ANISOTYPE GaAs BASED HETEROJUNCTIONS FOR III-V MULTIJUNCTION SOLAR CELLS

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ABSTRACT: The design of anisotype heterojunctions with an n-type wide band gap emitter layer (GaInP, AlInP or AlGaAs) and a p-type GaAs base layer was analyzed for application as a middle subcell of multijunction cells. Theoretical estimations made by numerical simulations have demonstrated that, when performance of conventional GaAs homojunction subcell is limited by the charge carrier recombination in an n+ GaAs emitter, the proposed design could increase the open circuit voltage as well as the cell efficiency. The influence of the defect density at the wide gap emitter/base heterointerface on the solar cell performance was also analyzed. The efficiency of n-AlInP/p-GaAs and n-AlGaAs/p-GaAs heterojunctions was shown to be independent of the interface density of states up to the value of 10^{11} cm^{-2} eV^{-1} (for the capture cross section value equal to 10^{-14} cm^2). This fact makes them attractive for application in high efficiency solar cells. In contrary, the n-GaInP/p-GaAs heterojunction exhibits a strong sensitivity of the efficiency to the interface states that can limit its application.
Keywords: Heterojunction, III-V Semiconductors, Multijunction Solar Cell

1 INTRODUCTION

Multijunction solar cells based on III-V compounds have reached the highest efficiency, while many efforts for the further efficiency increase are still being made. There are different concepts for the further III-V multijunction solar cells development like an increase of the number of subcells or a variation of the subcell band gaps using metamorphic growth [1]. However, all of them are based on the use of p-n homojunctions as photoactive junctions.

Another approach to the III-V multijunction solar cells design is explored in the paper, namely the usage of anisotype heterojunction with wide a band gap emitter layer for the photoactive GaAs junction of the middle subcell instead of a conventional p-n homojunction. The heavily doped GaAs emitter layer may be very defective having the small charge carrier lifetime that results in significant recombination losses in this layer. In case of the emitter layer with a wider band gap compared to GaAs (GaInP, AlInP or AlGaAs) one can expect a reduction of the recombination losses in the emitter. Because the recombination rate is determined by the minority charge carrier concentration [2], the potential barriers at the heterointerface formed due to band discontinuities can limit the minority charge carrier transport from the base to the emitter. Additionally, less photons are absorbed in the wide band gap emitter (short wavelength photons are mostly absorbed by the top subcell) and, therefore, less charge carriers are generated in this layer compared to GaAs emitter. From this point of view the lifetime of wide band gap emitter layer should have lower influence on solar cell performance.

The potential advantage of middle GaAs (or GaInAs with low In content) subcell with different wide band gap emitter layers (GaInP, AlInP AlGaAs) is analyzed in this paper using computer simulations.

2 SIMULATION DETAILS

The computer simulations were made using AFORS-HET 2.2 software [3]. Four different solar cell structures based on traditional n-p GaAs homojunction and n-AlInP/p-GaAs, n-GaInP/p-GaAs and n-AlGaAs/p-GaAs heterojunctions with $Al_{0.53}In_{0.47}P$, $Ga_{0.52}In_{0.48}P$ and $Al_{0.8}Ga_{0.2}As$ emitter layer, respectively, were simulated. In order to analyze the properties of the middle subcell the additional absorbing AlInP, GaInP and GaAs layers, which reproduce the absorption of the GaInP top subcell and the tunnel junction, were introduced at front. The layers sequences, thicknesses and doping levels of the simulated solar cells are presented in Table I. The main material parameters used in the calculations are given in Table II. The values of the minority carrier lifetime in the emitter and base layers were varied.

