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Original paper

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CHARGE PROPERTIES AND CURRENTS IN THE SILICON/NANOPARTICLES OF ZINC OXIDE HETEROSTRUCTURE IRRADIATED BY THE SOLAR LIGHT

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Abstract. Silicon/zinc oxide heterostructures have shown themselves to be promising for use in photovoltaics. This paper presents the results of modeling the charge properties and currents in a Si/nanosized ZnO particle with different types of conductivity under sunlight irradiation. The simulation was carried out using the Comsol Multiphysics software package. The energy diagrams of the investigated heterostructures were plotted, the charge properties and currents flowing in the structure were investigated, the dependences of the rate of generation of charge carriers on wavelength on the surfaces of silicon, zinc oxide, and at the interface between silicon and zinc oxide, the rate of recombination of charge carriers at various wavelengths of incident radiation was obtained. The regularities of the influence of wavelength of the incident radiation on the charge density and electric potential on the surface of heterostructures have been established. It is shown that the potential on the surface of the p-Si / n-ZnO heterostructure is positive, depends on the wavelength of the incident radiation and reaches the maximum of 0.68 V. For other structures, it is negative and does not depend on the wavelength: n-Si / p-ZnO –0.78 V, p-Si / p-ZnO –0.65 V, n-Si / n-ZnO –0.25 V.

Keywords: nanoparticle; zinc oxide; silicon; heterostructure; charge properties; modeling; photovoltaics.

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Introduction

Zinc oxide is a wide-gap (3.37 eV) semiconductor that is used in a variety of fields of photovoltaics, such as photocatalytic water and air purification, photolysis of water, optoelectronics, and gas sensors [1]. Zinc oxide has a number of advantages over other materials used in photocatalysis: low cost, non-toxicity, low reflectance in the solar spectrum, the ability to create low-dimensional structures using chemical etching (amphotericity), resistance to high-energy radiation, flexible change of electrophysical and optical properties by doping with various impurities [2].

The conductivity of zinc oxide depends significantly on the stoichiometric composition of the material. The deviation from the stoichiometric ratio [Zn]:[O] = 1 causes the formation of point defects: interstitial atoms and vacancies of oxygen and zinc atoms. An excess of zinc or oxygen vacancies is a characteristic of the n-type conductivity of ZnO obtained under nonequilibrium conditions or due to the partial transition of oxygen to the gas phase. Moreover, hydrogen atoms [3]

injected into the material during growth or deposition in a hydrogen-containing enviroment or during post-processing of the sample with water solutions can be responsible for the n-type conductivity.

At the same time, attention is now focused on obtaining and studying the properties of the p-type zinc oxide. Obtaining the p-type conductivity is complicated by the presence of natural oxygen vacancies, which act as donor states [4]. Today the following elements are acceptors for ZnO: Zn vacancies; IA group: Li, Na, K; IB group: Cu, Ag, Au; VA group: N, P, As, Sb [5]. On the other hand, much attention is paid to the creation and study of silicon/zinc oxide heterostructures containing ZnO nanoparticles. This is important for the formation of composite materials with a developed surface for photovoltaics.

Charge properties modeling methodic

Modeling of currents, charge properties, and electron-hole processes were carried out using the Comsol Multiphysics package, a two-dimensional diffusion-drift model for calculating current transfer in semiconductors, as well as the Maxwell system of equations. The main properties of silicon [6] and zinc oxide [2, 7–9] used in the simulation are presented in Tab. 1.

Table 1. Material parameters (temperature 300 K)

Parameter	n,p-Si	n,p-ZnO
Bandgap, eV	1.12	3.37
Affinity, eV	4.05	4.3
Permittivity	11.7	8.5
Effective density of states, cm^{-3} *– conduction band* *– valence band*	 $2.8 \cdot 10^{19}$ $1.04 \cdot 10^{19}$	 $4.124 \cdot 10^{18}$ $1.138 \cdot 10^{19}$
Charge carries lifetime, μs	10	$9.7 \cdot 10^{-4}$
Impurity concentration, cm^{-3}	10^{17}	10^{16}
Electron mobility, $cm^2/(V \cdot s)$	1450	200
Hole mobility, $cm^2/(V \cdot s)$	500	50

The real parts of the refractive index for silicon and zinc oxide n(Si) and n(ZnO), as well as the imaginary parts of the refractive index k(ZnO) and k(Si) are given in a table depending on the wavelength [10, 11]. The heterostructure is a zinc oxide nanoparticle with a size of 500×500 nm in a silicon substrate.

