temperature, degree of alloying and the geometrical sizes on characteristics of photoconverters. The generation of current carriers is characterized by the rate of optical generation and for the interpretation of photoconductivity, the following models of recombination are used such as zone-tail, which occurs when a nonequilibrium carrier is captured from the free zone to the tail state of the opposite zone, which has captured the carrier of another sign and acts as a recombination center. The number of tail states increases as the temperature decreases. Tail - broken link recombination occurs when captured carriers are tunneled from the tail zone state to the broken link state. The dependence of the photoconductivity on the temperature of these structures is calculated.
Key words: monocrystalline silicon, amorphous silicon, heterojunction, photoconductivity.

1. Introduction

The end of the twentieth and early twenty-first centuries were marked by large-scale achievements in the development, creation, optimization of optical converters, their electrical parameters and the study of physical phenomena in semiconductor structures based on heterojunctions of amorphous-monocrystalline silicon (a-Si:H) - (C-Si), widely used as materials for the creation of solar photovoltaic energy. The study of such structures is located on the border of different scientific areas, and there are many scientific publications devoted to them. These are papers of foreign scientists: Martin A. Green, Jianhua Zhao, A. I. Shkrebtii, C. B. Honsberg; scientists from Russia: J. I. Alferov, V. G. Budagyan, O. A. Golikova, A. G. Kazansky, M. M. Kazanin; scientists from Ukraine: V. G. Litovchenko, A. M. Gorban, D. I. Levinzon, N. I. Kluy, V. P. Kostylev, V. N. Borschev, G. S. Khripunova, A. V. Sachenko, V. A. Skrichevskiy. It is necessary to develop new semiconductor materials in order to improve the parameters of photovoltaic converters. At the same time, semiconductor structures with high

photoelectric conversion capacity are needed along with low production cost. The importance and timeliness of using such structures is directly related to the increasing energy consumption and trends in the transition from traditional to renewable energy resources, including solar energy. Certain hopes in solving this problem are pinned on the development of technology for photosensitive elements production on the basis of heterostructures amorphous-monocrystal silicon (GAMS). They combine a good photoelectric conversion in amorphous silicon with the possibility of rapid withdrawal of carriers at the heterojunction. The considered semiconductor GAMS structures have promising photo convector parameters in combination with acceptable technological production costs. Insufficiently developed in terms of theory, experiment and technology are the issues related to the physics of processes that affect the formation of broken bonds and the possibility of their compensation, with the withdrawal of non-equilibrium carriers that arose as a result of photogeneration from the amorphous silicon area before their recombination [1, 2].

Must be considered that lack of an in-depth understanding of the physics of the process occurring in the photopreforming structures based on GAMS makes it necessary to conduct numerical and analytical modeling to study the physics of photogeneration and current transfer processes on the basis of broken connections statistics with the conclusion of non-equilibrium carriers, and to conduct experimental verification of the simulation results.

In works [3, 5-7] the dependence of p-type photoconductivity α-Si:H on the doping level and hydrogen concentration with argon-hydrogen plasma and defects in the structure was studied. The studies were carried out using both a numerical model and experimental samples. An energy model of amorphous silicon photoconductivity is proposed. In work [5], the properties and structure of α-Si:H films obtained by the method of silane decomposition (silicon-hydrogen compound) in a high-frequency glow discharge from external influences, including the annealing temperature, were studied. In works [4, 5] a simpler and more cost-effective magnetron sputtering method for thin films of amorphous hydrogenated silicon with similar characteristics is proposed.

The effectiveness of photopleasure equally depends on the characteristics of the film and geometry of the transducers.

The purpose of this work is to develop the basic principles of the numerical model to study the dependence of the photoconductivity of heterojunctions α-Si:H – c-Si and its approbation.

2. Model of current transfer carriers

To solve this problem it is advisable to carry out the calculation in the kinetic approximation. The model proposed in [6, 7, 10-12] supplemented with representations from [4, 5] can be used to describe the processes of carrier transfer in silicon.

Carrier transport in amorphous silicon is described in terms of hopping conductivity for an unordered system with a random field of randomly located charged point centers. The conductivity process is described by media transitions between different localized positions.

The correlation function of an additional random field is represented as [8]:

$$\phi(r) = \frac{2\pi n_t e^4}{\varepsilon^2} r_0 \exp\left(-\frac{r}{r_0}\right), \tag{1}$$

when $r_0 = \left(\dfrac{4\pi n_0 e^2}{\varepsilon T}\right) = \alpha^{-1}$ is the radius of screening, n_t is a concentration of centers, e is the electron charge, ε is the dielectric constant of the exemplar, and $r = r_1 - r_2$ is a distance between two points in the exemplar.