Table I: Layers' thickness and doping level

	n-p GaAs	n-wide gap emitter/ p-GaAs
Absorbing layer	$Al_{0.53}In_{0.47}P$ 15 nm	
Absorbing layer	$Ga_{0.52}In_{0.48}P$ 500 nm	
Absorbing layer	GaAs 15 nm	
Window	n-$Al_{0.8}Ga_{0.2}As$ 30 nm/ 3×10^{18} cm^{-3}	none
Emitter	n-GaAs 100 nm / 3×10^{18} cm^{-3}	n-wide gap emitter 30 nm / 3×10^{18} cm^{-3}
Base	p-GaAs 2500 nm / 4×10^{17} cm^{-3}	
BSF	p-$Al_{0.8}Ga_{0.2}As$ 30 nm / 10^{18} cm^{-3}	

Table II: Values of the band gap (E_g) and the electron affinity (χ) of the materials used in the simulations

Material	E_g (eV)	χ (eV)
GaAs	1.42 [2]	4.07 [2]
$Ga_{0.52}In_{0.48}P$	1.85 [4]	4.01 [7]
$Al_{0.53}In_{0.47}P$	2.35 [5]	3.78 [7]
$Al_{0.8}Ga_{0.2}As$	2.09 [6]	3.53 [8]

When the carriers recombination at the interface states was analyzed the interface was described by introducing a very thin (d = 1 nm) defective GaAs layer between the n-type wide band gap emitter and the p-GaAs base layers. The energetic defect distribution (g_{it}) in this interface layer was taken constant through the bandgap, assuming donor/acceptor-like defects in the lower/upper half of the bandgap. The interface defect density is described as $D_{it} = g_{it} \times d$.

3 RESULTS AND DISCUSSIONS

The fragment of the calculated band diagram of the n-p GaAs homojunction solar cell is presented in Fig.1. For this structure, a potential barrier in the valence band formed by the n-AlGaAs window layer prevents the hole transport from the emitter to the tunnel junction. This conventional design allows one to avoid the recombination in the n+ tunnel junction layer of holes generated in the emitter and the depletion region. But it does not allow one to avoid the carrier recombination in the emitter layer, which can be significant. For example, the calculated generation and recombination rates for n-p GaAs homojunction solar cells under AM1.5D illumination at short circuit current condition is given in Fig.2.

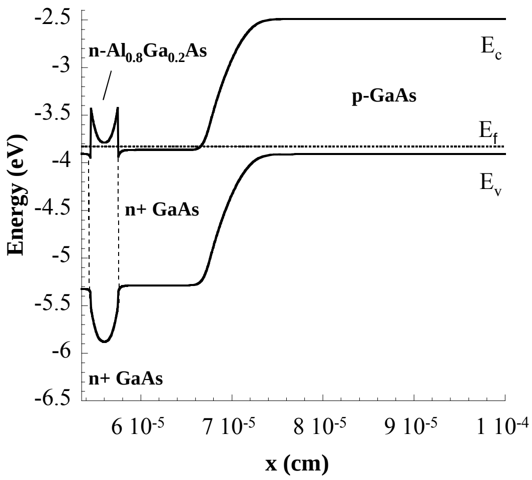

Figure 1: The calculated equilibrium band diagrams of the n-p GaAs homojunction

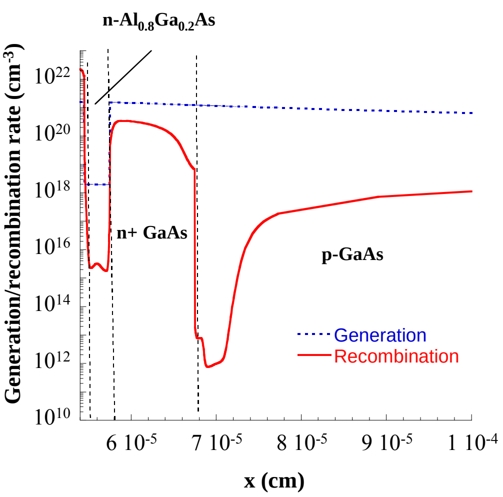

Figure 2: The calculated profile of the generation and recombination rates for the n-p GaAs homojunction solar cell under AM1.5D illumination at short circuit current condition.

