Effect of Passivation on III-Nitride/Silicon Tandem Solar Cells

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Abstract

We have studied the impact of mesa sidewall passivation by SiO_2 on characteristics of III–nitride/silicon tandem solar cells. These dual junction solar cells were fabricated from standard n-type Si (111) substrates with III–nitride epitaxial layers grown by plasma-assisted molecular beam epitaxy (PAMBE). Photovoltaic testing was experimentally carried out under a solar simulator before and after the 100nm-thick SiO_2 passivation of these solar cell mesa side walls. We have found that the sidewall passivation improves the efficiency of these solar cells. The open-circuit voltage (V_{OC}) increased from 1.45 to 1.53 V, the short-circuit current density (J_{SC}) enhanced from 0.116 to 0.121 mA/cm^2, the fill factor increased from 39.7 to 41.5% under the solar simulator illumination yielding 13.3% conversion efficiency improvement after passivation. Moreover, IPCE (the incident monochromatic photon to current conversion efficiency) also moderately increased by approximately 13% in the visible region after passivation.

1. Introduction

The design of solar cells that use multiple semiconductor materials with different energy bandgaps is an important area of research for improving conversion efficiency. Each photovoltaic material in these 'tandem' or 'multi-junction' devices is sensitive to different parts of the solar spectrum, yielding higher absorption rates and reducing thermal losses [1,2].

Considering the short diffusion length of high energy photons, a tandem solar structure is typically designed with a wider band-gap semiconductor for the top cell and a smaller band-gap semiconductor for the bottom cell [3]. This architecture design can improve the light harvesting over a wider portion of the solar emission spectrum than that of a single cell. The power-conversion efficiency of the tandem solar cells is innately better than that of a single cell made from the smaller bandgap material unless the current mismatch between sub-cells is considerably large.

The open circuit voltage (V_{oc}) in a tandem solar cell is the sum of the V_{OC}'s of the individual cells due to their serial connection. On the other hand, the tandem short circuit current is limited strictly to the smaller current generated in either sub-cell [4]. In the case of greater carrier generation in either sub-cell, there is no contribution from these excess charges to the photocurrent, therefore they compensate for the built-in potential across the respective sub-cell which results in a reduced Voc in the tandem structure [5].

The III-nitrides semiconductors, which consist of InN, GaN, AlN and their alloys, have become a topic of much discussion for photovoltaic space and terrestrial devices applications mainly due to their wide range of direct-bandgap, electronic, optical and mechanical properties [6,7,8]. Very large spectral ranges from the extreme deep ultraviolet to the near infrared spectral region can be covered by the energy bandgaps of group III-nitride alloys. The tunable band gaps (0.7 – 3.4eV) of InGaN alloys cover nearly the complete solar spectrum, and make them excellent materials for solar cells, which can be designed with multiple junctions to achieve maximum efficiency [9,10,11,12].

The direct bandgap structure of III-N alloys over the entire material composition is also superior to conventional III-V alloys, which suffer from indirect band gaps for higher material compositions. In addition, III-N materials have excellent absorption coefficients (~10^5 cm^{-1}) at the band edge [13,14]. This allows even a few hundred nanometers of material to absorb a great percentage of light, unlike conventional solar cells made from indirect materials, which can require hundreds of microns [15].

Adding a passivating layer may further improve the performance of a tandem solar cell by suppressing current leakage and reducing surface damage during fabrication. Determining the effect of passivated mesa sidewalls on the III-N/Si tandem solar cell structure motivated our research.

2. Experimental Details

The sample was grown with plasma-assisted molecular beam epitaxy (PA-MBE) using n-Si (111) wafers. The III-nitride/silicon tandem solar cell structure, shown in Fig. 1, consisted of (top to bottom): a ~100 nm layer of p-GaN, a 600 nm layer of n-GaN, and a 50 nm thin AlN buffer layer on the n-Si (111) wafer. The AlN buffer layer was intended to bridge the lattice mismatch between the epitaxial GaN layer and the Si wafer. The p-GaN was achieved by incorporating magnesium, and the nominally undoped GaN layer acts as an n-type to form the GaN pn junction on the top of the tandem structure. The Si pn junction at the bottom was formed as a by-product of the buffer layer where aluminum in-diffusion caused the wafer surface to be heavily p-type doped [16,17,18].

Before the metal stack deposition, the sample was ultrasonically degreased in acetone, methanol and rinsed using deionized (DI) water. The degreasing procedure was followed by a treatment in $HCl:H_2O$ (3:1) solution for 10 min at room temperature. The treatment was completed with a DI water rinse and subsequent drying in high purity N_2 gas. A semitransparent Au (5 nm)/Ni (5 nm) bilayer was then deposited in an electron beam evaporator with base pressure less than 2x10^{-7} Torr. The $HCl:H_2O$ (3:1) surface preparation for the semitransparent metal stack was found to yield the lowest specific contact resistance (ρ) for *p*-GaN [19]. Standard photolithography and wet etching

were employed to pattern the semitransparent bilayer as the front contact on the p-type GaN top layer.

