Simulation of double-junction III-phosphides/silicon solar cells

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Abstract. The characteristics of two-junction solar cells were calculated in this work, in which phosphides of group III are used as the top junction, and Si as the bottom junction. The following ternary phosphide compounds Ga\textsubscript{0.52}In\textsubscript{0.48}P (1.85 eV), GaPN\textsubscript{0.02} (1.9 eV), and GaPN\textsubscript{0.04} (1.7 eV) were considered as the active material of the top junction. The use of GaPN\textsubscript{0.04} allowed one to reach the current matching with the bottom Si junction and an efficiency of 30\% was achieved. In addition, the influence of the layer thickness, the lifetime of minority charge carriers and the electronic affinity on the efficiency of solar energy conversion were considered.

1. Introduction
The development of solar energy requires a further increase in conversion efficiency. However, silicon single-junction solar cells (SCs), which are the basis of terrestrial photovoltaics, have practically reached the efficiency limit [1]. A further increase in efficiency is possible with an increase in the number of junctions. One of the most promising ways to create two-junction SC based on Si is an integration with III-V compounds. The formation of III-V layers on the silicon surface is a complex technological task that requires the use of expensive epitaxial methods, high growth temperatures, and also imposes restrictions on the choice of materials in terms of the crystal lattice parameter, which together is a significant obstacle to the development of this path. However, it has recently been shown that epitaxial and microcrystalline layers of III-phosphides can be obtained by plasma deposition at low temperatures [2]. The possibility of mass production of this technology is promising for photovoltaics. In this work, using computer simulation, an assessment was made of the potential possibility of using III-phosphides as the top junction of a double-junction SC with a bottom junction based on a Si substrate. The key feature of this simulation is that potentially defective phosphide layers (for instance due to microcrystalline structure) were taken into account. Therefore, the p-i-n structure was considered, and the effect of defects was also taken into account.

2. Simulation of top junction
Computer simulations were carried out using the AFORS-HET v2.5 software. The modeling was carried out in two stages. At the first stage of modeling, the calculation was carried out without taking into account the effect of defects, at the second stage the defects were taken into account. The following phosphides were considered as active materials of the top junction: Ga\textsubscript{0.52}In\textsubscript{0.48}P with a band gap of
1.85 eV, in which Al$_{0.53}$In$_{0.47}$P and GaP layers were used as a wide-gap window and a back potential barrier (BSF). For subsequent calculations, the doping level was taken equal to $10^{18}$ cm$^{-3}$ for the n- and p-layers and $10^{12}$ cm$^{-3}$ for the i-layer. Schematic representations of these structures are presented in Figure 1 a, b.

![Schematic representation of the top junction on GaP (a) and Al$_{0.53}$In$_{0.47}$P (b).](image)

The radiative recombination rate was taken equal to $1\cdot10^{-13}$ cm$^3$/s, the values of the Auger recombination coefficients for electrons and holes were $1\cdot10^{-30}$ cm$^6$/s. The phosphides GaPN$_{0.02}$ and GaPN$_{0.04}$ were also considered for the top junction. The given nitrogen concentrations of 2% and 4% provide the band gap equal to 1.9 eV and 1.7 eV, respectively. Schematic representations of these structures are presented in Figure 2 a, b.

![Schematic representation of the top junction with an i-layer based on GaPN$_{0.04}$ (a) and GaPN$_{0.02}$ (b).](image)

The main parameters of the materials used in the calculation are shown in Table 1.

**Table 1.** Material parameters of the upper transition layers.

| Layers       | $\varepsilon_0$ | $E_g$, eV | $\chi_0$, eV | $\mu_e/\mu_h$, cm$^2$V$^{-1}$s$^{-1}$ | $N_C$, cm$^{-3}$ | $N_V$, cm$^{-3}$ |
|--------------|-----------------|----------|--------------|--------------------------------------|-----------------|-----------------|
| n-GaP        | 11.1            | 2.26$^{[5]}$ | 3.8          | 250/150                              | 1.8$\cdot10^{19}$ | 1.9$\cdot10^{19}$ |
| n- Al$_{0.53}$In$_{0.47}$P | 11.9            | 2.35$^{[4]}$ | 3.78$^{[6]}$ | 100/50                               | 2$\cdot10^{19}$ | 2$\cdot10^{19}$ |
| i- GaPN$_{0.04}$ | 11.8            | 1.9$^{[5]}$ | 3.8$^{[5]}$ | 500/30$^{[7, 8]}$                    | 1.9$\cdot10^{19}$ | 1.9$\cdot10^{19}$ |
| i- GaPN$_{0.02}$ | 11.1            | 1.7$^{[3]}$ | 4.08         | 50/50$^{[3]}$                       | 1.8$\cdot10^{19}$ | 1.9$\cdot10^{19}$ |
| p-GaP        | 11.1            | 2.26$^{[3]}$ | 3.8          | 250/150                              | 1.8$\cdot10^{19}$ | 1.9$\cdot10^{19}$ |
| p- Al$_{0.53}$In$_{0.47}$P | 11.9            | 2.35$^{[4]}$ | 3.78$^{[6]}$ | 100/50                               | 2$\cdot10^{19}$ | 2$\cdot10^{19}$ |