The values of the minority carrier lifetime were set equal to 0.1 ns for the emitter layer and 10 ns for the base layer. Significant recombination losses in the n+GaAs emitter is observed, which can affect the performance of the solar cell.

The way to avoid recombination losses in the emitter layer is to use the wide band gap emitter. In the design of heterojunction solar cells, one should take into account the band structure at the heterointerfaces which is determined by the band discontinuities. In case of the n-type wide band gap emitter/p-GaAs base heterojunction, the potential barrier in the conduction band should not prevent the electron transport from the base to the emitter. While in contrary, the potential barrier in the valence band should limit the hole transport from the depletion region to the emitter. The light absorption in the wide band gap material of the emitter placed below the top subcell is low, and, therefore, no window layer is required in this case.

The band diagrams of n-AlInP/p-GaAs, n-GaInP/p-GaAs and n-AlGaAs/p-GaAs heterojunctions calculated using material parameters given in Table II are presented in Fig.3-Fig.5. The potential barriers in the valence band

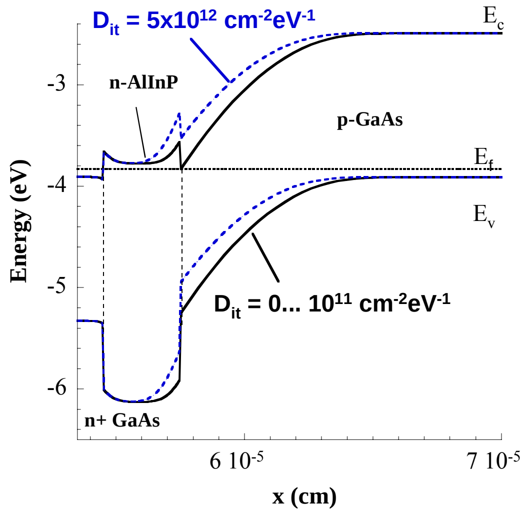

Figure 3: The calculated equilibrium band diagrams of the n-AlInP/p-GaAs heterojunction

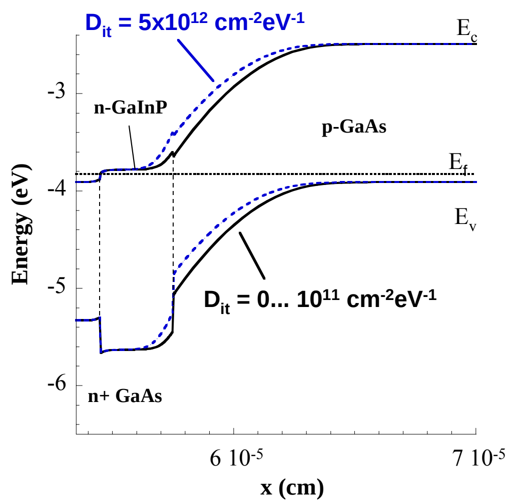

Figure 4: The calculated equilibrium band diagrams of the n- GaInP/p-GaAs heterojunction.

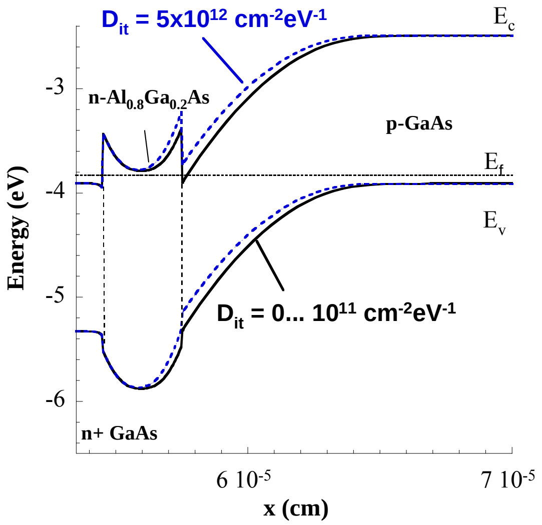

Figure 5: The calculated band diagrams of the n-AlGaAs/p-GaAs heterojunction.

