Journal of Nano- and Electronic Physics
Vol. **13** No 6, 06010(5pp) (2021)

Журнал нано- та електронної фізики
Том **13** № 6, 06010(5cc) (2021)

Distribution of Excess Charge Carriers in Bilateral Macroporous Silicon with Different Thicknesses of Porous Layers

V.F. Onyshchenko*

V.Ye. Lashkaryov Institute of Semiconductor Physics of National Academy of Sciences of Ukraine, 41, Nauky Ave, 03028 Kyiv, Ukraine

(Received 07 October 2021; revised manuscript received 01 December 2021; published online 20 December 2021)

The paper presents a system of equations describing the distribution of excess charge carriers in bilateral macroporous silicon with different thicknesses of porous layers. The system contains equations, which are the general solution to the diffusion equation written for a monocrystalline substrate and each porous layer. Also, it contains equations describing the boundary conditions on two surfaces of a bilateral macroporous silicon sample and on the boundaries of a monocrystalline substrate with macroporous layers. It was taken into account that light propagates through the pores and illuminates the monocrystalline substrate through the bottom of the pores. We calculated the distribution of excess charge carriers in bilateral macroporous silicon with different thicknesses of porous layers, provided that excess charge carriers are generated by light with wavelengths of 0.95 and 1.05 μm. At these wavelengths, the generation of excess charge carriers was uniform and non-uniform over the sample, respectively. The calculations were carried out for the cases when one layer of macropores had a thickness of 100 μm, while the other varied from zero to 400 μm. It is shown that one or two maxima are observed in the distribution of excess charge carriers in bilateral macroporous silicon with different thicknesses of porous layers. The maximum can be located near surfaces that are illuminated by light or in the middle of a monocrystalline substrate. The maxima decrease due to the diffusion of charge carriers to the recombination surfaces. The distribution of excess charge carriers in bilateral macroporous silicon with different thicknesses of porous layers is affected by the recombination of excess charge carriers on the pore surface of each macroporous layer and the diffusion of excess charge carriers from the substrate to the recombination surfaces in porous layers.

Keywords: Bilateral macroporous silicon, Porous silicon, Excess charge carriers.

DOI: 10.21272/jnep.13(6).06010 PACS number: 73.50.Pz

1. INTRODUCTION

Macroporous silicon is used in biological sensors, chemical sensors, photodetectors, integrated chips, and solar cells. Macroporous silicon has found applications in solar cells because it absorbs light efficiently by absorbing and scattering it in the pores. In a solar cell, the pores are located on one or both sides. Solar cells with a structured surface are characterized by optical and electrical parameters. The relationship between the pore size, the distance between pores in the macroporous layer and the absorption of light is calculated, thereby optimizing the optoelectrical parameters of the solar cell [1, 2]. Short-circuit current, open-circuit voltage and phototransformation efficiency in high-performance textured silicon solar cells are analytically calculated and modelled [3]. The simulation and optimization take into account the nonradiative Auger recombination of excitons and the recombination of excess charge carriers in the space charge region. A simple phenomenological expression is used to calculate the quantum efficiency of a textured silicon solar cell in the long wavelength part of the absorption spectrum. The dependence of the phototransformation efficiency on the thickness of the solar cell is calculated [4]. The surface of macroporous silicon is passivated by thermal oxidation. The thickness of silicon oxide on the surface of macropores is increased to improve passivation and decrease the relaxation time of photoconductivity in macroporous silicon [5]. The relaxation time of photoconductivity in macroporous silicon with one layer of macropores is determined from a system of two equations. The diffusion model of photoconductivity relaxation takes into account the diffusion equations both in the monocrystalline substrate and in the effective medium of the macroporous layer, as well as the boundary conditions written for the surfaces of the macroporous silicon layer and the monocrystalline substrate. The relaxation time of photoconductivity in one-sided macroporous silicon rapidly decreases with an increase in the macropore depth from zero to 25 μm and a decrease in the thickness of a monocrystalline substrate from 250 μm to zero [6]. The relaxation of photoconductivity in a sample of macroporous silicon is determined by the diffusion of charge carriers to the recombination surfaces in the pores. This is confirmed by experimental measurements of the kinetics of photoconductivity in macroporous silicon at temperatures from 100 to 300 K [7]. The effective lifetime of minority charge carriers in bilateral macroporous silicon is determined from a system of two equations. The system of equations was found by solving the diffusion equation written for excess charge carriers in a monocrystalline substrate and macroporous layers. The boundary conditions on the surface of the macroporous silicon sample and at the interface between the monocrystalline substrate with each macroporous layer are also taken into account. The effective lifetime of minority carriers in bilateral macroporous silicon is calculated as a function of the macropore depth. To check the accuracy of the calculations, a numerical method is used [8]. The photoconductivity of macroporous silicon depends on the an-

