NUMERICAL SIMULATION OF THE PHOTOCURRENT IN THE THIN METAL – SILICON STRUCTURES WITH QUANTUM WELLS

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Using the SimWindows program package, we have numerically calculated the photocurrents in the space-charge region of thin metal—silicon structures with quantum wells (QWs) as well as their dependences on the geometrical size and the number of the QWs, and on the doping level. A possibility of creating the photosensitive structures on the basis of the layers of porous silicon with various degree of porosity has been analyzed.

Introduction

Semiconducting structures with QWs are widely used in fabricating optoelectronic devices. For example, the infrared (IR) detectors with a low noise factor (1×10^{10} cm Hz/V at $T = 77$ K) were developed for the radiation range of 3—30 μm [1]. Making use of the epitaxial growth process of the structures, one can create comb IR detectors with a response at certain wavelengths [2]. The IR sensors with QWs are the basis for the fabrication of detector matrices of thermal imagers [3] and IR cameras [4, 5]. As the time of the carrier interception in structures with QWs is very small (of the order of picoseconds), they are the basis for developing the heterodyne oscillators with the frequencies up to 40 GHz, the parameters of the QWs determining the oscillating frequency of the laser [6, 7]. An additional introducing of QWs into the solar cells based on the GaAs and AlGaAs compounds results in improving the output parameters [8, 9]. Really, while comparing such a solar cell with a homojunction made up of the barrier substance, the QW solar cell (QWSC) has a larger short-circuit current $I_{\rm sc}$. On the other hand, while comparing it with a cell made up of a semiconductor, which participates in the formation of the QWs, the QWSC has a larger open-circuit voltage $V_{\rm oc}$.

The diagram in Fig. 1 shows an example of the photosensitive structure of the Schottky-barrier type with the QWs in the space-charge region (SCR), where the quantization of the energy levels takes place. If the selection rules allow the transitions of type *2* at the absorption of a photon, this results in a shift of the absorption threshold into the region with energies $h\nu < E_g$ of the material of the barrier. For an additional photocurrent to appear, it is necessary that photo-induced electrons and holes can be thermally thrown out into the allowed energy bands (processes *5* and *6*) and, afterwards, routed to relevant electric junctions. With this aim in view, the QWs are placed in the SCR of the p—i—n structure or the Schottky barrier (processes *7* and *8*). The increase of the current, induced by the introducing of QWs, may override, at certain values of the parameters, some decrease of $V_{\rm oc}$, which is typical of those structures.

The calculation of the efficiency of the photoconversion in such a structure is rather complicated in the general case and requires taking into account the generation-recombination and diffusion-drift processes in the space-charge and quasi-neutral regions, which can be fulfilled only numerically. It this work, we consider the simpler case, where the QWs are built-in into the SCR of the metal–semiconductor junction and the thickness of the whole structure is no more than the size of the depletion region. It allows us to suggest that all the photo-induced current carriers are arranged by the SCR field.

1. Method of Calculation

For the numerical simulation, we used a SimWindows computer program (http://ucsu.colorado.edu/~winston/simwin.html), which allows one to evaluate the parameters of the microelectronic devices taking advantage of the solution of the diffusion-drift equations, namely, to simulate one-dimensional structures with QWs and heterojunctions, both sharp and gradient.

For the simulation, we used a structure, shown in Fig. 1, where the total thickness of the structure was no more than the width of the SCR and the wells were rectangular. The dependences of the optical absorption and photocurrents on the specimen thickness L, the QW