is high enough to avoid the hole transport from the depletion region in all cases. The calculated generation and recombination rates for those three heterojunction solar cells are presented in Fig.6. The conditions and the values of the carrier lifetime in the emitter and the base layers (0.1 ns and 10 ns, respectively) are the same as in the case of the homojunction. The recombination rate in the emitter of all three heterojunctions is much lower compared to that of the homojunction. While in case of the GaInP emitter, the recombination rate is by two orders of magnitude higher than for the AlInP and AlGaAs emitter. It is due to the higher absorption in the GaInP layer, which has the narrower band gap. Indeed, the recombination rate in the wide band gap emitter is caused mostly by the hole generation in this layer.

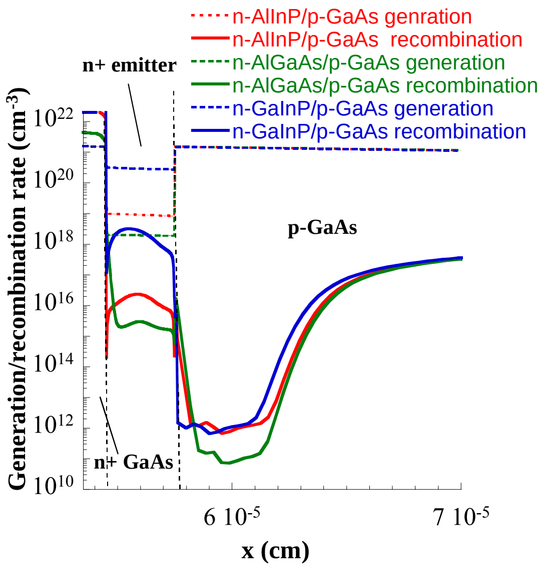

Figure 6: The calculated profile of the generation and recombination rates for n-AlInP/p-GaAs, n-GaInP/p-GaAs and n-AlGaAs/p-GaAs heterojunction solar cells under AM1.5D illumination at short circuit current condition.

The performance of the n-p GaAs homojunction and n-AlInP/p-GaAs, n-GaInP/p-GaAs and n-AlGaAs/p-GaAs heterojunction solar cells under AM 1.5D illumination was calculated for different values of the base and emitter layers carrier lifetime. The obtained dependences of the open circuit voltage (V_{oc}) as a function of the GaAs base electron lifetime (τ_b) for various values of the emitter hole lifetime (τ_e) being in the range of 0.01…1 ns are presented in Fig.7. The efficiency (η) has a similar dependence (insert in Fig.7). For low values of minority carrier lifetime in p-GaAs base (τ_b < 1 ns) homojunction and heterojunction solar cells exhibit an increase of V_{oc} with increasing τ_b which is independent on τ_e. In this region V_{oc} is limited by p-GaAs base minority carrier lifetime. With further increase of τ_b, the rise of V_{oc} for the n-p GaAs homojunction solar cell becomes to be dependent of τ_e and has a tendency to saturate, i.e V_{oc} is limited by the emitter minority carrier lifetime. While V_{oc} for heterojunction solar cells continues to rise with τ_b independent of τ_e. The emitter hole lifetime does not limit V_{oc} in this case. It means that heterojunctions with wide band gap emitter allow one to avoid recombination losses in the emitter. In other words, if the efficiency of homojunction solar cell is limited by the carrier recombination in the emitter layer, it could be improved using the wide band gap emitter.

