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GaN-nanowire/Si solar cell: numerical modeling, fabrication and characterization

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Abstract. A silicon (111) based solar cell with an emitter layer of an array of GaN nanowires was proposed, synthesized, and studied. Theoretical and experimental volt-ampere and spectral characteristics of the solar cell were compared and analyzed. The density of surface states and lifetime of minority carriers in the active region were obtained with the use of numerical modeling. A significant effect of recombination on efficiency was demonstrated. The modeling results correspond well to the experimental data obtained via the characterization of the SC prototype.

1. Introduction

Today, the most promising alternative and renewable energy source on Earth is the sun. The percentage of annual production of solar photovoltaic energy in the total world energy output increased from 0.01% to 1.3% from 2004 to 2016 (according to the BP Statistical Review of World Energy 2017). Despite the fact that solar photovoltaics eliminate a number of problems caused by hydrocarbon and atomic energy sources solar cannot fully compete with them due to the maintenance costs of solar power plants, which are still several times more expensive than thermal power plants. Cost-effectiveness is the main problem facing the global realization of solar energy. Thus, scientists all over the world are trying to find a way to improve the efficiency of solar cells (SCs) and at the same time make them cheaper.

As silicon remains the main material in photovoltaics, its integration with other semiconductors is of great importance. Over the last few years, gallium nitride (GaN) has become one of the most popular semiconductor materials [1], and this compound is currently the focus of intensive research.

GaN, like most AlInN compounds, is a wide-band semiconductor with high electron mobility [2], which makes it an appropriate candidate as a wide-gap window material. Good thermal stability of GaN allows it to work under high operating temperatures [2], consequently making it a good candidate to be used in multi-junction concentrator SCs.

For SC optimization, it is necessary to have a quantitative understanding of the parameters that determine the operation of the structure. Since the operation and properties of heterostructure devices cannot be obtained analytically in most cases, computer modeling is usually used.

Semiconductor nanowires (NWs) represent perspective platform for realization of efficient optoelectronic and photovoltaic devices on inexpensive mismatched substrates [3, 4]. Our work is devoted to theoretical and experimental study of the characteristics of n-GaN NW/p-Si heterojunction SCs.

2. Experimental

In our experiment, n-GaN NWs/p-Si heterostructures were fabricated using plasma-assisted molecular beam epitaxy (MBE). The emitter layer (GaN) is presented in the form of a NW array. It should also be mentioned that such a NW array makes it possible to improve the light absorption without the use...
of special multilayer antireflection coatings [5, 6]. As previously reported, optimization of the NW morphology can provide low reflective losses [7].

Due to a significant lattice mismatch between GaN and silicon [8], buffer layers are known to be used in the MBE synthesis of GaN/Si. In this paper, we consider the structure without a buffer layer: after the oxide removal, the substrate was cooled down to a temperature of 810 °C (according to thermocouple measurements), and then growth of NWs was initiated.

Development of the SC involves fabrication of top and bottom contacts. At first, an aluminum bottom contact was thermally deposited and then annealed at 700°C in nitrogen atmosphere. At the next technological step, the structure was treated in hydrogen plasma in a plasma-enhanced chemical vapor deposition machine (PECVD) to reduce the number of the surface states. A SU-8 photoresist was used as an insulating layer to avoid the short-circuit between the top contact and silicon substrate. The top transparent contact in the form of an ITO film was deposited using magnetron sputtering technology. Several silver paste drops were placed over the ITO layer so as not to pierce the ITO film with the probe used for electronic measurements. The fabrication process is schematically shown in figure 1.

![Figure 1. Technological steps of the structure post-growth processing.](image)

The current-voltage characteristics (I-V characteristics) were measured using a Keithley 2400 SourceMeter multimeter and a thermo-stabilized stage under illumination conditions of the AM 1.5G solar spectrum. During the measurements, the temperature was maintained at 25 °C.

The spectral dependence of the external quantum efficiency (EQE) as well as the reflection spectrum were measured in the 400 – 1200 nm wavelength range using a M266 (Laser Solar) monochromator and a calibrated silicon photodiode with known spectral characteristics. An aluminum mirror was used as a reference for reflection measurements (figure 2).
Figure 2. Experimental reflection spectrum of the fabricated SC used in the modeling.