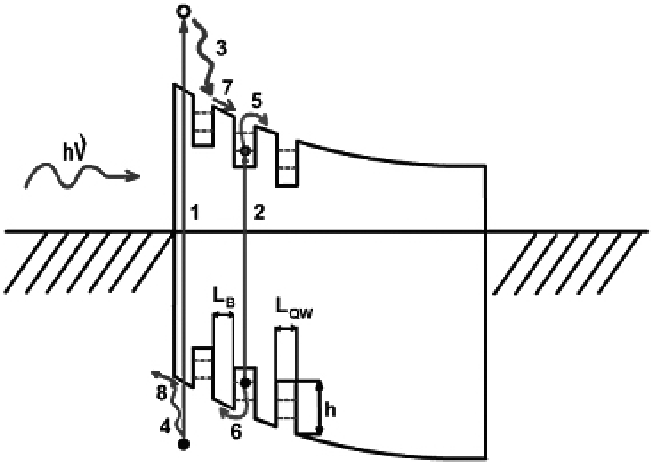

Fig. 1. The energy diagram of the Schottky barrier with QWs in the SCR: *1* denotes the photo-induced generation in the barrier substance, *2* shows the interlevel transitions between the QWs, *3* and *4* correspond to the electron and hole thermalization, respectively, *5* and *6* indicate the thermal throwing out of electrons and holes, respectively, onto the conduction level, *7* and *8* are the drift of nonequilibrium electrons and holes, respectively

number N_{QW}, the QW width L_{QW}, the doping level N_d, and the height of the Schottky barrier were also simulated. The following parameters of the structure were selected for the simulation: 1) for $L = 0.1$ μm, $L_{\mathrm{QW}} = 3.5$ nm ($N_{\mathrm{QW}} = 1 \div 10$), $L_{\mathrm{QW}} = 5$ nm ($N_{\mathrm{QW}} = 2 \div 8$), and $L_{\mathrm{QW}} = 10$ nm ($N_{\mathrm{QW}} = 1 \div 4$); 2) for $L = 0.25$ μm, $L_{\mathrm{QW}} = 10$ nm ($N_{\mathrm{QW}} = 1 \div 10$) and $L_{\mathrm{QW}} = 25$ nm ($N_{\mathrm{QW}} = 1 \div 4$); 3) for $L = 0.5$ μm, $L_{\mathrm{QW}} = 25$ nm ($N_{\mathrm{QW}} = 1 \div 9$), $L_{\mathrm{QW}} = 50$ nm ($N_{\mathrm{QW}} = 1 \div 4$), and $L_{\mathrm{QW}} = 100$ nm ($N_{\mathrm{QW}} = 1, 2$); and 4) for $L = 1$ μm, $L_{\mathrm{QW}} = 50$ nm ($N_{\mathrm{QW}} = 1 \div 9$). The doping level N_d was varied within the limits of $10^{15} - 10^{17}$ cm^{-3}. A semiconductor with $E_g = 1.5$ eV and other characteristics being those of the porous silicon (PS) [10] was considered as the barrier substance, with the quasi-crystalline silicon being selected as a material for the QW formation. The irradiation level corresponded to the AM1.5 conditions. All the light was assumed to be absorbed.

2. Results of Simulation and their Discussion

The dependences of the current I_{sc} on the QW thickness for the specimens with various doping levels are shown in Fig. 2. The minimum value of L_{QW} was selected to be 3.3 nm, which, according to the calculations, corresponds to a single discrete energy level E_1 available in the well. The thickness of the structure was selected in accordance with the value of the width of the SCR in the Schottky barrier at the given doping level of silicon. It is seen that I_{sc} grows to the saturation as the width of the well increases.

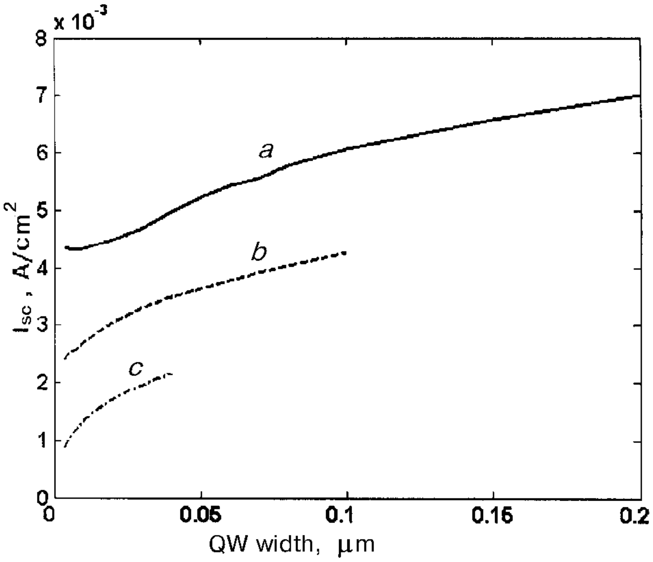

Fig. 2. I_{sc} as a function of the QW width at various doping levels N_d and specimen thicknesses L: *a* — $L = 0.5$ μm and $N_d = 10^{15}$ cm^{-3}, *b* — $L = 0.25$ μm and $N_d = 10^{16}$ cm^{-3}, *c* — $L = 0.08$ μm and $N_d = 10^{17}$ cm^{-3}