* onyshchenkovf@isp.kiev.ua

gle of incidence of light. Light is reflected and absorbed by the walls of the macropores and is also scattered at the bottom of the macropores. Scattered light has a longer optical path and is better absorbed at the corresponding wavelengths [9]. If the wavelength of light incident on a porous silicon sample is comparable to the average distance between macropores, then the light is reflected from macropores as from an effective medium. The effective medium of porous silicon has a lower effective refractive index than silicon due to air in the pores; therefore, the reflection from porous silicon will be less than from the surface of a single crystal [10].

The aim of this work is to calculate and study the distribution of minority charge carriers in bilateral macroporous silicon with different thicknesses of porous layers depending on the thickness of each macroporous layer and to reveal the features of the distribution of minority charge carriers associated with illumination of the bottom of the pores and diffusion of charge carriers.

2. DIFFUSION MODEL OF EXCESS CHARGE CARRIER DISTRIBUTION IN BILATERAL MACROPOROUS SILICON

Consider a bilateral macroporous silicon wafer. Let one side of the bilateral macroporous silicon wafer be illuminated with light. The side of the plate that is illuminated by light will be called the front side of the bilateral macroporous silicon sample; the other side will be called the back side. The layer of macroporous silicon, on which the light is incident, will be called the frontal macroporous layer, and the other layer will be called the back macroporous layer. We select the origin of coordinates on the front side of the sample. The x axis is directed to the depth of the pores of the frontal macroporous layer. The pores of the frontal macroporous layer have the same direction as the back macroporous layer. The general solution of the diffusion equation under stationary conditions in bilateral macroporous silicon in the x direction is written as:

$$\delta p_1(x) = C_1\cosh(X_1) - C_2\sinh(X_1) - \delta p_{g1}(x), \quad (2.1)$$

$$\delta p_2(x) = C_3\cosh(X_2) - C_4\sinh(X_2) - \delta p_{g2}(x), \quad (2.2)$$

$$\delta p_3(x) = C_5\cosh(X_3) - C_6\sinh(X_3) - \delta p_{g3}(x). \quad (2.3)$$

Here $\delta p_1(x)$, $\delta p_2(x)$, $\delta p_3(x)$, $X_1 = x/L_1$, $X_2 = x/L_2$, $X_3 = x/L_3$, $L_1 = \sqrt{D_p\tau_1}$, $L_2 = \sqrt{D_p\tau_2}$, $L_3 = \sqrt{D_p\tau_3}$, τ_1, τ_2, τ_3 are the concentration, dimensionless coordinate, diffusion length and the bulk lifetime of excess minority charge carriers in the frontal macroporous layer, monocrystalline substrate and back macroporous layer, respectively, C_i ($i = 1, 2, \ldots, 6$) are constants. The bulk lifetime of charge carriers in macroporous layers is effective [8]. Here $\delta p_{g1}(x) = g_0\alpha\tau_1\exp(-\alpha x)/((\alpha L_1)^2 - 1)$, $\delta p_{g2}(x) = g_0\alpha\tau_2 E(x)/((\alpha L_2)^2 - 1)$, $\delta p_{g3}(x) = g_0\alpha\tau_3 E(x)/((\alpha L_3)^2 - 1)$, $E(x) = (1 - P_1)\exp(-\alpha x) + P_1\exp(-\alpha x(x - h_1))$ are the surface generation velocity of excess minority charge carriers on the surface of the bilateral macroporous silicon sample, on the monocrystalline substrate, and on the monocrystalline substrate with a back macropoporous layer, respectively, $P_1 = \pi D_{por1}{}^2/(4a_1{}^2)$ is the pore volume fraction, h_1, D_{por1}, a_1 are the pore depth, pore diameter and the distance between the pore centers of the frontal macroporous layer, respectively. Constants C_i ($i = 1, 2, \ldots, 6$) are found from a system of equations that describes the boundary condition written at the boundary of porous layers with a monocrystalline substrate and at the boundaries of the sample. The boundary condition on the front surface of the sample is written as:

