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NUMERICAL SIMULATION OF OPERATING MODES OF HETEROSTRUCTURAL PHOTODIODES BASED ON INDIUM ARSENIDE NANOWIRES ON THE SILICON SUBSTRATES

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Abstract. The paper presents the results of numerical simulation of the heterostructural diodes operation based on the array of indium arsenide nanowires on the silicon substrates with different polarities, namely *n*- or *p*-types. It has been found that it is possible to achieve theoretical values of the ideality factor equal to 1.1 and 2.1 respectively. The high quantum efficiency values are typical for the investigated heterostructures during separation of photogenerated charge carriers in the temperature range of 150–300 K.

Keywords: indium arsenide, nanowire, heterostructure, silicon substrate, numerical calculation

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ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ РЕЖИМОВ РАБОТЫ ГЕТЕРОСТРУКТУРНЫХ ФОТОДИОДОВ НА ОСНОВЕ НИТЕВИДНЫХ НАНОКРИСТАЛЛОВ АРСЕНИДА ИНДИЯ НА КРЕМНИЕВЫХ ПОДЛОЖКАХ

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Аннотация. В работе представлены результаты численного моделирования работы гетероструктурных диодов на основе массива нитевидных нанокристаллов арсенида индия (InAs) на кремниевых подложках, обладающих разными полярностями, а именно – *n*- и *p*-типов. Установлено, что в этих случаях удается достичь теоретических значений коэффициента идеальности, равных 1,1 и 2,1, соответственно. Для исследованных гетероструктур в температурном диапазоне 150 – 300 K характерны высокие значения квантовой эффективности при разделении фотогенерированных носителей заряда.

Ключевые слова: арсенид индия, нитевидный нанокристалл, гетероструктура, кремниевая подложка, численное моделирование

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Introduction

A promising direction in seminconductor physics is the development of photodetector devices based on crystalline nanowires (NW). This is of particular importance due to the obvious advantages of NW over thin-film structures of the same composition.

Firstly, relaxation of elastic stresses occurs on the lateral surface of NW during synthesis due to the difference in the lattice constants of the semiconductor crystals comprising the substrate and the NW. This circumstance makes it possible to carry out epitaxial synthesis of a number of semiconductor materials, such as InGaN, GaPAs, InAsP [1, 2], for which lattice-matched substrates are either difficult to procure or completely unavailable. In particular, semiconductor devices can be constructed for axial NW with diameters below the critical value (24–110 nm) [3] and lattice-mismatched thick layers. The thicknesses of the layers exceed the critical value (several nanometers) for similar planar structures [4].

Secondly, an equally important advantage of NW is their applications in devices with electronic size effects or subwavelength-scale localization of the electromagnetic field. Such devices can be used to create effective photodiodes, single-photon sources, etc. [5].

A third advantage of NWs is that the structure of the devices can be formed not only in the axial direction (normal to the substrate), but also on the lateral face of the NW (radial geometry, or core–shell geometry). This circumstance makes it possible to distinguish between physical processes, such as, for example, light absorption and separation of charge carriers, which is fundamentally impossible in the case of planar geometry.

This work analyzes the effect of doping type of silicon substrates in the system of indium arsenide nanowires (referred to as InAs/Si) on the characteristics of the photodetector diode structure. The study was conducted within the framework of numerical simulation.

Experimental samples and computational procedure

The paper considers two simplified configurations of axial diode heterostructures based on indium arsenide nanowires on silicon substrates:

n-InAs/*i*-InAs/*p*-Si (configuration *n*–*i*–*p*);
p-InAs/*i*-InAs/*n*-Si (configuration *p*–*i*–*n*).

The choice of NW sizes was dictated by the optimal waveguide geometry for constructing a photodiode structure in the communication wavelength range for such NW [6]: length of 2.5 μm, diameter of 300 nm. Notably, with these characteristic sizes of NW, there are no size effects of energy level quantization in them.

The thickness of the upper emitter was chosen to be 50 nm at a doping level of 10^{18} cm^{-3}, which provided a sufficient number of charge carriers for the formation of a space-charge region mainly inside the NW.