While calculating, we also took into account the fact that, as the width of the well H_w increases, the values of ΔE_l in the QW and, correspondingly, of $E_{g\mathrm{eff}}$ also increase. Moreover, if the current carriers occupy the lowest level E_{w1} in the QW, the probability of their tunneling into the allowed energy band decreases. But if $E_{w2} > E_{w1}$ for the level E_{w2}, i.e. when it is situated above the bottom of the well, then its population is smaller, but the relevant probability for the current carries to quit the well through either the thermal throwing out or tunneling is higher.

An introducing of the QWs into the SCR of the structure extends the interval of the spectral sensitivity towards lower energies due to the absorption of the low-energy photons in the QWs (see Fig. 3). Figs. 4 and 5 show the dependences of the current I_{sc} on the QW number for the Schottky barrier at the PS with various structure thicknesses, well widths, and barrier heights. It is seen that the introducing of additional number of QWs into the SCR is accompanied at first by a linear growth of I_{sc} due to extra long-wave absorption, but at a certain number of the QWs that dependence saturates. The current increases for the larger heights of the barrier, as it was in the case of the structure with the Schottky barrier but without wells.

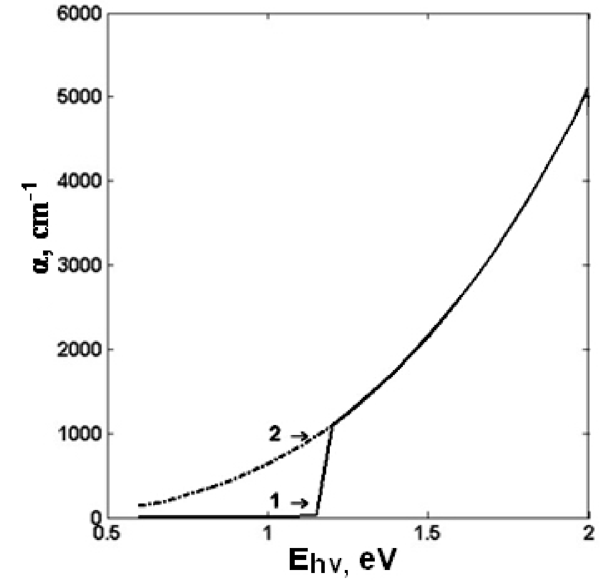

Fig. 3. The energy dependences of the absorption coefficient of the direct-band-gap semiconductor with $E_g = 1.5$ eV and (*1*) without QWs and (*2*) with QWs ($L = 80$ nm, $L_{\mathrm{QW}} = 10$ nm, $N_d = 10^{15}$ cm^{-3}, $N_{\mathrm{QW}} = 3$)

Conclusions

With the use of the numerical simulation methods, it has been shown that if the QWs are introduced into the SCR of the Schottky barrier in silicon, the absorption of the radiation, whose energy is determined by the lowest consistent levels in the QWs, is observed. It results in an extension of the photogeneration interval of the structure towards the long-wave range. The QW geometry influences the effective gap width of the QWs, with the following mechanisms, by means of which the current carriers quit the wells, playing an important role in creating the photocurrent: the thermal throwing out of the current carriers upwards, tunneling, and the energy level occupation. An increase in the number of QWs causes the growth of the photocurrent and the situation where a certain number of the QWs finds themselves in the region of the small band bending, where the probability of tunneling for the current carriers decreases. Therefore, when using a semiconductor with the small SCR, it imposes a limitation on the specimen length and, correspondingly, on the depth of the active zone, where the QWs can be introduced into.