The kinetic equation for amorphous silicon in a stationary positions can be written in the form proposed in [8], rewriting the right part taking into account all the main processes of generation and recombination of current carriers.

$$\frac{\partial f_\lambda}{\partial t}=-\sum_{\lambda'}\left\{W_{\lambda\lambda'}f_\lambda\left(1-f_{\lambda'}\right)-W_{\lambda\lambda'}f_{\lambda'}\left(1-f_\lambda\right)\right\},$$

when f_λ - the diagonal element is non-equilibrium one-particle density matrix, $W_{\lambda\lambda'}$ - probability of transition between positions λ and λ'. The probability of scattering corresponding to different types of transitions is determined through the scattering cross sections.

This equation describes the evolution of the diagonal part of the density matrix, and in the localized positions it describes the balance of electronic transitions between different positions. The probability of jumps between different pairs of centers varies randomly and in a wide range. As a result of changes in population conditions, the easiest directions of jumps can be blocked.

Current carrier generation is characterized by the rate of optical generation. The following models of recombination are used for the interpretation of photoconductivity:

1) recombination of "zone - tail" occurs when the capture of nonequilibrium media of the free zone on the condition of the tail opposite the zone, seized the front of this carrier other character, and acting as a recombination center. The number of tail positions increases as the temperature decreases;

2) recombination "tail - dangling bonds" occurs when the tunneling of the captured carriers from the condition of the tailings areas in the state of dangling bonds;

3) tail -to-tail recombination is a tunneling recombination between electrons trapped in the tail positions of the conduction band and holes trapped in the tail states of the valence band.

In [8] it is shown that in reality it is necessary to take into account all possible mechanisms of recombination and to allocate from them the basic depending on a spectrum of carriers positions, type and concentration of defects, external conditions (temperature, light intensity, etc.).

When describing the processes of carriers recombination and their capture to the appropriate traps, you can use the model proposed in [8, 9], supplementing it with the concepts described in [8].

The density of positions in disordered semiconductor at $|E|\gg\sqrt{\psi_1}$ [9]:

$$\rho(E)=\frac{\psi_1\exp\left(-\dfrac{E^2}{2\psi_1}\right)}{2\pi^2|E|^{3/2}}+\frac{\alpha\cdot\exp\left(-\dfrac{E^2}{2\psi_1}\right)}{8\sqrt{2}\pi^{3/2}\sqrt{\psi_1}}\left(E-\frac{\alpha|E|^{3/2}}{\sqrt{2\pi\psi_1}}\right),\tag{2}$$

when $\psi_1=2\pi n_t e^4 r_0/\varepsilon^2$, E - energy of positions, $\alpha^{-1}=r_0$ - characteristic length, the role of which is played by the radius of the shield.
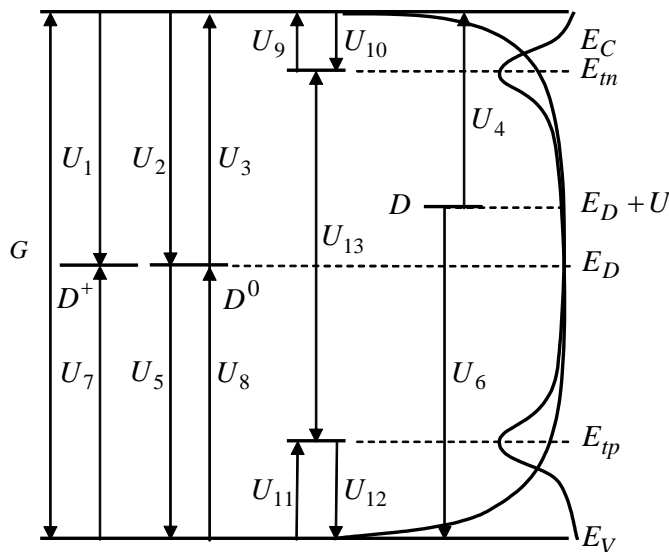

Figure 1. Schematic representation of electronic transitions for a simplified state density model and a view of the state density in the mobility gap.

Calculations are carried out for a simplified model of the density of positions in the mobility gap, consisting of four discrete levels. Levels E_{tp} and E_{tn} with density of positions N_{tp} and N_{tn} - effective tail levels of the valence band and conduction band respectively. Levels E_D and $E_D + U$ - energy levels of positions of dangling bonds.

We consider the positions of the zone tails as small traps in thermodynamic equilibrium with the nearest zone, i.e. "traps for holes" and "traps for electrons". This simplified representation of the density of positions in the mobility gap, as shown in [5], does not lead to qualitative changes in the results of numerical calculation.