3. Modeling
The effective operation of the SC structure is highly dependent on the rate of carrier recombination. The presence of a heterointerface in the structure has a direct impact on its characteristics because of interface recombination. The surface of any semiconductor has a defined spectrum of surface states with energy levels inside the band gap, which act as recombination centers for charge carriers. The model we used in this study simulated surface states that are uniformly distributed over the band gap and located at the boundary of the active region (silicon surface), as well as Fermi level pinning at the interface due to recharging of these surface states. Another important parameter affecting the SC characteristics is the lifetime of minority carriers in the active region, which determines bulk recombination.

The main aim of computer modeling was to quantify the density of heterointerface surface states and the lifetime of minority carriers in the active region (silicon substrate).

Comsol Multiphysics was used as a software package to calculate the solar cell. The parameters of the materials used in this paper were taken from [9]. The simulation accounted for the Fermi-Dirac statistics for charge carriers, the model of band gap narrowing at a high doping level [10], the model of interband tunneling through the GaN / Si interface [11], the Shockley-Reed-Hall recombination [12], the carrier recombination at the GaN / Si interface [13], and Auger recombination [14]. Tunneling through barriers was also taken into account. To ensure accuracy, the optical properties of the studied structure were included in calculations (figure 2).

Figure 3 shows the calculated band diagram of the structure.

Figure 3. Modeled band diagram of SC.
4. Results and discussion
The variation in the lifetime of minority carriers in the substrate showed an effect on both open-circuit voltage (Voc) and short-circuit current (Isc), while the relative change of Isc with a lifetime decrease is more significant than for Voc. To calculate the density of surface states, the capture cross section of electrons and holes was fixed at a value of $10^{-14}$ cm$^2$. The simulation showed that an increase in the density of surface states leads to a rapid decrease in Voc, but Isc does not change up to a density of states of $10^{13}$ cm$^{-2}$, above which it begins to fall sharply. This phenomenon can be explained by analyzing the operation of SC in the following configuration of charge carrier traps. Since the direct separation of charge carriers occurs at the n-GaN / p-Si interface, free carriers such as electrons from GaN and holes from silicon predominate in recombination at this interface. Thus, the SC is shunted by the interface surface states. In this case, the recombination rate depends on the product of the concentrations of electrons and holes at the interface, and these values increase exponentially when a positive bias is applied to the element. Since Voc corresponds to the equality of the photogeneration rate and charge carrier recombination, an increase in the density of states leads to a voltage drop. However, at zero bias voltages the interface concentrations of electrons and holes are low and this leakage channel is significantly suppressed, so Isc does not change with increasing density of states. If the density of states is greater than $10^{13}$ cm$^{-2}$, the recombination rate at zero bias becomes comparable to the generation rate.

The best correspondence between theory and experiment was obtained with a lifetime of $10^{-5}$ seconds and a surface state density of $10^{13}$ cm$^{-2}$.

A comparison of the experimental external quantum efficiency (EQE) of the fabricated SC with the modeling results is shown in figure 4.

![Figure 4. Theoretical and experimental EQE spectral dependencies.](image)

As can be seen in figure 4, the EQE depends on the applied bias reverse voltage, which is associated with a change of the surface recombination rate as well as with a change of the series resistance of the structure. The long-wave parts of the experimental and calculated spectra, which mostly correspond to the current density and bulk lifetime, are in good agreement. A possible reason for the discrepancy of the short-wave parts may be the absorption of light in ITO grown at low temperature, or the reflection measurement error caused by the inability to measure the diffuse scattering and reflection with the lateral component.
Figure 5 shows a comparison of the experimentally measured and modeled dark and light I-V characteristics of the SC. Analysis of the graph allows us to conclude that the selected model describes the quantitative characteristics of the SC, such as open-circuit voltage, short-circuit current and fill factor with high accuracy. However, a large difference was obtained in the dark I-V characteristics as well as the presence of a kink in the experimental light I-V curve near the open-circuit voltage, which indicates the presence of a potential barrier for current. It should be mentioned that the fabricated SC has a high series resistance, which is explained by the presence of an unannealed ITO layer.

5. Summary
In our paper, we studied both the theoretical and experimental characteristics of the GaN-NWs/Si heterostructure SC. Optical properties were taken into account using the measured reflection spectrum of the processed sample. An analysis of the EQE spectra and current-voltage characteristics showed good agreement between the experimental data and simulation results. The best correspondence between theory and experiment was obtained with a lifetime of $10^{-5}$ seconds and a density of surface states of $10^{13}$ cm$^{-2}$. The high density of surface states in combination with the short lifetime of minority carriers in the active region causes a significant recombination impact on the SC efficiency. Further refinement of the model should be carried out for a more accurate calculation of the properties of the proposed SC.

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