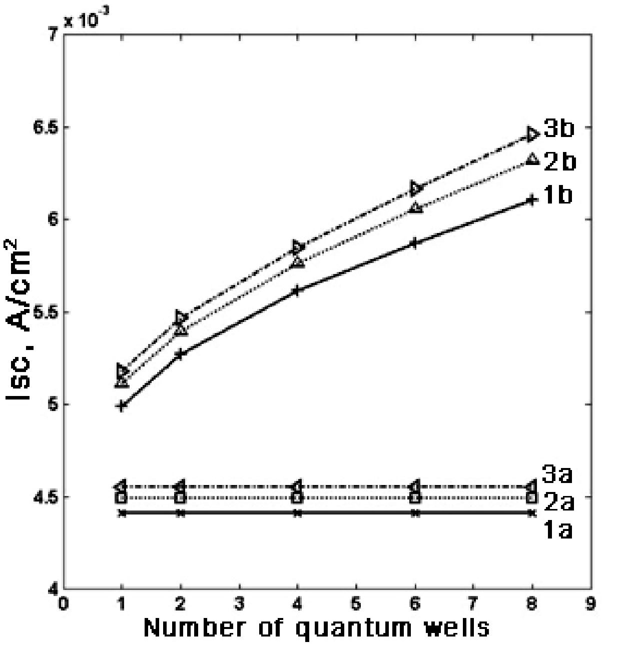

Fig. 4. I_{sc} as a function of the QW number for a specimen with $L = 0.5$ μm, $L_{\mathrm{QW}} = 0.025$ μm, and $N_d = 10^{15}$ cm^{-3} at the Schottky barrier height $e\varphi = 0.7$(*1*), 0.8 (*2*), and 0.9 eV (*3*); curves *a* correspond to a reference specimen, curves *b* to the QW cells

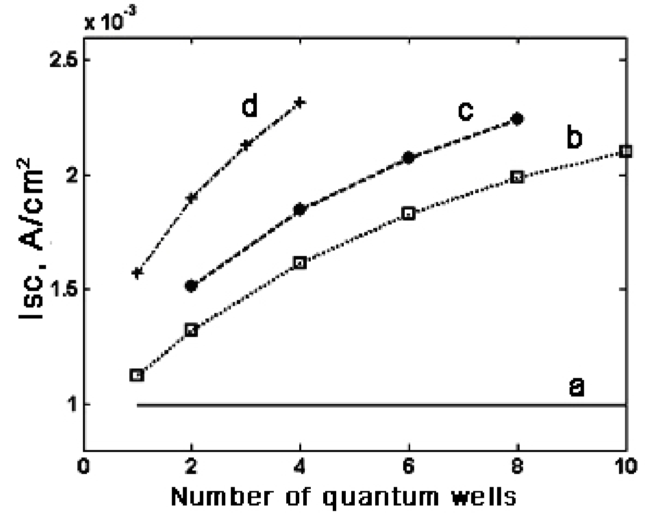

Fig. 5. I_{sc} as a function of the QW number for various well widths L_w (the doping level $N_d = 10^{16}$ cm^{-3}, $L = 0.1$ μm); curve *a* corresponds to a reference specimen without the QWs, curve *b* to $L_w = 3.5$ nm, curve *c* to $L_w = 5$ nm, and curve *d* to $L_w = 10$ nm

The calculated current densities for those structures amount to units of mA/cm^2 and are not competitive, for example, against the high-performance silicon solar cells. Nevertheless, taking into account the perspective of a broad use of those materials, such as PS, in optoelectronics, the considered elements can be proposed as functional ones for photodetectors and solar cells, as optical modulators, or for the enhancement of the conductivity of the PS layers.

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ЧИСЕЛЬНЕ МОДЕЛЮВАННЯ ФОТОСТРУМУ У ТОНКОПЛІВКОВИХ СТРУКТУРАХ МЕТАЛ—КРЕМНІЙ З КВАНТОВИМИ ЯМАМИ

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Резюме

За допомогою пакета SimWindows чисельно розраховані фотоструми для тонких структур метал—кремній з квантовими ямами (КЯ) в області просторового заряду в залежності від геометричних розмірів і кількості (КЯ) та ступеня легування. Проаналізовано можливість створення фоточутливих структур на основі шарів поруватого кремнію з різним ступенем поруватості.