Based on the results of the I-V curve calculations and the performed variation in thickness, it was found that the structure in which n and p layers based on GaP, and an i-layer based on Ga$_{0.53}$In$_{0.47}$P have a high FF, which indicates that there is no limitation for the transport of charge carriers. In addition, high $V_{OC} = 1651$ mV, $J_{SC} = 13.95$ mA/cm$^2$, FF = 91.55% and efficiency = 20% are provided. Also, according to the results of calculations, it was found that the structure based on GaPN$_{0.02}$ is significantly inferior in output parameters to the structure of GaPN$_{0.04}$. In particular, this affects the maximum achievable value of the short-circuit current density. It is significantly lower compared that for the structure based on GaPN$_{0.04}$. With a thickness of 1.4 μm, a current density of 17.5 mA/cm$^2$ is achieved for GaPN$_{0.02}$. For GaPN$_{0.04}$, at the same thickness, a current density of 22.5 mA/cm$^2$ was reached. This is due to the band gap difference, for the higher gap less solar radiation is absorbed in the material, therefore, the current density is lower. As a result, the efficiency value is also lower. For GaPN$_{0.04}$ the efficiency was 22.34%, for GaPN$_{0.02}$ - 20.79%.
At the second stage of the simulation, the calculation was carried out for heterostructures in which the Ga$_{0.52}$In$_{0.48}$P (1.85 eV) and GaPN$_{0.04}$ (1.7 eV) layers were used as the top junction. The peculiarity of the second stage of modeling was the introduction of defects. An acceptor-type defect with a point distribution was introduced into the Ga$_{0.52}$In$_{0.48}$P layer. The energy position of the defects was 1.1 eV, and the concentration was $1 \times 10^{14}$ cm$^{-3}$. The calculation of the dependence of the SC parameters on the lifetime of charge carriers in Ga$_{0.52}$In$_{0.48}$P (which was varied in the range of $10^7$ - $10^{15}$ s) due to the variation of the capture cross-section for electrons and holes ($10^{-14}$ ... $10^{-9}$ cm$^2$) was performed. The resulting dependencies are shown in Figure 3 (a). The $V_{OC}$ monotonically decreases with lifetime decrease, while $J_{SC}$ drastically drops for lifetime below $10^9$ s.

![Graph](image_url)

**Figure 3.** Influence of the lifetime on the current density and the voltage of Ga$_{0.52}$In$_{0.48}$P (a) and GaPN$_{0.04}$ (b).

An acceptor-type defect with a point distribution was introduced into the GaPN$_{0.04}$ layer. The energy position of the defects was 0.85 eV. The influence of the lifetime of charge carriers in GaPN$_{0.04}$ as well as the valence band offset ($\Delta E_V$) at the GaPN/GaP interface on the SC performance was explored. The variation of the lifetime is shown in Figure 3 (b). It showed that the values should be at least $10^9$ s to achieve the current matching with bottom Si junction. The value of $\Delta E_V$ at the GaPN/GaP interface, which is not exactly known, has a significant influence on transport properties. An increase of $\Delta E_V$ leads to the formation of a potential barrier at the i-GaPN/p-GaP interface that prevents the transport of holes (Figure 4 a) and, as a consequence, leads to a significant decrease in the fill factor of the I–V curve. Indeed, for $\chi = 4.08$ eV ($\Delta E_V = 0.3$ eV) FF is equal to 85.12%, while for $\chi = 3.8$ eV ($\Delta E_V = 0.6$ eV) FF = 63.69%. This transport limitation due to large $\Delta E_V$ significantly manifested in the dependence of the short-circuit current on the layer thickness, at which a sharp drop of $J_{SC}$ is observed when thickness reaches 0.8 µm (Figure 4 b). Thus, the influence of band discontinuities must be taken into account when analyzing experimental data. For the further calculations, $\Delta E_V$ at the interface was taken equal to 0.3 eV ($\chi = 4.08$ eV).

3. **Simulation of double-junction solar cell**

To achieve maximum efficiency of double-junction SC it is necessary to fit current matching condition. The top junction based on Ga$_{0.52}$In$_{0.48}$P or GaPN$_{0.04}$ (1.7 eV) should have practically the same short-circuit current as the bottom junction based on n-GaP/p-Si. The performed variation in thickness for GaPN$_{0.04}$ showed that the thickness at which the current matching is ensured is 0.48 µm, while for Ga$_{0.52}$In$_{0.48}$P this thickness is 0.3 µm.
The final stage of the calculation is the calculation of the characteristics of double-junction SCs based on group III phosphides - Ga$_{0.52}$In$_{0.48}$P and GaPN$_{0.04}$ (1.7 eV) and silicon. A schematic representation of the GaPN/Si and the I-V curves are shown in Figure 5 (a, b). The main parameters of the materials used in the calculation of bottom junction are given in Table 2. The values of doping levels and layer thicknesses for Ga$_{0.52}$In$_{0.48}$P/Si and GaPN$_{0.04}$/Si double-junction SC are given in Table 3, 4, respectively.

