Nitride solar cells - improving efficiency based on simulation

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Abstract. Solar cells model based on GaN/Si heterostructure was made. The optimum heterostructure design and doping profile were defined. Quite high solar cell efficiencies based on n-GaN–p-Si heterostructures such as 14.35 % at 1 · AM 1.5 and 21.10 % at 1000 · AM 1.5 were achieved.

1. Introduction
Nowadays, energy saving and renewable energy source are cruel popular and important. The rapid increase in energy consumption will be one of the most characteristic features of the technical activities of mankind in the second half of the 21-st century. The development of energy until recently did not meet fundamental difficulties.

One of the most reasonable renewable energy source is the sun. It can give the Earth power about $10^{17} \text{ W} / \text{ m}^2$ (for the side at our planet facing the sun). The intensity of sunlight at sea level in the southern latitudes, when the Sun is at its zenith, is $1 \text{ kW} / \text{ m}^2$. By developing highly efficient methods for converting solar energy, the sun can provide rapidly growing energy needs for hundreds of years.

Achieving maximum solar energy conversion now is one of the main goals. Now it is need to find cheap and effective material for such devices. The main performance characteristic of solar cells is the peak power, which is expressed in watts. This characteristic shows the output power of solar cells under optimal conditions: 1 kW / m² solar radiation, 25 °C ambient temperature, 45 ° wide solar spectrum (AM1.5). Under normal conditions, it is extremely rare to achieve such values, the illumination is lower, and the module heats up higher (up to 60-70 degrees).

By connecting the SC in-series, it is possible to increase the potential difference, by connecting in-parallel the current [1]. Thus, by combining the connections, it is possible to achieve the required parameters in current and voltage, and, consequently, in power. In addition, not only photocells in a single solar cell (SC), but also the SC as a whole can be connected in-series or in-parallel. If the solar cell has an ideal current-voltage characteristic, then the corresponding equivalent circuit is shown in figure 1, where a direct current source $I_s$ is connected in-parallel to the p-n– junction, which describes the nonequilibrium carriers excitation by solar radiation.

The current-voltage characteristic of such a device is determined by the expressions

$$I = I_s (e^{qV/kT} - 1) - I_L,$$

(1)
solar cells efficiency ($\eta$)

$$\eta = P_{EL} / P_{OPT},$$

where $I_L$ - a direct current that describes the nonequilibrium carriers excitation by solar radiation, $I_s$ - the diode saturation current, $A$ - the area of the device, $\tau_n$ - the electron lifetime, $\tau_p$ - the hole lifetime, $N_A$ - the acceptor concentration, $N_D$ - the donor concentration, $D_p$ - the hole diffusion coefficient, $D_n$ - the electron diffusion coefficient, $N_c$ - the concentration of charge carriers in the conduction band, $N_V$ - the concentration of charge carriers in the valence band, $P_{OPT}$ - the radiation power, $P_{EL}$ - electric power.

Efficiency measurements are typically obtained under conditions AM 1.5 solar radiation that imitates the spectral distribution of sunlight under a given atmospheric condition (figure 2). The solar spectrum AM 1.5 is shown, as well as the band gap for some materials [2, 3].

In the late 1990s, many research groups focused on the different types development of two-cascade solar cells. Later the third cascade with a p-n–junction in the germanium substrate was also included into the photoelectric conversion process. The complication of the multi cascade solar cells structure is due to the problem of growth the photoactive thinner region with flexible band gap to convert maximum solar energy. New materials for high efficiency solar cells can be direct-gap nitride
semiconductors with various bandgaps: InN (E_g ~ 0.65 eV), GaN (E_g ~ 3.4 eV), AlN, (E_g ~ 6.2 eV) and solid solutions based on them. Such materials can be grown by different contemporary method like MOCVD or MBE or others [4, 5]. Even for individual SCs, it is theoretically possible to achieve an efficiency of converting solar energy into electrical energy of more than 50 %, for example, using an InGaN heterostructure with an indium concentration 40 % grown on a silicon substrate. Unfortunately, these hopes remain theoretical because it is very difficult to grow high-quality InGaN with high indium concentration. The problem is that there is a mismatch between the constant lattices in InN and GaN (~ 11 %). Despite difficulties, now it is very promising to create nitride semiconductors for use in solar cells.