Numerical simulation of the diodes was carried out in the Comsol Multiphysics package. The calculations were performed within the framework of the drift-diffusion model, taking into account the Fermi–Dirac statistics for both types of charge carriers. The Shockley–Read–Hall model was used to account for the effects of charge carrier recombination, with carrier lifetimes in indium arsenide equal to 30 ns for electrons and 3 μs for holes [7, 8]. The parameters of semiconductor materials were taken from [8, 9].

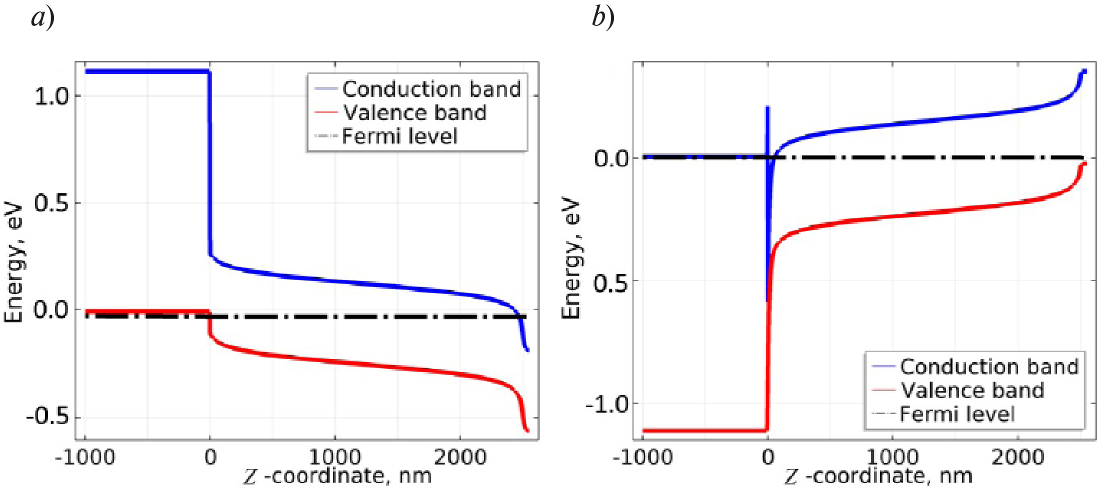

Fig. 1. Band structures of the diode at 200 K for cases of *p*- (*a*) or *n*-type (*b*) substrate chosen

To account for the imperfections in the NW structure, for example, the presence of point defects or the occurrence of various polytypes in the NW, the carrier diffusion length was varied during the simulation process. The considered values of carrier diffusion length ranged from 500 nm to 20 μm.

Importantly, the influence of surface conditions on the operation of the diode was not taken into account in this study.

Results and discussion

According to the literature data, the InAs/Si heterointerface is a type-II heterojunction, where the top of the valence band in both materials is located approximately at the same energy level, so it is natural to choose a silicon substrate with p-type conductivity for constructing diode structures (Fig. 1,*a*). In turn, a distinct characteristic of this configuration is the propagation of the space-charge region into the heterointerface region, which in the case of the considered geometry of the photodetector structure can lead to leakage currents under experimental conditions [10, 11]. Despite the large energy gap between the positions of the conduction band bottom in the two materials, a reverse-polarity diode can be formed due to the low effective mass for electrons in indium arsenide. Indeed, if an n-type substrate is chosen, electrons from the substrate must move to the NW, which can lead to the formation of an electron-depleted region in silicon and an electron-rich region in indium arsenide.

The position of the Fermi level E_F relative to the bottom of the conduction band for degenerate semiconductors can be expressed by the following formula [12]:

$$E_F = \frac{\hbar^2}{2m^*} \cdot (3\pi^2 n)^{\frac{2}{3}}, \tag{1}$$

where m^* is the effective electron mass, n is the carrier concentration, $\hbar$ is the reduced Planck constant.