$$\frac{dp_1}{dx}(0) = s_1 p_1(0). \quad (2.4)$$

The boundary condition written at the boundary of the frontal porous layer with a monocrystalline substrate:

$$(1 - P_1)\frac{dp_1}{dx}(h_1) = \frac{dp_2}{dx}(h_1) - \frac{P_1}{D}s_{por1}p_2(h_1). \quad (2.5)$$

The boundary condition at the boundary of a monocrystalline substrate with a back macroporous layer:

$$(1 - P_2)\frac{dp_3}{dx}(h - h_2) = \frac{dp_2}{dx}(h - h_2) - \frac{P_2}{D}s_{por2}p_2(h - h_2). \quad (2.6)$$

The boundary condition on the back surface of the sample is written as:

$$\frac{dp_3}{dx}(h) = s_2 p_3(h). \quad (2.7)$$

The concentration of excess minority charge carriers should not have a discontinuity at the boundary of the front porous layer with a monocrystalline substrate:

$$p_1(h_1) = p_2(h_1). \quad (2.8)$$

The concentration of excess minority charge carriers should not have a discontinuity at the boundary of a monocrystalline substrate with a back porous layer:

$$p_2(h - h_2) = p_3(h - h_2), \quad (2.9)$$

where $P_2 = \pi D_{por2}{}^2/(4a_2{}^2)$ is the pore volume fraction, h_2, D_{por2}, a_2 are the pore depth, pore diameter and the distance between the pore centers of the back macroporous layer, respectively.

The system of equations (2.4)-(2.9) has an exact solution; it can also be solved numerically.

3. DISTRIBUTION OF EXCESS CHARGE CARRIERS VERSUS THE PORE DEPTH OF THE FRONTAL MACROPOROUS LAYER

To calculate the distribution of excess charge carriers, the following parameters of bilateral macroporous silicon were used: the thickness of the macroporous silicon sample is 500 μm, the bulk lifetime in the monocrystalline silicon substrate is 10 μs, the other parameters characterize macroporous layers. We took the same parameters in each macroporous layer. The average diameter of macropores is 1 μm. The average distance between the pore centers is 2 μm. The effective bulk lifetime in both layers of macroporous silicon is 1 μs. The surface recombination velocity on the sample surface and on the pore surface is 1 m/s. Due to the fact that light falls on the surface of macroporous silicon parallel to the pores, it propagates through the pores and illuminates the surface of the bottom of the pores.