In 2009, the American company RoseStreet Energy Labs Inc announced the creation of a silicon nitride solar cell [6-9]. Researchers used a 12-period structure with multiple quantum well (QW) – combination – InGaN (QW) and GaN barriers (3 nm / 16 nm) with an In content in the QW about 35 %.

The problem with current silicon or GaAs solar cells (SC) is not their high efficiency, which is about 11-14 %. The goal of current work is to find possibility for SC efficiency rise based on nitride heterostructure.

2. Experiment

The SC efficiency is determined by the following expressions:

\[ \eta_i = FF \cdot (U_{oc} \cdot J_{sc}) / (1 \cdot AM1.5) , \]

\[ \eta_{1000} = FF \cdot (U_{oc} \cdot J_{sc}) / (1000AM1.5) , \]

\[ FF = (U_m \cdot J_m) / (U_{oc} \cdot J_{sc}) , \]

where U_{oc} - the voltage on the SC in an open circuit, I_{sc} - the short circuit current through the SC.

These parameters are determined from the current–voltage characteristics (I-V) simulation results at a solar illumination power - 1 · AM - 1.5 = 88.4 mW / cm^2 or 1000 · AM 1.5 = 84.4 W / cm^2. Based on I-V simulation, it is possible to determine the parameters U_m and I_m and by them the maximum value of the electric power P_a generated by the solar cell can be calculated.

The choice for SC heterostructure can be made based on three heterojunctions band diagrams: p-GaN – n-Si, n-GaN – p-Si and n-GaN – n-AlN – p-Si (figure 3).

Diagrams were created during simulation in Sim Windows software [10-14]. The n-GaN layer was 500 nm thick and an electron concentration was 10^{17} cm^{-3}, the p-GaN layer was 500 nm with hole concentration 10^{17} cm^{-3}, the n-AlN layer - 1 nm and the electron concentration - 10^{17} cm^{-3}, n-Si / pSi layers were 500 nm thick and carrier concentrations - 10^{-17} cm^{-3}.

The creation of SCs based on the p-GaN – n-Si heterojunction (figure 3a), is impossible, since the holes generated by radiation in the n-Si region cannot reach the p-GaN region due to the large gap of the valence bands at the heterojunction boundary.

The creation of SCs based on the n-GaN – p-Si heterojunction (figure 3b), is possible, since the electrons generated by radiation in the p-Si region can easily fall into the n-GaN region.

The creation of SCs based on the n-GaN – n-AlN – p-Si heterojunction (figure 3c), is possible, but complicated since the electrons generated by radiation in the p-Si region can reach the n-GaN region only if they can overcome the high energy barrier at the n-AlN – p-Si heterojunction due to tunneling. Tunneling simulations (using the Sim Windows software) at n-AlN layer (1 nm thickness) did not give possibility to create SC. As a result, the n-GaN – p-Si heterostructure was chosen as the main type for the solar cell (figure 4).

Initial data for typical n-GaN – p-Si heterostructure simulation was:

- the n-GaN upper heterostructure layer (a donor concentration - N_d = 10^{17} cm^{-3} and a 50 nm thickness);
- the lower p-type Si layer for maximum light absorption (an acceptor concentration \( N_a = 10^{16} \text{ cm}^{-3} \) and 20 \( \mu \text{m} \) thickness);
- the Si substrate (an acceptor concentration \( N_a = 10^{18} \text{ cm}^{-3} \) and 100 - 500 \( \mu \text{m} \) thickness).

**Figure 3.** Band diagrams for heterojunctions: p-GaN – n-Si (a), n-GaN – p-Si (b) and n-GaN – n-AlN – p-Si (c).
3. Result and Discussion

In figure 5 some results are presented.

Figure 5 shows band diagrams without and with irradiation, the optical generation and the nonradiative recombination rate according to the Shockley-Hall-Reed mechanism.

It is clearly seen that the recombination rate is lower than the electron–hole pairs generation rate in the p-Si base region. With increasing forward voltage $U_m$, the absolute value of $J_m$ will decrease to zero, which corresponds to the voltage $U_{ShC}$. $I–V$ characteristic for a lighting power $1000 \cdot AM\ 1.5$ is shown in figure 6. The data for the two lighting modes are given in table 1.

