GaP/Si anisotype heterojunction solar cells

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Abstract. Multijunction solar cells grown on Si substrates using III-V compounds are very promising due to potentially high efficiency (over 40%). In that case homojunction in silicon can be replaced with GaP heterojunctions which can be more effective in terms of lowering surface recombination. Silicon substrates of both n- and p-type doping were used to form GaP/Si anisotype heterostructures. It was demonstrated that for p-GaP/n-Si structures charge carrier transport is mainly blocked due to large value of valence band offset at the heterointerface. For n-GaP/p-Si solar cells optimal thickness and doping level were calculated using AFORS-HET software. The influence of interface states density and GaP layer parameters was investigated.

1. Introduction

Further development of silicon based multijunction solar cells requires new concepts to be applied. The use of anisotype heterojunctions may potentially increase the efficiency by lowering surface recombination. This approach was successfully used for GaAs based solar cells as reported here [1]. However, in case of GaP/Si heterojunctions the polar/nonpolar nature and band offsets at the interface must be taken into account.

Numeric simulations of band diagram (figure 1) for both p-GaP/n-Si and n-GaP/p-Si heterostructures were performed using AFORS-HET software [2]. According to data on band offsets [3, 4], high value of \(\Delta E_v\) (0.8-0.95 eV) results in significant barrier for majority carriers (holes) at the heterointerface for p-GaP/n-Si structure. This barrier may affect charge carrier transport even at room temperature. On the other hand, in this structure minority carriers (electrons) are effectively blocked off the surface due to band bending in GaP layer and \(\Delta E_c\) value, thus surface recombination is suppressed.

In case of n-GaP/p-Si structure, barrier height for majority carrier (electrons) is significantly lower due to conductance band offset \(\Delta E_c = 0.19-0.32\) eV. However, potential barrier at the interface for minority carrier, which is mostly because of valence band offset, still effectively blocks them off the surface and thereby lowers recombination rate.
2. Experiment
Both p-GaP/n-Si and n-GaP/p-Si heterostructures were fabricated using molecular-beam epitaxy. Silicon substrates of <100> orientation with 4° offcut towards <110> with doping level of $10^{16}$ cm$^{-3}$ were used. Thickness of GaP layer was 100 nm for both structures and the doping level was more than $10^{18}$ cm$^{-3}$. Al and In were used to form back contact to p-type and n-type substrates respectively. Top contact was In for both structures.

Admittance spectroscopy technique [5,6] was used to investigate charge carrier transport in GaP/Si structures. Potential barriers at the interface result in step-like increase in admittance signal as shown in figure 2. Obtained value of activation energy $E_a$, which is in fact an effective barrier height, is 0.7 eV and 0.12 eV for p-GaP/n-Si and n-GaP/p-Si structures respectively. This is less than values of band offsets reported in literature because of tunneling effect in highly doped GaP layer.

Current-voltage characteristics under illumination flux of ~1 sun, measured for these structures are presented in figure 3a. The potential barrier of 0.12 eV is not sufficient enough to affect charge carrier transport over the interface, so n-GaP/p-Si structure demonstrates decent values of short circuit current, $J_{sc} = 38$ mA/cm$^2$, and fill factor, FF=84%. Short circuit current for p-GaP/n-Si is about two orders of magnitude lower that that for n-GaP/p-Si due to potential barrier of 0.7 eV which blocks charge carrier transport over the interface.

Figure 1. Simulated band diagrams for p-GaP/n-Si and n-GaP/p-Si heterostructures.

Figure 2. Admittance spectra of p-GaP/n-Si and n-GaP/p-Si anisotype heterostructures.
The result above was also confirmed by spectral measurements of EQE for these structures (figure 3b). N-GaP/p-Si demonstrates noticeable EQE in the range of 300-1200 nm due to absorption in silicon substrate. However, for p-GaP/n-Si structure potential barrier for holes blocks transport over heterointerface, so this structure exhibits non-zero EQE only for wavelengths less than 400 nm and only charge carriers generated in GaP layer contribute to photocurrent.

Thus, there are fundamental problems, limiting the use of p-GaP/n-Si heterostructures for photovoltaic applications. However, GaP/Si structures grown on p-type substrates have no such limitations and can be used for high efficiency solar cells.

3. Simulation

It was demonstrated in previous section that p-GaP/n-Si heretostructure can be used as an effective photoconverter. In this section the influence of GaP thickness, doping level and interface states density on device properties is considered using numeric simulation.

Effective lifetime of charge carrier in GaP epi-layer is substantially less than that of substrate, so photocurrent through GaP/Si structure mostly depends on absorption in Si. Absorption in GaP layer result in short circuit current decrease when layer thickness is more than 50 nm as shown in figure 4a. However, $V_{oc}$ is only slightly depends on GaP thickness, but largely on interface trap density $D_{it}$. In order to reduce effect of $D_{it}$ on $V_{oc}$, the minimum doping level of GaP layer should be not less than $N_d > 10^{16}$ cm$^{-3}$ or else $(E_C - E_F) \leq 0.2$ eV. On the other hand, the surface state density should be less than $D_{it} < 10^{12}$ cm$^{-2}$eV$^{-1}$ (see figure 4b).

Figure 3(a, b). (a) I-V curves for GaP/Si heterostructures; (b) Quantum efficiency spectra (no ARC).
In figure 5 anisotype heterojunction n-GaP/p-Si is compared to conventional n-GaP/n-Si/p-Si solar cells (isotype). I-V curves demonstrate that both structures are sensitive to heterointerface trap density, but there is almost no difference between them in terms of open voltage circuit or fill factor at equal Dit. However, isotype structure is commonly formed by diffusion of phosphorus into substrate during GaP growth. This requires the use of high temperatures for any growth technique used. Anisotype heterostructures doesn’t rely on diffusion processes, so it can be possible to grow this structure at lower temperatures using ALD instead of MBE.

**Figure 5.** Simulated I-V characteristics for isotype and anisotype GaP/Si heterostructures.

4. Conclusion

In this paper new approach to high efficient Si based solar cell was discussed. It was demonstrated that charge carrier transport is mainly blocked in p-GaP/n-Si heterostructures, while n-GaP/p-Si does not concede to conventional isotype heterostructures, but can be grown at lower temperatures. The requirements to doping type, doping level and layer thickness for GaP/Si solar cells were investigated.
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