The distributions of the concentration of excess minority charge carriers in bilateral macroporous silicon versus the pore depth of the frontal macroporous layer, when light with a wavelength of 0.95 and 1.05 μm generates excess charge carriers, are shown in Fig. 1 and Fig. 2, respectively. The pore depth of the back macroporous layer is 100 μm. The pore depth of the frontal macroporous layer varies from zero, that is, there are no pores on the front surface of the sample, up to 400 μm, that is, the pores in the porous silicon sample are through. The distribution of the excess minority charge carrier concentration has a maximum, which is located on the front side of the sample if there are no pores on the front side of the macroporous silicon sample, as shown in Fig. 1. As shown in Fig. 1 and Fig. 2, the concentration of excess minority charge carriers in the back macroporous layer sharply decreases due to the fact that the recombination of excess charge carriers occurs on the pore surface. The concentration gradient of excess charge carriers, which arises due to the different concentration of excess charge carriers in the monocrystalline substrate and the back macroporous layer, generates the charge carrier current. The current transfers charge carriers to the recombination surfaces and reduces the difference in charge carrier concentration between the monocrystalline substrate and the back macroporous layer. The concentration of excess minority charge carriers on the frontal surface of the sample decreases with increasing pore depth from zero to 100 μm (Fig. 1), and then it does not change. When it stops changing, two maxima in the distribution function of the concentration of excess minority charge carriers are observed (Fig. 1). The maxima in the distribution of charge carriers are observed on the front surface of the sample and on the monocrystalline substrate, as shown in Fig. 1. The first maximum in the distribution of the concentration of excess minority charge carriers in the sample of bilateral macroporous silicon, which is observed on the front surface of the sample, exceeds the second maximum, when the pore depth of the frontal macroporous layer is greater than 100 μm. The second maximum in the distribution of the concentration of excess minority charge carriers in the bilateral macroporous silicon sample gradually decreases and disappears when the pores of the frontal and back macroporous layers join and become through in the sample of macroporous silicon.

The concentration distribution of excess minority charge carriers in bilateral macroporous silicon has one maximum, which is located in the middle of the monocrystalline substrate, when light with a wavelength of 1.05 μm generates excess charge carriers (Fig. 2). The maximum is observed for the pore depth of the frontal macroporous layer less than 200 μm and for through pores (the pore depth of the frontal macroporous layer is 400 μm). Two maxima in the distribution of the concentration of excess minority charge carriers are observed when the pore depth changes from 200 to 399 μm (Fig. 2). Two maxima in the distribution function of the concentration of excess minority charge carriers are observed when the depth of light penetration into silicon is comparable to the pore depth of the frontal macroporous layer. The presence of pores in macroporous silicon causes the incidence of light on the surface of the bottom of the pores, which creates an additional generation of excess charge carriers in the monocrystalline substrate. In addition, the concentration of excess minority charge carriers in the monocrystalline substrate is higher than in macroporous layers due to the fact that the bulk lifetime of minority charge carriers in the monocrystalline substrate is longer than the effective bulk lifetime of minority carriers in the frontal and back macroporous layers. A decrease in the generation of excess charge carriers in the monocrystalline substrate and diffusion of charge carriers from the monocrystalline substrate into the frontal macroporous layer creates a maximum of the distribution of excess charge carriers in the monocrystalline substrate, near the bottom of the pores of the frontal macroporous layer.

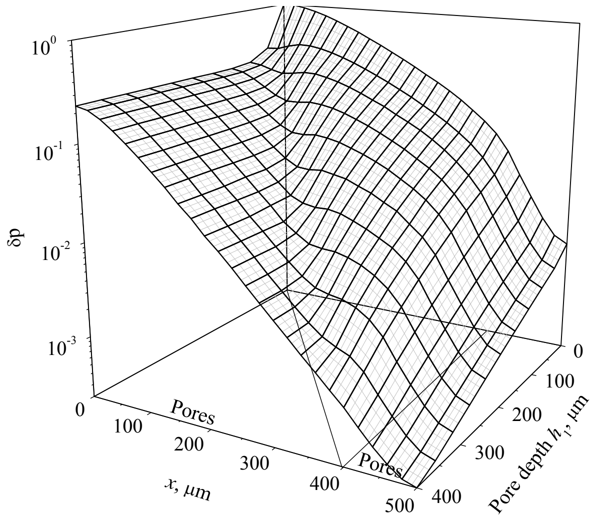

Fig. 1 – Distribution of the excess minority carrier concentration versus the pore depth of the frontal macroporous layer, when light with a wavelength of 0.95 μm generates excess charge carriers