Table 1 also shows the data for the electric power $P = U \times J \times 1 \ cm^2$ generated by the solar cell at various voltage on the SC. It can be seen that with radiation $1 \cdot AM\ 1.5$, the maximum power value is achieved at a voltage $U_m = 0.45 \ V$ and a current $J_m = 26.9 \ mA$ at level - $1000 \cdot AM\ 1.5$, the maximum power value is achieved at $U_m = 0.60 \ V$ and a current $J_m = 26.9 \ A$. In figure 6 the maximum value of the generated power is equal to the areas of the graphically inserted rectangles.
Figure 6. I – V characteristic for illumination power 1 ∙ AM 1.5 and 1000 ∙ AM 1.5.1 - at 1 ∙ AM1.5; 2 - at 1000 ∙ AM1.5.

Table 1. The data for the two lighting modes.

| U_opt, V | J, mA/cm² | P_el=U_el×J×1 cm², mW | J, A/cm² | P_el=U_opt×J×1 cm², W |
|----------|-----------|------------------------|----------|-----------------------|
| 0        | J_sc=27.8 | 0                      | J_sc=30.9 | 0                     |
| 0.05     | 27.8      | 1.390                  | 30.90    | 1.55                  |
| 0.10     | 27.8      | 2.780                  | 30.90    | 3.09                  |
| 0.15     | 27.8      | 4.170                  | 30.90    | 4.64                  |
| 0.20     | 27.8      | 5.560                  | 30.85    | 6.17                  |
| 0.25     | 27.8      | 6.950                  | 30.85    | 7.71                  |
| 0.30     | 27.7      | 8.310                  | 30.80    | 9.24                  |
| 0.35     | 27.7      | 9.700                  | 30.80    | 10.8                  |
| 0.40     | 27.6      | 11.04                  | 30.80    | 12.3                  |
| U_m=0.45 | J_m=27.9  | 12.11                  | 30.80    | 13.9                  |
| 0.50     | 22.2      | 11.10                  | 30.75    | 15.4                  |
| U_oc=0.542 | 0.06   | 0.035                  | -        | -                     |
| 0.55     | -0.01     | -                      | 30.60    | 16.8                  |
| U_m=0.60 | -0.01     | -                      | J_m=29.60| 17.8                  |
| 0.65     | -         | 24.50                  | J_m=29.60| 17.8                  |
| 0.70     | -         | 4.670                  | 4.670    | 3.27                  |
| U_oc=0.707 | -     | -                      | -2.720   | -                     |
| 0.75     | -         | -10.70                 | -50.70   | -                     |

Table 2 shows the main data for calculating the form factors FF and the efficiency for the solar cells η₁ and η₁₀₀₀ according to formulas (4), (5) and (6).
Table 2. The data for calculating the form factors FF and the efficiency for the solar cells $\eta_1$ and $\eta_{1000}$.

|                  | 1 · AM 1.5 (S=1cm$^2$) | 1000 · AM 1.5 (S=1cm$^2$) |
|------------------|-------------------------|-----------------------------|
| $U_{OC}$, V      | $J_{sc}$, mA           | $J_{lm}$, mA               | FF, % | $\eta_1$, V | $U_{OC}$, V | $J_{sc}$, mA | $J_{lm}$, mA | FF, % | $\eta_{1000}$, % |
| 0.542            | 27.8                    | 0.45                        | 26.9  | 0.803        | 14.35        | 0.707         | 30.9          | 0.60  | 29.6         | 0.813 | 21.1 |

The results of the n-GaN – p-Si solar cell characteristics simulation relate to a heterostructure with the following parameters; n-GaN layer thickness $d_{GaN} = 50$ nm; the p- Si layer thickness in which the nonequilibrium charge carriers generation by radiation occurs, $d_{Si} = 20$ μm; the donor concentration in the n-GaN layer is $N_d = 10^{17}$ cm$^{-3}$, the acceptor concentration in the p-Si layer is $N_a = 10^{16}$ cm$^{-3}$, and the lifetime of the injected charge carriers in the p-Si layer is $\tau = 10^{-6}$ s. It was found that changes in $d_{GaN}$ in the range from 30 nm to 500 nm, $N_d$ in the range $10^{17}$ - $10^{19}$ cm$^{-3}$, and $\tau$ in the range from $10^{-6}$ s to 100 · $10^{-8}$ s practically do not influence on the SC simulation results.

4. Conclusion
Detected efficiencies such as 14.35 % at 1 · AM 1.5 and 21.10 % at 1000 · AM 1.5 are quite high. The advantages of using these elements on silicon versus AlGaAs solar cells are the significantly lower cost of the substrates, significantly higher thermal conductivity and due to this longer device life time.

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