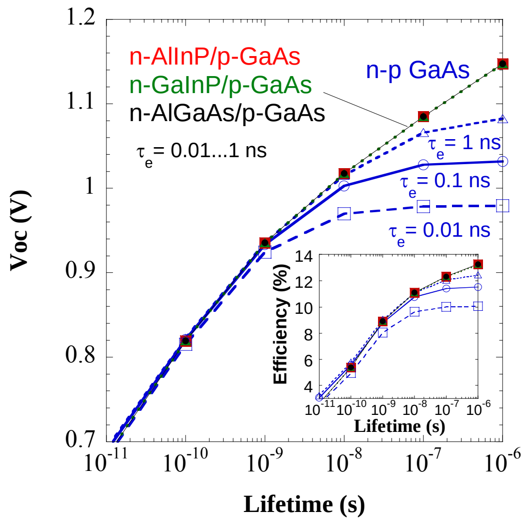

Figure 7: The calculated dependences of the open circuit voltage (V_{oc}) as a function of GaAs base minority carrier lifetime (τ_b) for n-p GaAs homojunction and n-AlInP/p-GaAs, n-GaInP/p-GaAs and n-AlGaAs/p-GaAs heterojunction solar cells under AM 1.5D illumination. In insert, the dependences of the efficiency (η) are given.

To estimate the possibility for the improvement, the performance of the homojunction and heterojunction solar cells with low defect density p-GaAs base layer was calculated. The minority carrier lifetime in this case is determined by the radiative (B) and Auger (C) recombination coefficients. The values of B=1.7× 10^{-10} cm^3s^{-1} and C= 7× 10^{-30} cm^6s^{-1} were used [9] giving τ_b to be in the order of 10^{-8} s. The value of the emitter minority carrier lifetime, τ_e, was set equal to 10^{-10} s. Multiple reflection calculations were performed and TiO_2/SiO_2 antireflection coating was considered.

However, the photon recycling effect was not taken into account. The calculated I-V curves for AM1.5D one sun illumination are presented in Fig.8. The corresponding values of the open circuit voltage (V_{oc}), the short circuit current (J_{sc}), the fill factor (FF) and the efficiency (η) are given in Table III. The heterojunction solar cells have higher V_{oc}, J_{sc} and FF compared to those of the n-p GaAs homojunction resulting in about 0.7 % rise of efficiency. The n-GaInP/p-GaAs heterojunction solar cells has slightly lower short circuit current (and efficiency) than n-AlInP/p-GaAs and n-AlGaAs/p-GaAs heterojunctions due to the higher absorption in the GaInP layer.

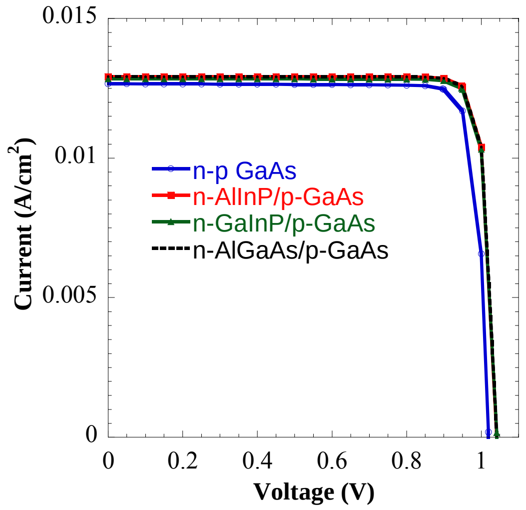

Figure 8: Calculated I-V curves of n-p GaAs homojunction and n-AlInP/p-GaAs, n-GaInP/p-GaAs and n-AlGaAs/p-GaAs heterojunctions solar cells with the low defect GaAs base layer under AM1.5D one sun illumination. See details in the text.

Table III: Parameters of the calculated I-V curves in Fig.8.

	V_{oc}(V)	J_{sc} (mA/cm^2)	FF(%)	η(%)
GaAs	1.019	12.66	86.72	11.19
AlInP/GaAs	1.043	12.92	88.51	11.92
GaInP/GaAs	1.042	12.84	88.49	11.84
AlGaAs/GaAs	1.043	12.92	88.51	11.92