In order to define the mesa structure, a 100nm-thick Ni mask and a 500nm-thick SiO_2 mask were deposited using the e-beam evaporator and PECVD respectively. A variety of mesas of different diameters from 120 to 400 µm were then defined by inductively coupled plasma reactive ion etching (ICP-RIE) to reach the n-type silicon substrate. The etch system used has been described elsewhere [20]. The dry etching process was carried out in a chlorine-based plasma. The ICP power, RIE power and the chamber pressure were held constant at 250 W, 200 W and 8 mTorr, respectively, during the etch procedure.

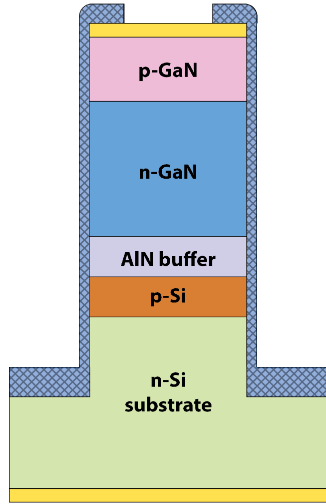

Fig. 1. Schematic of the III-nitride/silicon tandem solar cell structure with front and rear contacts. SiO_2 passivation is depicted on the sidewalls.

Rear contact was formed with Ti (50 nm)/Au (50 nm) using the electron beam evaporator onto the back side of the Si wafer. The sample was annealed in a rapid thermal annealing (RTA) at 500 °C in 90% N_2 and 10% O_2 ambiance for 10 min.

Before and after passivation of the mesa sidewalls with 100nm of SiO_2 deposited by PECVD at 250 °C, the current-voltage (I-V) characterization was performed in dark and under illumination of a solar simulator operating at 75 mW/cm^2. The current–voltage measurements were acquired through a Keithley 2400 source meter. External quantum efficiency of the tandem solar cell was investigated by employing the incident photon-to-current conversion efficiency (IPCE) with a characterization system consisting of a Xenon lamp, a chopper controller, a monochromator, and a lock-in amplifier.

3. Results and Discussion

Before discussing the results of the tandem structure, it is useful to investigate the pn-Si sub-cell alone. This structure was realized by removing of the p-GaN layer and part of the n-GaN epitaxial layer. This single pn-Si junction solar cell was measured under the solar simulator; the photovoltaic characteristics are listed in Table 1. Current density versus voltage (J-V) characteristics of the single pn-Si sub-cell are shown in Fig. 2.

Table 1. Photovoltaic characteristics of the single pn-Si junction solar cell

Photovoltaic characteristic	Value
J_{sc} (mA/cm^2)	9.55
V_{oc} (V)	0.29
Fill factor (%)	55.33
Conversion efficiency (%)	2.06

The tandem pn-GaN/pn-Si cell is expected to suffer from poor power conversion efficiency as a consequence of the sizable current mismatch between the top and bottom cells. This is due to a smaller fraction of the terrestrial solar spectrum existing above the GaN band gap (3.4 eV). From a theoretical point of view, such an ideal tandem structure has the following photovoltaic parameters. Assuming 100% quantum efficiency limits the current density to at most 0.6 mA/cm^2, and estimating an 80% fill factor results in a maximum conversion efficiency of only 1.5% [17].

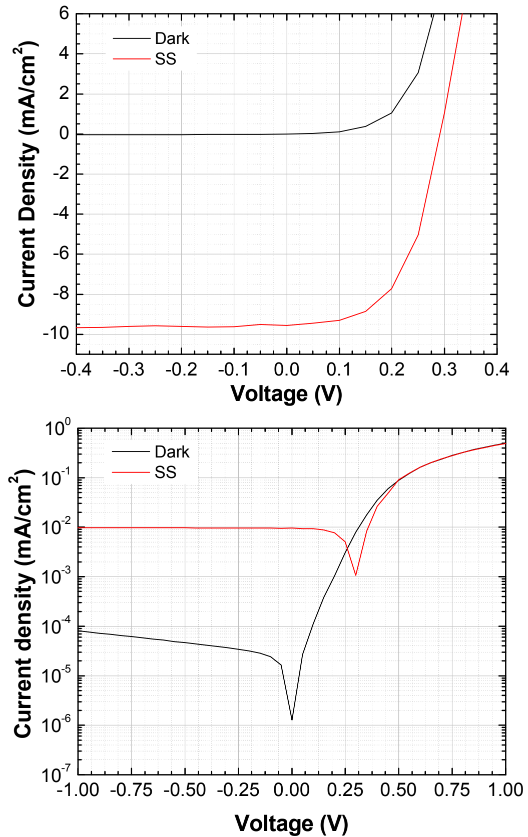

Fig. 2: Current density versus voltage characteristics of single pn-Si under the solar simulator (SS) illumination in linear (top) and logarithmic (bottom) scales.