Results and discussion

Fig. 1 shows the energy diagrams of heterostructures for various combinations of types of conductivity of a silicon substrate and zinc oxide nanoparticles.

The barrier height for electrons from the silicon side in the n-Si/n-ZnO heterostructure is 0.133 eV, after passing through which, they enter the depletion region for electrons in zinc oxide, thereby creating an excess negative charge at the edge (length ≈ 70 nm) of the oxide nanoparticle zinc. The hole barrier on the zinc oxide side is 0.092 eV. In the n-Si/p-ZnO heterostructure, the barrier for electrons on the silicon side is 0.104 eV, and for holes on the zinc oxide side it is 0.567 eV. For the p-Si/p-ZnO heterostructure, these values are 0.028 eV and 0.57 eV, respectively. For the p-Si/n-ZnO heterostructure, there are no such barriers, it allows electrons generated in silicon and holes generated in zinc oxide to flow freely into another semiconductor.

Fig. 2 shows the dependences of the generation rate G of charge carriers on the wavelength of incident radiation on the surface of a zinc oxide nanoparticle (curve 3), the surface of a silicon substrate (curve 1), and silicon under a zinc oxide nanoparticle under the radiation transmitted through a ZnO nanoparticle (curve 2).

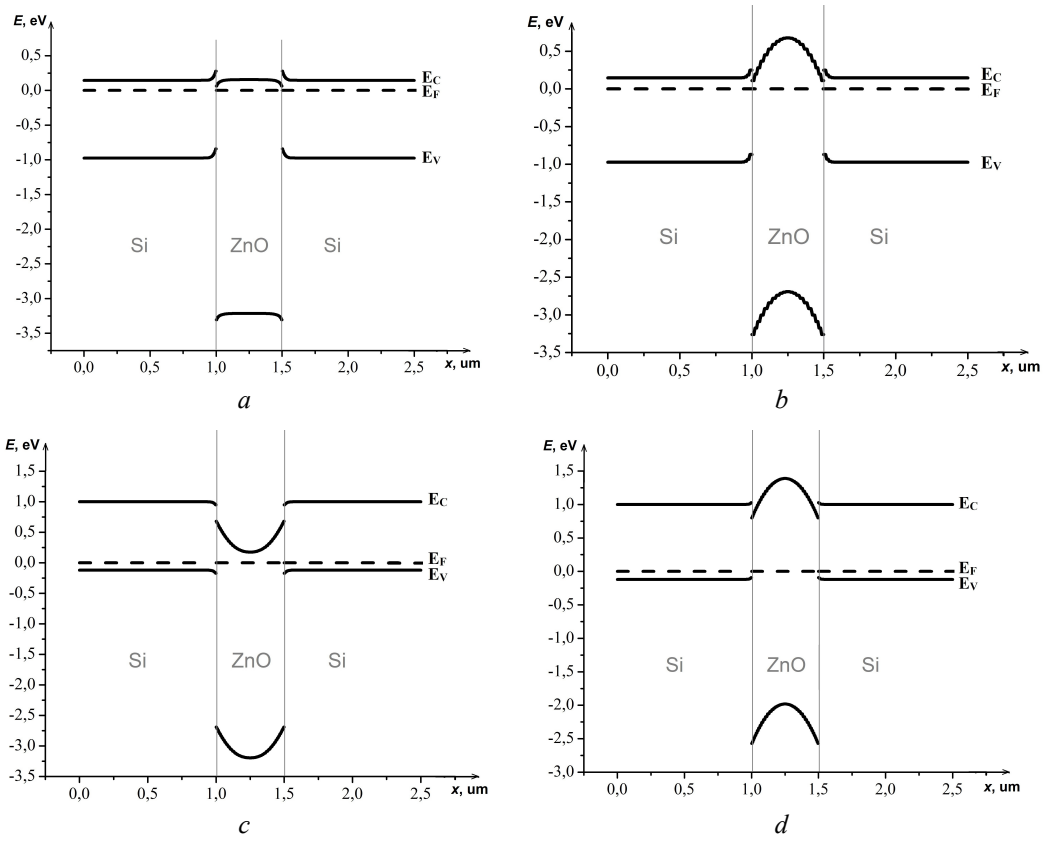


Fig. 1. Energy diagrams of heterostructures: *a* – n-Si/n-ZnO; *b* – n-Si/p-ZnO; *c* – p-Si/n-ZnO; *d* – p-Si/p-ZnO

