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MODELING OF PHOTOCONDUCTIVITY OF POROUS SILICON WITH SPHERICAL AND CYLINDRICAL GEOMETRY OF PORES

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This paper investigates by the finite element method the influence of inhomogeneity in the distribution of pores on the photoconductivity of porous silicon.

For cylindrical pores the significant influence the Gaussian distribution of pore radii takes place for small distances between the centers of pores (R* ~ 0,2) and at low velocities of surface recombination of photocarriers (S* ~ 5). Typical part of the photoconductivity growth with increasing the distance between the centers of pores has a saturation region for low surface recombination velocity (S* ~ 5). For porous silicon with a cylindrical pore geometry the photoconductivity decrease due to recombination processes at the same radii of pores between the centres and surface recombination velocities is several times more substantial than for the porous silicon with a spherical pore geometry. The results obtained can be used for creating sensory devices operating on the peculiarities of the photoconductivity effect of porous materials.

Key words: porous silicon, photoconductivity, computer modeling, finite element method, pore geometry.

Chemical sensors based on crystalline semiconductors, particularly, on porous silicon attract increased interest nowadays. It is known, that a gas environment has a significant impact on fluorescent and optical properties of porous silicon has and this stimulates the growing efforts focused on the design of photosensitive detection systems [1-3].

Unlike conventional semiconductors, porous silicon combines a unique combination of crystal structure and a giant outer surface (200-500 m^2/cm^3), which can lead to strongly enhanced absorption effects. Alternatively, the surface activity of porous silicon can be selectively altered in case of various treatments and modifications in organic solvents, thermal annealing, or when exposed to light. Among these sensors of particular interest are photosensitive porous silicon structures, the principle of which is based on the effect of changes in photoconductivity when the structure is exposed to light and gas adsorption occurs. In order to develop such sensors one needs to know how photoconductivity depends on the type of gas medium, concentration, surface properties of porous silicon – *i.e.* the geometry of pores, pore radius and the average distance between them. The fact that the adsorption of gas molecules changes the rate of surface photocarriers recombination ensures the sensitivity of porous silicon to the type of gas and to the gas concentration.

Let us consider a porous silicon plate having parallel cylindrical or spherical pores of the radius r_0, periodically distributed in a semiconductor with an average distance between the centers $2R$. We assume these pores form a square lattice in the xOy plane which is perpendicular to the axis of the pore. Semiconductor with p-type conductivity is irradiated by the light from the fundamental absorption region for where the photocarriers generation

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function G, *i.e.* the number photocarriers generated in one second per unit volume, independent of the location. It has to be noted, that the condition of homogeneous photocarriers generation is met in the absorption of light is not very intensive.

Generated photocarriers recombine in the bulk semiconductor and at the pore surfaces. Furthermore, in case of stationary irradiation, there is an inhomogeneous spatial distribution of photocarriers concentration, which ensures the balance between the processes of generation and recombination of non-equilibrium carriers.

Spatial distribution of concentrations photocarriers Δn in $r_0 \le r \le R$ described by the equation:

$$\frac{\partial^2 \Delta n}{\partial x^2} + \frac{\partial^2 \Delta n}{\partial y^2} + \frac{\partial^2 \Delta n}{\partial z^2} - \frac{\Delta n}{L_n^2} = -\frac{\tau_n G}{L_n^2}\,, \tag{1}$$

where L_n - diffusion path length of electrons; τ_n - the lifetime of electrons. Note that for porous silicon $L_n \sim 10^{-7}$ m, $\tau_n \sim 10^{-6}$ sec [4].

Equation (1) two complementary boundary conditions, the first of which describes the surface recombination time

$$\frac{1}{\sqrt{x^2+y^2+z^2}} \left[x\frac{\partial \Delta n}{\partial x} + y\frac{\partial \Delta n}{\partial y} + z\frac{\partial \Delta n}{\partial z} \right]\Bigg|_{x^2+y^2+z^2=r_0^2} = \frac{S\tau_n}{L_n^2}\Delta n\Bigg|_{x^2+y^2+z^2=r_0^2}\,. \tag{2}$$

here S - photocarriers surface recombination velocity, which depends on the physical and chemical state of the pores, such as the presence of gas molecules in the pores, which can alter the electrostatic potential and, consequently, the rate of recombination photocarriers.