Determining the probability of finding the D-center in the state D^+, D^0 and D^- how , f^+, f^0 and f^- accordingly. Because the D-center can only be in three positions $f^+ + f^0 + f^- = 1$. You can record on the basis of the formalism of Shockley-Reeda[8]:

$$U_1 = nN_D f^+ c_n^+, \quad U_2 = nN_D f^0 c_n^0, \quad U_3 = N_D f^0 e_n^0, \quad U_4 = N_D f^- e_n^-, \quad U_5 = pN_D f^0 c_p^0,$$

$$U_6 = pN_D f^- c_p^-, \quad U_7 = N_D f^+ e_p^+, \quad U_8 = N_D f^0 e_p^0, \quad U_9 = nN_{tn}\left(1 - f_{tn}\right)c_{tn}, \tag{3}$$

$$U_{10} = N_{tn} f_{tn} e_{tn}, \quad U_{11} = pN_{tp} f_{tp} c_{tp}, \quad U_{12} = N_{tp}\left(1 - f_{tp}\right)e_{tp}, \quad U_{13} = N_{tp} f_{tp} N_{tn} f_{tn} T_{np},$$

when c_n^0 and c_n^+ - the coefficients of electron capture on D^0 - and D^+ - position; c_p^0 and c_p^- - the coefficients of capture of holes on D^0 - and D^- - position; e_n^0, e_n^-, e_p^0 and e_p^+ - coefficients of thermal emission of electrons from D^0 - and D^- - position and holes of D^0 - and D^+ - position; f_{tn}, f_{tp} - the probability of filling of traps for electrons and holes; c_{tn}, c_{tp} and e_{tn}, e_{tp} - the capture coefficients of electrons and holes at the respective traps, and heat release of these; N_D - concentration D-centers; T_{np} - the ratio of the tunneling recombination «tail - tail».

The increase in electron density in the conduction band is due to optical generation G and transitions U_3, U_4, U_{10}. The decrease of the density due to the transitions U_1, U_2 and U_9. It can be written that the change in the concentration of conduction electrons:

$$\frac{\partial n}{\partial t} = G - U_1 - U_2 + U_3 + U_4 - U_9 + U_{10}. \tag{4}$$

Similarly, it can be written for the density of holes in the valence band and the filling density of the levels: E_{tn}, E_{tp} and D:

$$\frac{\partial p}{\partial t} = G - U_5 - U_6 + U_7 + U_8 - U_{11} + U_{12},$$

$$\frac{\partial\left[N_{tn} f_{tn}\right]}{\partial t} = U_9 - U_{10} - U_{13}, \qquad \frac{\partial\left[N_{tp} f_{tp}\right]}{\partial t} = U_{11} - U_{12} - U_{13},$$

$$\frac{\partial\left[N_D f^+\right]}{\partial t} = U_3 + U_5 - U_1 - U_7. \tag{5}$$

These relations allow us to determine the probability of generation and recombination of carriers included in the right part of the kinetic equation.

The kinetic equation in the nonstationary state can be written for the distribution function of carriers in the following f form:

$$\frac{\partial f_\lambda}{\partial t}+\left(\vec{v}\vec{\nabla}_r f_\lambda\right)+\frac{1}{\hbar}\left(\vec{F}_i\vec{\nabla}_k f_\lambda\right)=\left(\frac{\partial f}{\partial t}\right)_i-\sum_{\lambda'}\left\{W_{\lambda\lambda'}f_\lambda\left(1-f_{\lambda'}\right)-W_{\lambda\lambda'}f_{\lambda'}\left(1-f_\lambda\right)\right\}$$

when $\vec{v}_i$ - charge carrier speed e_i, $\vec{F}_i$ - force, acting on the charge from the external electromagnetic field and other charge carriers, $\left(\frac{\partial f}{\partial t}\right)_i$ – collision integral, ρ – bulk charge density of ions in the sample, $\sum_i e_i \int f_i d\vec{v}_i$ - density of the volume charge generated by free current carriers.

Force $\vec{F}_i$ is electric and can be defined as the field gradient which is the solution of the Poisson equation:

$$\Delta\phi=-\frac{1}{\varepsilon}(\rho(\vec{r})-\sum_i e_i \int f_i d\vec{v}_i)$$

with the addition of a random field (1).

The method of solving the above system of equations is described in detail in the works [6, 7].