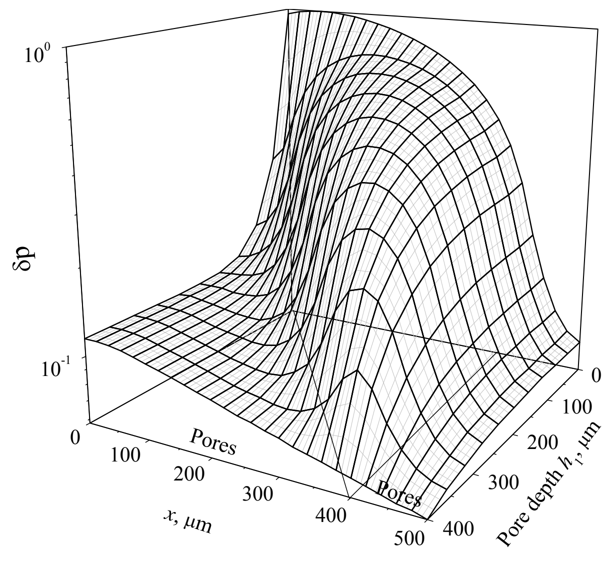

Fig. 2 – Distribution of the excess minority carrier concentration versus the pore depth of the frontal macroporous layer, when light with a wavelength of 1.05 μm generates excess charge carriers

4. DISTRIBUTION OF EXCESS CHARGE CARRIERS VERSUS THE PORE DEPTH OF THE BACK MACROPOROUS LAYER

The distributions of the excess minority carrier concentration in bilateral macroporous silicon on the pore depth of the back macroporous layer, when light with wavelengths of 0.95 and 1.05 μm generates excess charge carriers, are shown in Fig. 3 and Fig. 4, respectively. For the calculation, we used the following parameters of the bilateral macroporous silicon sample: the thickness of the sample of macroporous silicon is 500 μm, the bulk lifetime in the monocrystalline silicon substrate is 10 μs. The parameters are the same in each macroporous layer. The average diameter of macropores is 1 μm. The average distance between the pore centers is 2 μm. The effective bulk lifetime in both layers of macroporous silicon is 1 μs. The surface recombination velocity on the surface of the macroporous silicon sample and on the surface of the pores of the frontal and back macroporous layers is 1 m/s. The pore depth of the frontal macroporous layer is 100 μm. The pore depth of the back macroporous layer varies from zero, that is, there are no pores on the back surface of the sample, up to 400 μm, that is, the pores in the porous silicon sample are through. The concentration of excess minority charge carriers on the front surface of the bilateral macroporous silicon sample does not change (Fig. 3), when light with a wavelength of 0.95 μm generates excess charge carriers. The concentration of excess minority charge carriers on the back surface of the bilateral macroporous silicon sample sharply decreases when the pore depth of the back macroporous layer changes from zero to 300 μm. When the pore depth of the back macroporous layer changes from 300 to 400 μm, the concentration of excess minority charge carriers does not change (Fig. 3). In the distribution of the concentration of excess minority charge carriers, two maxima are constantly observed. The maxima in the distribution of charge carriers are observed on the front surface of the sample and on the monocrystalline substrate, as shown in Fig. 3. The concentration distribution of excess minority charge carriers has one maximum, when there are through pores in the sample of macroporous silicon (Fig. 3 and Fig. 4).

Fig. 4 shows that the concentration of excess minority charge carriers on the front surface of the sample changes little when light with a wavelength of 1.05 μm generates excess charge carriers. The concentration of excess minority charge carriers on the back surface of the bilateral macroporous silicon sample sharply decreases when the pore depth of the back macroporous layer changes from zero to 200 μm, and then it does not change (Fig. 4). One maximum is constantly observed in the distribution of the excess minority carrier concentration. The maximum located in the middle of the monocrystalline substrate is constantly shifting due to the fact that the thickness of the monocrystalline substrate decreases as the pore depth of the back macroporous layer increases (Fig. 4). When the pore depth of the back macroporous layer is 400 μm, the pores of the frontal and back macroporous layers are connected, that is, they become through for the macroporous silicon sample; we observe one maximum, which is located on the front surface of the bilateral macroporous silicon sample.