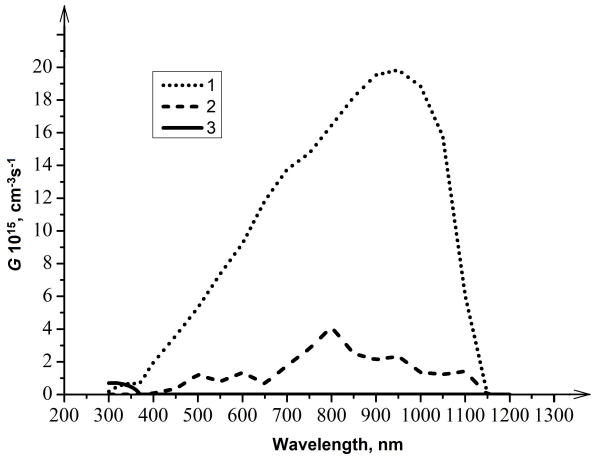
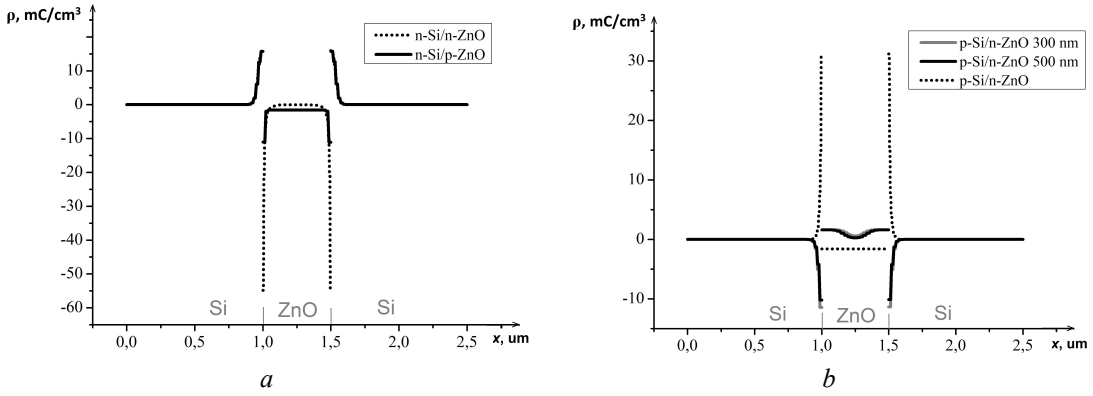


Fig. 2. The rate of generation of charge carriers on the surface of a silicon substrate (1), in silicon after the passage of radiation through a zinc oxide nanoparticle (2), and on the surface of a zinc oxide nanoparticle (3)

Due to the charge carriers redistribution during irradiation an excess electric charge is formed on the surface of heterostructures, the bulk density of which is shown in Fig. 3. The charge density slightly depends on the wavelength of incident radiation in the p-Si/n-ZnO heterostructure on the surface of the ZnO nanoparticle as can be seen from Fig. 3, *b*.

The electric charge is generated on the surface of a zinc oxide nanoparticle and its boundary is with silicon during irradiation, which leads to the potential difference and the emergence of the current of charge carriers generated by the radiation. For the n-Si/n-ZnO structure the potential difference ΔV between the ZnO/Si interface and the ZnO nanoparticle volume is 0.11 V, and for the n-Si/p-ZnO heterostructure it is $\Delta V = 0.63$ V. The difference in values of the negative electric potential V_{surf} on the surface of n-Si/n-ZnO and n-Si/p-ZnO heterostructures (Fig. 4) is the cause. In these structures the observed hole current density from the surface is about 10^{-6} A/m^2. The current density of electrons from the surfaces of the n-Si/p-ZnO and n-Si/n-ZnO heterostructures is