The second boundary condition is based on the fact that in between seasons photocarriers concentration reaches a maximum value:

$$\left.\frac{\partial \Delta n}{\partial x}\right|_{x=\pm R} = 0\,,\ \left.\frac{\partial \Delta n}{\partial y}\right|_{y=\pm R} = 0\,,\ \left.\frac{\partial \Delta n}{\partial z}\right|_{z=\pm R} = 0\,. \tag{3}$$

Based coordinate photocarriers concentration distribution can be calculated photocarriers total number N of "unit cell"

$$N = \iiint \Delta n(x,y,z)\,dxdydz\,, \tag{4}$$

where are integrating the region with volume A, which is a cube of side $2R$, which is at the center of a round neckline radius r_0. Depending on the geometry of the pores may be a cylinder or sphere. Note that the total number N photocarriers up to a constant factor dependent carrier mobility determines photoconductivity of porous silicon.

The problem (1)–(3) is solved by finite element method [5], which is particularly effective in the case of payments systems with a complex geometric configuration.

Experimental data show that a porous silicon have pores of different sizes, ie different radius, and the distribution of pore radius corresponds to a normal distribution (Gaussian distribution)

$$f(r_0) = \frac{1}{\delta\sqrt{2\pi}} \exp\left(-\frac{(r_0-\mu)^2}{2\sigma^2} \right), \tag{5}$$

where μ - expectation; δ - standard deviation; σ^2 - variance.

Therefore, after calculation the values photoconductivity carrier concentration for different values of r_0 averaged by the formula:

$$N_c = h\sum f(r_0)N(r_0)\,. \tag{6}$$

where η – step summation; $f(r_0)$ - function of pore radius distribution; $N(r_0)$ - photoconductivity in pore radius r_0.

The distribution function of pore radius $f(r_0)$ determined the weight value photoconductivity corresponding to r_0. Distribution functions asked the following parameters: variance $\delta^2 = 1$, the expectation $\mu = 0{,}05$. In such settings, this feature will be a function of the normal distribution (Fig. 1, curve 1). If you are increasing the variance $\delta^2 = 4$, we obtain the distribution function of the greater spread of weighting coefficients (Fig. 1, curve 2).

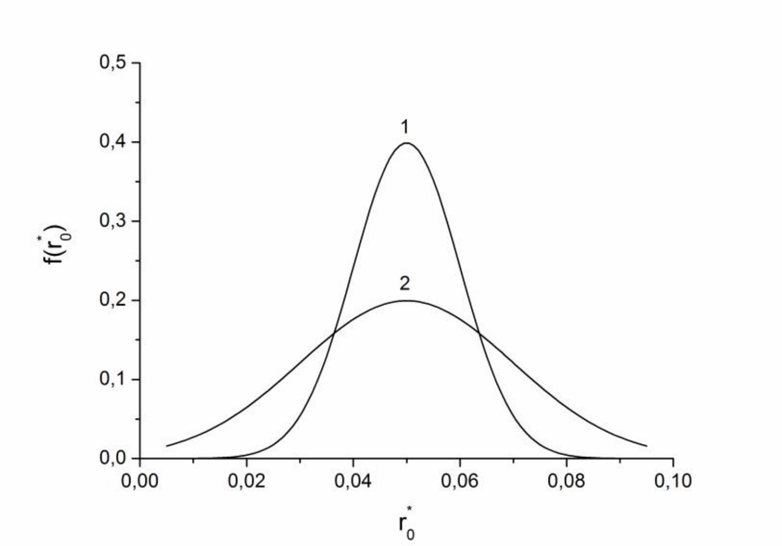
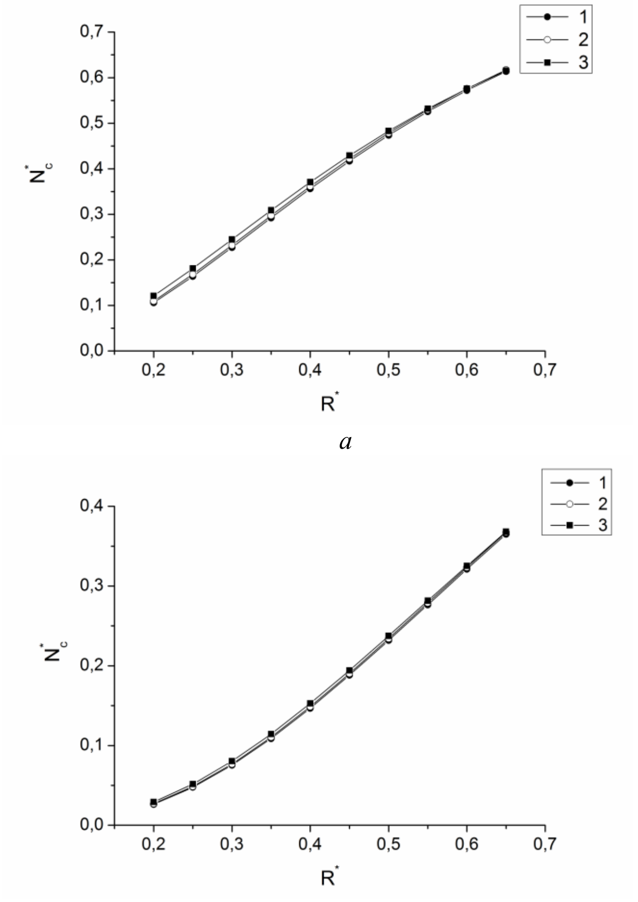