The obtained I-V curves of the heterojunction structure demonstrates the best current matching and also provides high values of the open circuit voltage. Thus, it is possible to achieve a high value of the short-circuit current density $J_{SC} = 18.75$ mA/cm$^2$ and $V_{OC} = 1.92$ V. As a result, the reaches 30%. A schematic representation of the structure based on GaInP/Si and the I-V characteristic of the heterojunction are shown in Figure 6 a, b, respectively.

Table 2. Material parameters of heterostructure layers.

| Layers       | $\varepsilon_0$ | $E_g$, eV | $\chi$, eV | $\mu_n/\mu_p$, cm$^2$V$^{-1}$s$^{-1}$ | $N_C$, cm$^{-3}$ | $N_V$, cm$^{-3}$ |
|--------------|-----------------|-----------|------------|-----------------------------------|-----------------|-----------------|
| p-Si         | 11.7            | 1.124     | 4.05       | 1107/424.6                        | 3.2-10$^{19}$   | 1.8-10$^{19}$   |
| (p) a-Si     | 11.9            | 1.6       | 3.85       | 10/1                              | 2.10$^{20}$     | 2.10$^{20}$     |

Table 3. Ga$_{0.52}$In$_{0.48}$P/Si 2J SC structure.

| Layers       | Thickness, µm | Doping level, cm$^{-3}$ |
|--------------|---------------|-------------------------|
| n-GaP        | 0.1           | 10$^{18}$               |
| i- Ga$_{0.52}$In$_{0.48}$P | 0.3           | 10$^{12}$               |
| p-GaP        | 0.1           | 10$^{18}$               |
| Tunnel junction | n-GaP        | 0.05                    | 10$^{19}$ |
|              | p - Si        | 300                     | 10$^{16}$ |
|              | (p) a-Si      | 0.03                    | 10$^{19}$ |

Table 4. GaPN$_{0.04}$/Si 2J SC structure.

| Layers       | Thickness, µm | Doping level, cm$^{-3}$ |
|--------------|---------------|-------------------------|
| n-GaP        | 0.1           | 10$^{18}$               |
| i- GaPN$_{0.04}$ | 0.448       | 10$^{12}$               |
| p-GaP        | 0.1           | 10$^{18}$               |
| Tunnel junction | n-GaP        | 0.05                    | 10$^{19}$ |
|              | p - Si        | 300                     | 10$^{16}$ |
|              | (p) a-Si      | 0.03                    | 10$^{19}$ |
respectively. As a result, the efficiency is also higher: 30.8% for GaPN$_{0.04}$ (1.7 eV) versus 29.5% for Ga$_{0.52}$In$_{0.48}$P. The calculation results are presented in Table 5.

| Structure        | V$_{OC}$, mV | J$_{SC}$, mA/cm$^2$ | FF, % | Eff, % |
|------------------|--------------|---------------------|-------|--------|
| GaPN$_{0.04}$/Si | 1.92         | 18.75               | 85.6  | 30.8   |
| Ga$_{0.52}$In$_{0.48}$P/Si | 2.14 | 15.47               | 89.2  | 29.5   |

The calculation of the spectral characteristics was also carried out. The spectral dependences of the quantum efficiency of two-junction SC based on GaPN/Si and GaInP/Si are shown in Figure 7.

The spectral characteristic also shows that the structure based on GaPN$_{0.04}$ makes it possible to achieve a higher short-circuit current due to a wider spectrum of absorbed photons. However, the influence of defects in the layers and band offset at the GaP/GaPN$_{0.04}$ interface can minimize this advantage. Thus, further experimental studies of the properties of layers and structures based on group III phosphides grown on silicon are required.
Figure 7. Spectral characteristics of two-junction SCs based on GaPN$_{0.04}$ (1.7 eV) and Ga$_{0.52}$In$_{0.48}$P.

4. Conclusion

The simulation showed that the use of SCs based on group III phosphides and silicon such as GaPN$_{0.04}$/Si and Ga$_{0.52}$In$_{0.48}$/Si is a promising way to reach high efficiency. The influence of the thickness of the i-layer of the upper junction on the filling factor of the I–V characteristic is shown. The influence of the lifetime of charge carriers on the efficiency of solar energy conversion was also considered, and it was found that in order to achieve the best matching in terms of current density, this value should reach at least $10^{-9}$ s for both structures. In addition, for the GaPN$_{0.04}$ structure, the influence of band discontinuity on the transport of charge carriers was considered. Based on the results of calculations, it was found that the most promising application can find a structure based on GaPN$_{0.04}$, since higher $J_{SC}$ values are provided for it and the efficiency reaches 30%.

Acknowledgments

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