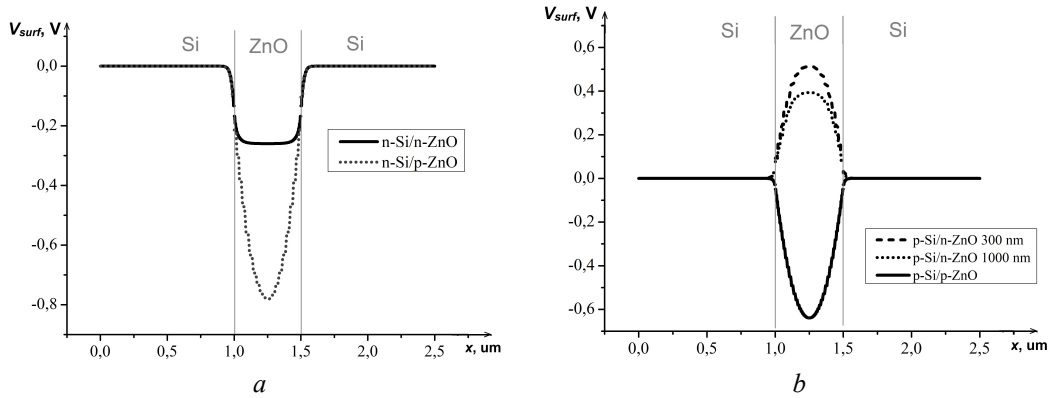
also about 10^{-6} A/m^2. In the p-Si/p-ZnO heterostructure the potential difference ΔV is 0.61 V. It forms the current of holes generated in zinc oxide from the surface of the heterostructure (hole current density is about 10^{-5} A/m^2).



a *b*

Fig. 3. Electric charge density on the surface of the structures: *a* – n-Si/n-ZnO and n-Si/p-ZnO; *b* – p-Si/n-ZnO and p-Si/p-ZnO under irradiation

The electron current density at the surface of the structure at the wavelengths of 300 nm and 350 nm is about 10^{-7} A/m^2. In the p-Si/n-ZnO heterostructure the potential difference ΔV depends on the wavelength of the incident radiation: –0.47 V (λ = 300 nm), –0.43 V (λ = 400 nm), –0.38 V (λ = 500 nm), and –0.35 V (λ = 1000 nm). Due to the absence of potential barriers for electrons from the silicon side at the p-Si/n-ZnO interface (Fig. 1, *c*) the electron current density reaches 7 A/m^2 at the radiation wavelength of 600 nm. The hole current density at the radiation wavelengths of 300 nm and 350 nm on the surface is about 10^{-6} A/m^2.



a *b*

Fig. 4. Electric potential on the surface of structures: *a* – n-Si/n-ZnO and n-Si/p-ZnO; *b* – p-Si/n-ZnO and p-Si/p-ZnO at different radiation wavelengths

The positive electric potential depends on the wavelength of the incident radiation and occurs only in the p-Si/n-ZnO heterostructure. Its value reaches 0.68 V in the absence of incident radiation and decreases in the presence of radiation by 0.06 V at the wavelength of 300 nm by 0.1 V at λ = 400 nm, by 0.15 V at λ = 500 nm, and by 0.18 V at λ = 1000 nm. In other cases, the potential on the surface of a zinc oxide nanoparticle is negative, but in the n-Si/p-ZnO structure, it is higher in modulus (–0.78 V) than in the n-Si/n-ZnO structures (–0.25 V) and p -Si/p-ZnO (–0.65V).

Conclusions

The simulation of the charge properties and currents in a zinc oxide nanoparticle in silicon heterostructures for the cases of n- and p-types of conductivity demonstrated differences in the electric charge and potential on the surface of heterostructures without significant differences depending on the wavelength of incident radiation. It is shown that the silicon/p-type zinc oxide nanoparticle heterostructure provides a negative potential and a negative surface charge on the surface of a zinc

oxide nanoparticle regardless of the wavelength of the solar radiation. It opens up additional possibilities for the photocatalytic use of zinc oxide in a wider emission spectrum than its own absorption spectrum. Achieving stable p-type conductivity of zinc oxide opens up many possibilities for creating optoelectric devices based on wide gap semiconductor materials. This will require better control over the natural n-type conductivity of zinc oxide which can compensate acceptor impurities.

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Authors' contribution

Kuraptsova A.A justified the choice of physical parameters, performed numerical solutions of the current transport equations and participated in the interpretation of the results.

Danilyuk A.L. defined the tasks that needed to be solved during the research and participated in the interpretation of the results.

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