Fig. 1. Density distribution of pore radius: *1* – δ^2= 1, μ = 0,05; *2* – δ^2 = 4, μ = 0,05.

Finite element solutions obtained equation (1) with boundary conditions (2) and (3) in the case of the cylindrical geometry of pores. These solutions shown in graphs depending averaged photoconductivity of porous silicon surface recombination velocity and distance between pores (Fig. 2).

Fig. 2 shows the dependence of the photoconductivity of porous silicon for cylindrical pores r_0 = 0,05 (curve 1) and the averaged dependence of photoconductivity on the distance between the pores. To determine the average value of the photoconductivity N^*_c using the expression (6). In this expression tripped photoconductivity value N^* for pore radius from 0.005 to 0.095.



a

б

Fig. 2. Dependence of the average photoconductivity of porous silicon on the distance between the cylindrical pores: *a* – S^* = 5; *б* – S^* = 95. Curve 1 - photoconductivity of porous silicon when r_0 = 0,05; curves 2, 3 - averaged photoconductivity PC with $\delta^2 = 1$ end $\delta^2 = 4$, respectively.

As shown in Fig. 2, the average value of the photoconductivity of porous silicon $\delta^2 = 1$ almost coincide with the values of the photoconductivity of porous silicon for r_0 = 0,05. However, the value of N^*_c at $\delta^2 = 4$ are somewhat different. This is due to the fact that with increasing deviation from the expected value increases the number of significant weights. Note that with increasing distance between the pores of the three curves coincide.

Fig. 3, 4, the dependence of N^*_c surface recombination velocity and distance between spherical and cylindrical pores, respectively.

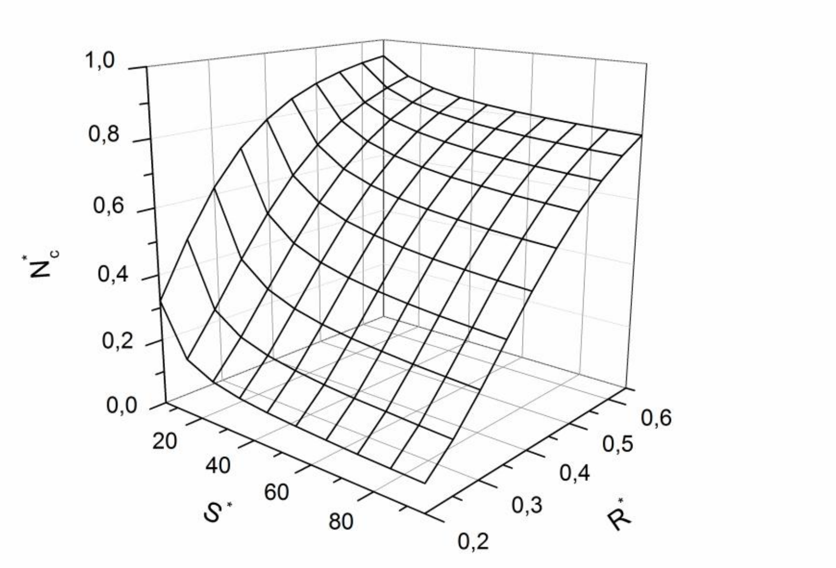


Fig. 3. The dependence of photoconductivity averaged *R** and *S** for porous silicon with a spherical geometry of pores.