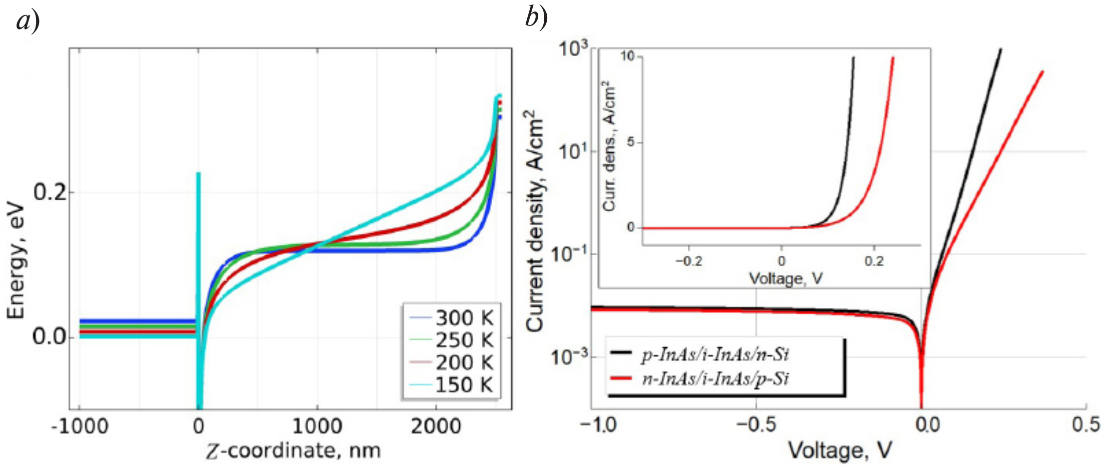

Fig. 2. Simulation of photodiode operation: positions of conduction band bottom forp-InAs/i-InAs/n-Si heterostructure at different temperatures (*a*); current–voltage characteristics for two types of diodes at 200 K on logarithmic (modulus) and linear scales (*b*)

Substituting the effective mass of InAs equal to 0.023 m_0 (m_0 is the electron mass) into this formula, we obtain that the doping level of the substrate about 10^{19} cm^{-3} is sufficient to compensate for the band discontinuity between *n*-Si and InAs.

Notably, such substrates are commercially available. The required value may be actually even lower, due to the appearance of size quantization in InAs along the NW axis with sharp band bending and a consequent decrease in electron filling density (Fig. 1,*b*).

Fig. 1 shows the band diagrams for diodes of both polarity types at a temperature of 200 K, above which (as we discuss below) thermogenerated charge carriers begin to effectively shield the potential difference between the emitters of the structure.

Apparently, in the case of choosing an *n*-type substrate, the doping level of 10^{19} cm^{-3} is sufficient to ensure the required band bending. The height of the potential barrier for electrons in silicon turns out to be relatively small and provides high conductivity of the heterointerface.

To determine the optimal operating conditions of the considered photodetector structures, simulation was carried out for various temperatures of the system. It was found for both configurations at room temperature that shielding of the electric field occurs in the NW volume due to intrinsic carrier concentration (Fig. 2,*a*). The intrinsic concentration decreases with a decrease in temperature, ensuring an increase in the space-charge region in NW, which is most noticeable at temperatures below 200 K. Thus, it can be expected that additional cooling of the structure may be required for efficient operation of the NW array as a photodiode.

The next stage of the simulation was the analysis of the current—voltage (*I—V*) characteristics of the considered diode heterostructures (Fig. 2,*b*) for a characteristic temperature of 200 K determined earlier. We established that the reverse currents practically coincide for both configurations and correspond to the value of the current formed by the separation of charge carriers arising in the NW volume due to the thermogeneration process. The forward-bias region of the current—voltage characteristic exhibits a significant difference between the two configurations, namely, that the diode formed on n-type silicon substrate opens earlier.