Finally, additionally to the described above model with the low defect p-GaAs base layer, the interface states were introduced at the wide band gap n-emitter/p-base heterointerface. The interface defect density (D_{it}) was varied, while the electron and hole capture cross-sections (σ) were set at 10^{-14} cm^2. The calculated dependence of V_{oc} on the product of $D_{it}\times\sigma$ for the n-AlInP/p-GaAs, n-GaInP/p-GaAs and n-AlGaAs/p-GaAs heterojunctios solar cells under AM 1.5D illumination is presented in Fig.9. The efficiency exhibits the similar dependence (see insert in Fig.9). For the n-AlInP/p-GaAs and n-AlGaAs/p-GaAs heterojunctions, up to $D_{it}\times\sigma = 10^{-3}$ eV^{-1} (corresponds to $D_{it}=10^{11}$ cm^{-2} eV^{-1} and $\sigma = 10^{-14}$ cm^2), the interface states do not affect V_{oc} and η. It should be noted that the value of $D_{it}=10^{11}$ cm^{-2} eV^{-1} can be considered as relatively high for epitaxially grown heterostructures. The increase of $D_{it}\times\sigma$ to 10^{-2} eV^{-1} leads to a small decrease of V_{oc} and η followed by drastic drop with further $D_{it}\times\sigma$ rise. This drop of V_{oc} and η for $D_{it}>10^{12}$ cm^{-2} eV^{-1} ($\sigma = 10^{-14}$ cm^2) is caused by the change in band bending at the heterointerface. From the calculated band diagrams for $D_{it}=5\times10^{12}$ cm^{-2} eV^{-1} given in Fig.3 and Fig.5, one can see that the Fermi level moves toward the midgap at the interface due to the pining effect. This results in decrease of the distance between valence band and the Fermi level at the interface leading to the hole concentration increase. While the recombination rate at the interface is proportional to the hole concentration as can be seen from [10]:

$$U \approx c_p p \int_{E_1}^{E_2} D_{it}(E)dE \qquad (1),$$

where p is the hole concentration at the interface, $c_p = v_p\sigma_p$ is the hole capture coefficient, v_p is the hole thermal velocity, $E_2 = E_F^e$, $E_1 = E_i - (E_F^e - E_i) - k_B T\ln(c_n/c_p)$, E_i and E_F^e being the intrinsic and electron quasi-Fermi levels, respectively. Thus, the change in the band bending at the heterointrface leads to enhance of the recombination rate at the interface. When similar product $D_{it}\times\sigma = 10^{-1}$ eV^{-1} is used with lower $D_{it}=10^{10}$ cm^{-2} eV^{-1} and higher $\sigma = 10^{-11}$ cm^2, no changes in the band bending and no drastic decrease of V_{oc} and η are observed (filled symbol in Fig.9).

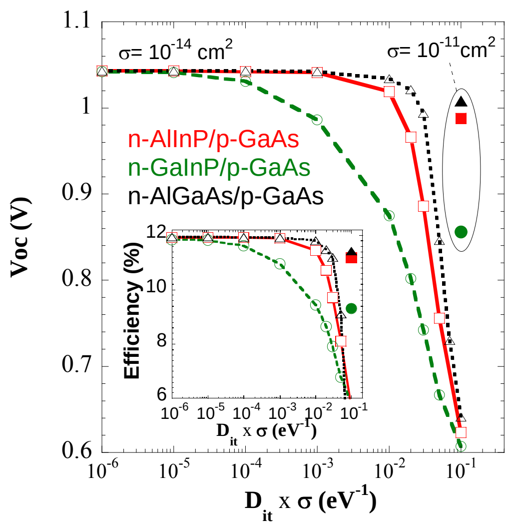

Figure 9: The calculated dependence of V_{oc} on the product of the interface defect density and the capture cross-sections ($D_{it}\times\sigma$) for heterojunction solar cells under AM1.5D illumination. In insert, the dependences of the efficiency (η) is given.