3. Results of numerical calculations

To compare the efficiency of GAMS and amorphous silicon structures, such characteristics as VAC were used. The developed software package made it possible to obtain numerically the VAC of the studied samples. In the course of numerical experiments using the proposed method, light load VAC for structures based on GAMS (Fig.2, curve 2) when illuminated by monochromatic light with a quantum energy of 1.85 eV (0.67 μm)and intensity of 1017 sm^{-2}·s^{-1} and structures of amorphous silicon grown on glass with the same irradiation parameters (Fig.2, curve 1). In the case of a lighted transition (Fig.2, curve 2) at negative voltage, the current is significantly different from zero. The increase in the back branch of the VAC in the case of GAMS is due to the retraction of the photoconductivity electrons in the p-region of monocrystalline silicon.
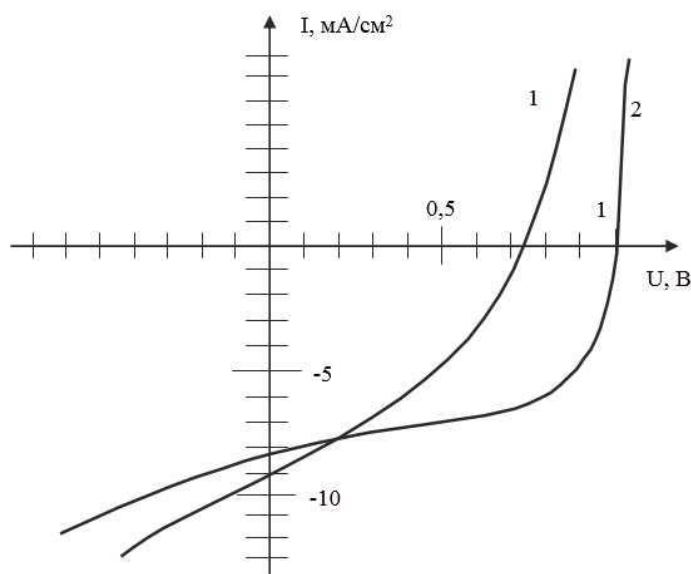

Figure 2. Light load VAC of amorphous structure (1) and GAMS-based structure (2).

Comparative analysis of these curves in Figure 2 allows you to set the share of generated carriers in the total current. Using numerically obtained VAC, the efficiency was calculated in GAMS, while it was possible to achieve an increase in efficiency up to 15%. From the curve comparison in Fig.2 shows that the GAMS photogrammetrists better performance amorphous structure.

The model parameters were chosen in accordance with the literature data and data obtained from experimental studies [4, 5]. The calculation was carried out for amorphous silicon with different degree of hydrogenation. The width of the mobility slit was taken to be 1.8 eV. The position of the Fermi level relative to the ceiling of the valence band was set to 1.05 eV. For the parameters of broken links the following values were taken: $E_D = 0.9\,\text{eV}$, $U = 0.3\,\text{eV}$. The rate of photogeneration was taken to be equal to $G = 10^{19}\,\text{sm}^{-3}\text{s}^{-1}$, $c_n^0 = c_p^0 = 3 \cdot 10^{-15}\,\text{sm}^{-2}$ and $c_n^+ = c_p^- = 1.5 \cdot 10^{-13}\,\text{sm}^{-2}$.

The calculation was carried out for conductivity in the region of low external field stresses up to 3 kV/cm. For fig.3 the results of numerical simulation of thermal conductivity for different values of hydrogen concentration are presented.

The results of modeling the specific conductivity dependences are in good agreement with the experimental data.
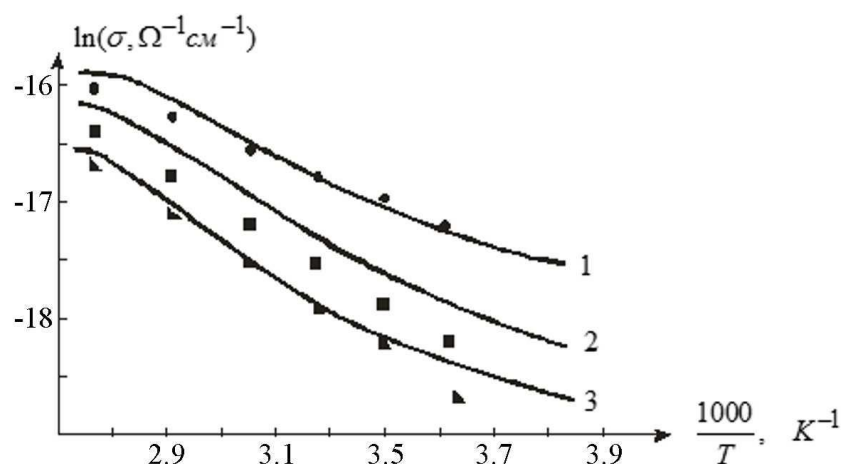

Figure 3. The thermal dependence of the calculated (solid lines) and experimental (points) conductivity a-Si films obtained by magnetron sputtering method at a concentration of hydrogen: 1 - 10%, 2 – 30%, 3- 40%.

4. Conclusion

In this paper, the basic principles of the model to study the dependence of the photoconductivity of heterojunctions α-Si:H – c-Si in the kinetic approximation are developed. The use of a simplified model of the positions density in the mobility gap of hydrogenated amorphous silicon is justified. This model allows us to study the effect of temperature, doping degree and geometric dimensions on the characteristics of the photoconverters.

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