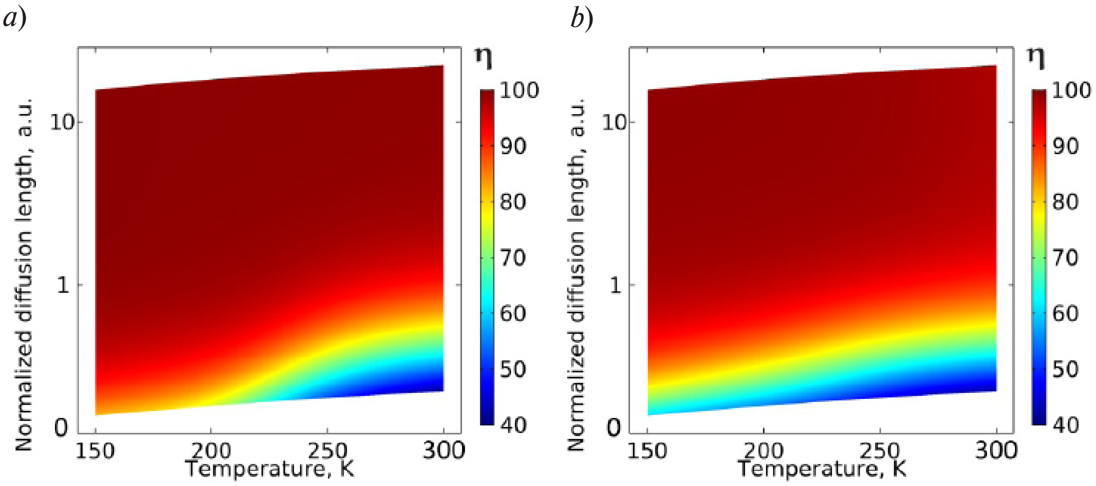

Fig. 3. Maps for dependence of quantum efficiency of separation of photogenerated charge carriers on temperature and carrier diffusion length normalized by the length of active region of the NW for configurations *n—i—p* (*a*) and *p—i—n* (*b*)

Approximation of the forward-bias region of the current—voltage characteristic using the Shockley equation [13] for a loaded diode shows that this circumstance is due to the difference in the ideality factor for two configurations: the *p—i—n* system has an ideality factor equal to 1.1, while this value for the *n—i—p* system is 2.1, which leads to an increase in the open-circuit voltage of the diode. Analysis of this result allows to conclude that the *p—i—n* system is more suitable in cases when low open-circuit voltages are important, for example, as detector diodes in high-frequency mixers.

At the next stage, we studied the operation of heterostructures as photodiodes. For this purpose, we carried out numerical simulation of the dependence of separation processes of photogenerated charge carriers in NW on temperature and diffusion length for two configurations at zero bias voltage. The electron—hole pairs were produced under optical irradiation of a photoactive structure by setting a fixed uniform generation rate equal to $1.4 \cdot 10^{19}$ cm^{-3}/s, which corresponds to the absorption of optical radiation with a wavelength of 1.55 μm and an intensity of 1 W/m^2 by a semiconductor material.

The quantum efficiency η was used as a comparative characteristic, calculated as the ratio of the carrier flux formed in the structure to the total generation rate over the NW volume. Fig. 3 shows maps for the dependence of quantum efficiency η on the temperature of the structure and the carrier diffusion length normalized by the length of the active region of the NW.

Evidently, almost complete separation of photogenerated charge carriers is achieved for both configurations at high diffusion lengths. A further decrease in the carrier diffusion length reveals the difference between the configurations. A decrease in the diffusion length down to values below the NW length leads to the appearance of a temperature dependence of quantum efficiency. In particular, there is an increase in quantum efficiency from 0.4 to 0.8 with a decrease in temperature from 300 to 150 K for the *n—i—p* system. In turn, the *p—i—n* system turns out to be more sensitive to a decrease in the diffusion length: the quantum efficiency at 300 K also corresponds to a value of 0.4, but it increases only to a value of 0.6 with a decrease in temperature. In addition, the *p–i–n* system demonstrates a lower quantum efficiency even for high values of the diffusion length. This phenomenon is likely related to the difference between the configurations, that is, the presence of an electron-rich region near the heterointerface, which leads to an increased recombination rate of holes near the interface and, as a result, their exclusion from the total photocurrent.

Conclusion

In this paper, we carried out numerical simulation to study the operational modes of two configurations of a heterostructure photodetector diode based on indium arsenide nanowires on silicon substrates. As a result of the simulation, we found that the diode structure on the *n*-type silicon substrate demonstrates a lower value of the ideality factor and it is more suitable for problems where low open-circuit voltages are required. The structures had almost identical parameter values for both systems in photodiode mode, however, the system using the *p*-type substrate gives higher values of quantum efficiency. Despite this, both configurations can be used to build photodiodes based on them, and the choice of specific configuration should be determined by the technological requirements for synthesis of the structure or the requirements for the polarity of the system.

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