The n-GaInP/p-GaAs heterojunction solar cell exhibits much higher sensitivity to the interface state density. A significant reduction of V_{oc} and η is observed at $D_{it}\times\sigma = 10^{-3}$ eV^{-1}, when no band bending changes occurs. This is due to the band structure at the n-GaInP/p-GaAs interface (Fig. 4). A low conduction band offset at the interface leads to the lower band bending and the lower distance between the valence band and the Fermi level resulting in higher hole concentration. This, according to (1), leads to the higher carrier recombination rate at the interface compared to n-AlInP/p-GaAs and n-AlGaAs/p-GaAs interfaces for the same values of $D_{it}\times\sigma$.

The performance of the n-AlInP/p-GaAs, n-GaInP/p-GaAs and n-AlGaAs/p-GaAs hetrojunction subcells for

D_{it}=10^{11} cm^{-2} eV^{-1} and σ = 10^{-14} cm^2 calculated for AM1.5D one sun illumination is presented in Table IV. The higher sensitivity of the n-GaInP/p-GaAs heterojunction to the interface state density leads to about 1% reduction of the cell efficiency. While the efficiency of the n-AlInP/p-GaAs and n-AlGaAs/p-GaAs heterojunction subcells remains the same as in the case, when no interface states were taken into account.

Table IV: Performance of the heterojunction subcells with the low defect GaAs base layer and D_{it}=10^{11} cm^{-2} eV^{-1}, σ = 10^{-14} cm^2 calculated for AM 1.5D one sun illumination.

	V_{oc}(V)	J_{sc} (mA/cm^2)	FF(%)	η(%)
AlInP/GaAs	1.041	12.92	88.46	11.9
GaInP/GaAs	0.986	12.85	86.57	10.97
AlGaAs/GaAs	1.042	12.92	88.51	11.92

4 CONCLUSIONS

The way to reduce the recombination losses in the emitter layer of the GaAs based subcell using the wide band gap emitter layer (GaInP, AlInP or AlGaAs) was demonstrated by numerical simulations. In case, when performance of a conventional GaAs homojunction subcell is limited by the carrier recombination in n+GaAs emitter the proposed design could increase the open circuit voltage as well as the cell efficiency.

The influence of the defect density at the wide gap emitter/base heterointerface on the solar cell performance was also analyzed for different types of n-p heterojunctions. The efficiency of the n-AlInP/p-GaAs and n-AlGaAs/p-GaAs heterojunctions was shown to be independent of the interface states up to $D_{it}\times\sigma = 10^{-3}$ eV^{-1} demonstrating a high potential of those heterojunctions for application in multijunction solar cells. While the n-GaInP/p-GaAs heterojunction exhibits a strong sensitivity to the interface states that can limit its application for solar cells.

Acknowledgments

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5 REFERENCES

[1] A.W. Bett, F. Dimroth, W. Guter, et al, Proceedings of the 24th European Photovoltaic Solar Energy Conference (2009) 1.
[2] S. M. Sze, 1981 Physics of Semiconductor Devices, 2nd Edition (John Wiley & Sons, New-York).
[3] R.Stangl, M.Kriegel, M.Schmidt, Proceedings of the 4th World Conf. on Photovoltaic Energy Conversion (Hawaii, USA, 2006) 1350.
[4] A. Gomyo, T. Suzuki, and S. Iijima, Phys. Rev. Lett. 60 (1988) 2645.
[5] D. P. Bour, J. R. Shealy, G. W. Wicks, and W. J. Schaff, Appl. Phys. Lett. 50 (1987) 615.
[6] I. Vurgaftman, J. R. Meyer, L. R. Ram-Mohan, J. Appl. Phys. 89 (2001) 5815.
[7] C.-S. Jiang, D.J. Friedman, H.R. Moutinho, and M.M. Al-Jassim, Proceedings of the 4th World Conf. on Photovoltaic Energy Conversion (Hawaii, USA, 2006) 853.
[8] S. Adachi, J.Appl. Phys. 58 (3) (1985) R1.
[9] U. Strauss and W. W. Rlihle, Appl. Phys. Lett. 62 (I) (1993) 55.
[10] J. P. Kleider, A. S Gudovskikh, Proceedings of the MRS Spring Meeting, (San Francisco, USA, 2008) Vol. 1066, 75.