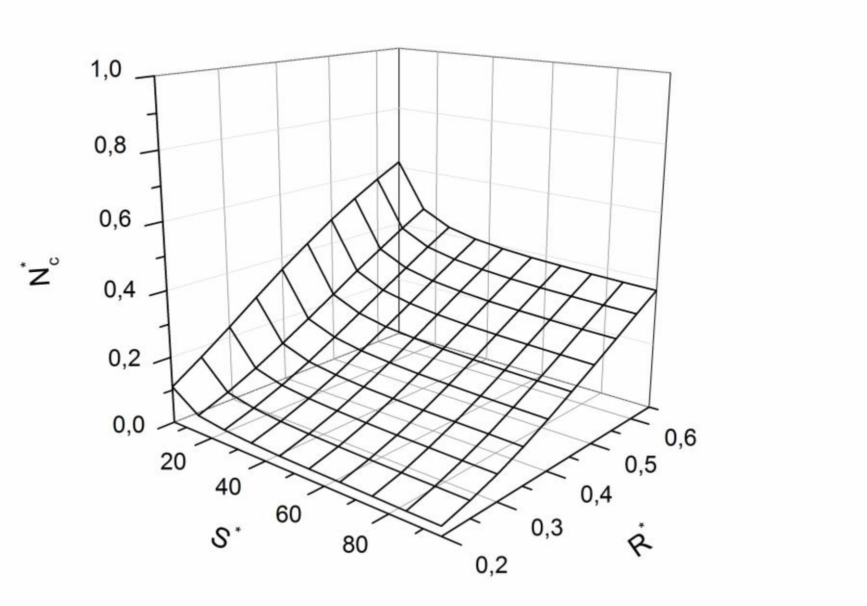


Fig. 4. The dependence of photoconductivity averaged *R** and *S** for porous silicon with cylindrical geometry of pores.

For spherical and cylindrical geometry averaged photoconductivity of porous silicon increases with the distance between the pores and decreases when increasing the rate of surface recombination.

Thus, the finite element method the effect of heterogeneity of pore sizes in photoconductivity of porous silicon. For cylindrical pores more substantial impact Gaussian distribution of pore size is for small distances between the centers of the pores ($R^* \sim 0{,}2$), and at low surface recombination velocities ($S^* \sim 5$). Typical character growth photoconductivity with increasing distance between the centers of pore saturation area is only for small surface recombination velocity ($S^* \sim 5$).

For porous silicon with a cylindrical pore geometry photoconductivity decrease due to recombination processes on the same radii of pores, pore center distance and surface recombination velocity is several times more significant than the porous silicon with a spherical geometry of pores.

The results can be used in the course of sensor devices that run on the features photoconductivity effect of porous materials.

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МОДЕЛЮВАННЯ ФОТОПРОВІДНОСТІ ПОРУВАТОГО КРЕМНІЮ ЗІ СФЕРИЧНОЮ ТА ЦИЛІНДРИЧНОЮ ГЕОМЕТРІЄЮ ПОР

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Наведено результати числового моделювання фотопровідності макропоруватого кремнію зі сферичними і циліндричними порами методом скінченних елементів. Проаналізовано залежність фотопровідності від швидкості поверхневої рекомбінації за різних радіусів пор та середніх відстаней між ними. Враховано гаусівський розподіл значень радіусів пор.

Ключові слова: поруватий кремній, фотопровідність, комп’ютерне моделювання, метод скінченних елементів, геометрія пор, розміри пор.

МОДЕЛИРОВАНИЕ ФОТОПРОВОДИМОСТИ ПОРИСТОГО КРЕМНИЯ СО СФЕРИЧЕСКОЙ И ЦИЛИНДРИЧЕСКОЙ ГЕОМЕТРИЕЙ ПОР

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Методом конечных элементов исследовано влияние неоднородности распределения пор на фотопроводимость пористого кремния.

Для цилиндрических пор существеннее влияние гауссовского распределения величин радиусов пор проявляется для небольших расстояний между центрами пор ($R^* \sim 0{,}2$) и при малых скоростях поверхностей рекомбинации фотоносителей ($S^* \sim 5$). Типичный характер роста фотопроводимости при увеличении расстояния между центрами пор имеет участок насыщения только для низких скоростей поверхностной рекомбинации ($S^* \sim 5$). Для пористого кремния с цилиндрической геометрией пор уменьшение фотопроводимости за счет рекомбинационных процессов при одинаковых радиусах пор, расстояниях между центрами пор, скоростях поверхностной рекомбинации в несколько раз существеннее, чем для пористого кремния со сферической геометрией пор. Полученные результаты можно использовать при создании сенсорных устройств, работающих на особенностях эффекта фотопроводимости пористых материалов.

Ключевые слова: пористый кремний, фотопроводимость, компьютерное моделирование, метод конечных элементов, геометрия пор, размеры пор.