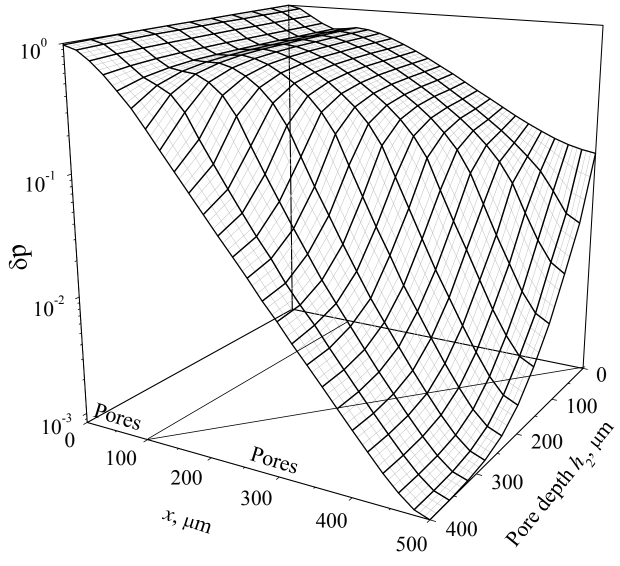

Fig. 3 – Distribution of the concentration of excess minority charge carriers versus the pore depth of the back macroporous layer, when light with a wavelength of 0.95 μm generates excess charge carriers

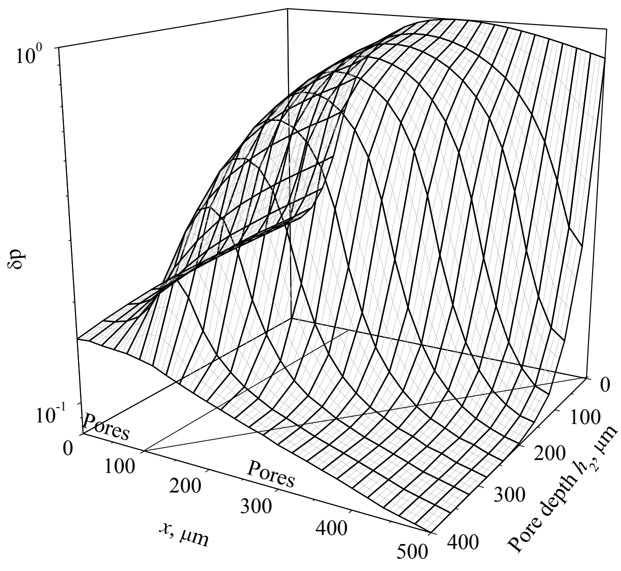

Fig. 4 – Distribution of the concentration of excess minority charge carriers versus the pore depth of the back macroporous layer, when light with a wavelength of 1.05 μm generates excess charge carriers

5. CONCLUSIONS

In the distribution of the excess minority carrier concentration in bilateral macroporous silicon with different thicknesses of macroporous layers, two maxima are observed. One maximum is located on the front surface of the sample, and the second is on the monocrystalline substrate. The maximum on the monocrystalline substrate is located near the boundary of the substrate with the frontal macroporous layer, in the case when the sample is illuminated with light with a wavelength of 0.95 μm, and in the middle of the monocrystalline substrate, in the case when the sample is illuminated with light with a wavelength of 1.05 μm.

In the distribution of the concentration of excess charge carriers in the sample of bilateral macroporous silicon on the pore depth of the back macroporous layer, one maximum is observed when the sample is illuminated with light with a wavelength of 1.05 μm.

A decrease in the generation of excess charge carriers in the monocrystalline substrate and the diffusion of excess charge carriers from the substrate into the frontal macroporous layer creates a maximum of the distribution of excess charge carriers in the substrate, on the surface of the bottom of the pores of the frontal macroporous layer.

A decrease in the generation of excess charge carriers in the frontal macroporous layer and the diffusion of charge carriers from the front surface of the sample into the depth of the frontal macroporous layer create a maximum of the distribution of excess charge carriers near the front surface of the sample. Recombination of excess charge carriers on the sample surface and on the pore surface of the frontal macroporous layer reduces the maximum of the distribution of excess charge carriers in the frontal macroporous layer.

REFERENCES

1. J.R. Maiolo, H.A. Atwater, N.S. Lewis, *J. Phys. Chem. C* **112** No 15, 6194 (2008).
2. M. Ernst, R Brendel, *IEEE J. Photovolt.* **3** No 2, 723 (2013).
3. A.V. Sachenko, V.P. Kostylyov, R.M. Korkishko, V.M. Vlasyuk, I.O. Sokolovskyi, B.F. Dvernikov, V.V. Chernenko, M.A. Evstigneev, *Semiconductor Physics, Quantum Electronics and Optoelectronics* **24** No 2, 175 (2021).
4. A.V. Sachenko, V.P. Kostylyov, R.M. Korkishko, V.M. Vlasiuk, I.O. Sokolovskyi, B.F. Dvernikov, V.V. Chernenko, M.A. Evstigneev, *Semiconductor Physics, Quantum Electronics and Optoelectronics* **24** No 3, 319 (2021).
5. L. Karachevtseva, M. Kartel, V Kladko, O. Gudymenko, Wang Bo, V. Bratus, O. Lytvynenko, V Onyshchenko, O. Stronska, *Appl. Surf. Sci.* **434**, 142 (2018).
6. V.F. Onyshchenko, L.A. Karachevtseva, M.I. Karas', *Emerg. Sci. J.* **4** No 3, 192 (2020).
7. L.A. Karachevtseva, V.F. Onyshchenko, A.V. Sachenko, *Ukr. J. Phys.* **53** No 9, 874 (2008).
8. V.F. Onyshchenko, L.A. Karachevtseva, *Semiconductor Physics, Quantum Electronics & Optoelectronics* **23** No 1, 29 (2020).
9. L. Karachevtseva, M. Karas', V. Onishchenko, F. Sizov, *Proc. SPIE* **5360**, 381 (2004).
10. P.O. Gentsar, A.V. Stronski, L.A. Karachevtseva, V.F. Onyshchenko, *Phys. Chem. Solid State* **22** No 3, 453 (2021).

Розподіл нерівноважних носіїв заряду в двосторонньому макропористому кремнії з різною товщиною пористих шарів

В.Ф. Онищенко

Інститут фізики напівпровідників імені В.Є. Лашкарьова НАН України, пр. Науки, 41, 03028 Київ, Україна

У роботі представлена система рівнянь, яка описує розподіл надлишкових носіїв заряду в двосторонньому макропористому кремнії з різною товщиною пористих шарів. Система містить рівняння, які є загальним розв'язком рівняння дифузії, записаного для монокристалічної підкладки та кожного з пористих шарів. Також вона містить рівняння, які описують граничні умови на двох поверхнях зразка двостороннього макропористого кремнію та на межах монокристалічної підкладки з макропористими шарами. Враховується, що світло розповсюджується по порах та освітлює монокристалічну підкладку через дно пор. Ми розрахували розподіл надлишкових носіїв заряду в двосторонньому макропористому кремнії з різною товщиною пористих шарів за умови, коли надлишкові носії заряду генеруються світлом з довжиною хвилі 0,95 мкм та 1,05 мкм. При цих довжинах хвиль генерація надлишкових носіїв заряду була однорідною та неоднорідною по зразку, відповідно. Розрахунки проводились для випадків, коли один шар макропор мав товщину 100 мкм, а інший змінювався від нуля до 400 мкм. Показано, що в розподілі надлишкових носіїв заряду в двосторонньому макропористому кремнії з різною товщиною пористих шарів спостерігаються один або два максимуми. Максимум може розташовуватися біля поверхонь, які освітлюються, або посередині монокристалічної підкладки. Максимуми зменшуються завдяки дифузії носіїв заряду до рекомбінаційних поверхонь. На розподіл надлишкових носіїв заряду в двосторонньому макропористому кремнії з різною товщиною пористих шарів впливає рекомбінація надлишкових носіїв заряду на поверхні пор кожного макропористого шару та дифузія надлишкових носіїв заряду з підкладки до рекомбінаційних поверхонь в пористих шарах.

Ключові слова: Двосторонній макропористий кремній, Пористий кремній, Надлишкові носії заряду.