When the full pn-GaN/pn-Si tandem structure was measured under solar simulator illumination, the V_{oc} was 1.45 V (almost 5 times the voltage of the Si bottom cell). The short circuit current density J_{sc} was 0.116 mA/cm^2 (over two orders of magnitude lower than in the Si bottom cell). These two distinct changes (reduction of the J_{sc} and increase of the V_{oc}) in the photovoltaic parameters of the tandem solar cell proves that the GaN pn-junction on top is functioning effectively, and limiting the

generated photocurrent in the bottom sub-cell. With these J-V measurements, a fill factor of 39.7% was measured, limiting the power conversion efficiency to 0.1%. These results confirm the large current mismatch between the top and bottom cells, with the latter providing much greater current density.

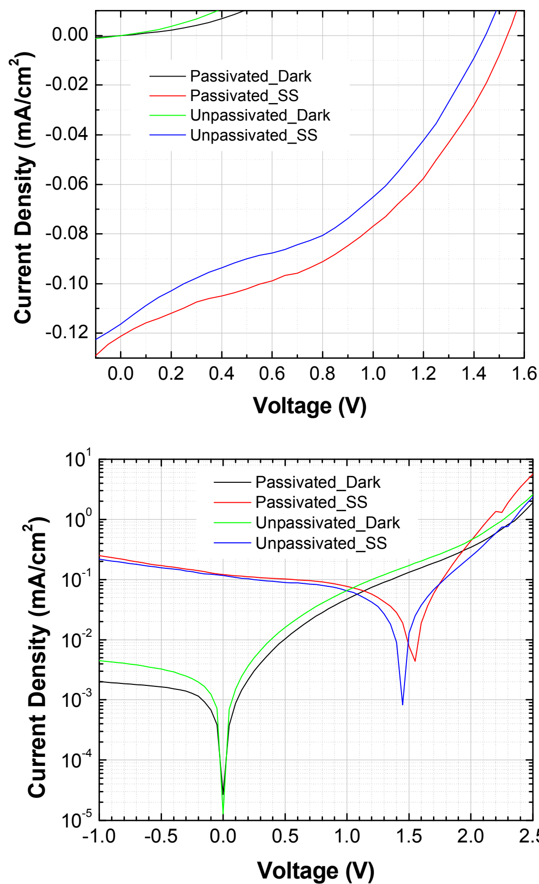

Fig. 3: Current density versus voltage characteristics of pn-GaN/pn-Si before and after passivation of the mesa sidewalls under the solar simulator (SS) illumination in linear (top) and logarithmic (bottom) scales.

Passivation may be useful for optoelectronic devices to achieve highly efficient operation [21]. Also, passivation may help reduce plasma-induced damage on semiconductor devices during their fabrication process. Plasma etching techniques can cause abruptly terminated mesa side walls with defects which trigger band bending and carrier accumulation. It is expected that passivation also tends to prevent oxidation of the mesa side walls. Furthermore, it saturates dangling bonds to avoid surface states. Passivation of mesa sidewalls by SiO_2 is found to be effective in suppressing reverse leakage [22].

Mesa sidewall passivation with 100nm-thick SiO_2 deposition by PECVD was carried out. Subsequently, the photovoltaic parameters were again measured to see the effect of passivation on device performance. We observed a slight enhancement in the *J-V* performance after passivating the mesa sidewalls. The passivated devices had open circuit voltage improved from 1.45 V before passivation to 1.53 V afterwards, and short circuit current density from 0.116 to 0.121 mA/cm^2. The devices with the passivation at their sidewalls also demonstrated a relatively higher fill factor of 41.5%, indicating slightly better solar cell performance. Given these improved values, the conversion efficiency increased by 13.3%. The solar cell parameters determined from the current–voltage measurements before and after passivation are summarized in Table 2. Also, current density versus voltage (J-V) characteristics of pn-GaN/pn-Si tandem structure before and after passivation of the mesa sidewalls under the solar simulator are shown in Fig. 3.

Table 2. Photovoltaic characteristic of the tandem solar cell before and after sidewall passivation

Passivation status	Before	After
J_{sc} (mA/cm^2)	0.116	0.121
V_{oc} (V)	1.45	1.53
Fill factor (%)	39.7	41.5
Conversion efficiency (%)	0.09	0.102

In order to characterize the photo-electrical performance of solar cells, the incident monochromatic photon to current conversion efficiency (IPCE) is crucial, which is also called the external quantum efficiency (EQE). IPCE is defined as the ratio between the number of generated charge carriers by light in the external circuit and the number of incident photons impinging on a solar cell. It is expressed as a function of excitation wavelength.

IPCE measurements of the tandem solar cell before and after mesa sidewall passivation were carried out using an Oriel xenon lamp source, a spectrometer, a SR850 lock-in amplifier, a chopping frequency of 200 Hz, and a calibrated silicon reference photodiode. It was observed that the IPCE spectrum after passivaton moderately increased by approximately 13% at around 600 nm wavelength in the visible region.

6. Conclusions

The fabrication and characterization of a Si-GaN tandem solar cell was demonstrated and the effect of passivation investigated.

Limited solar cell performance, in terms of short-circuit current density and efficiency was observed. This was attributed to the large current mismatch between the top and bottom sub-cells, formation of extended crystalline defects in the epilayers, and the energy band structure of the tandem device that does not cover the most effective middle part of the solar spectrum.

After passivation, it was noted that the device response was slightly dependent on the passivation along the sidewall. The open-circuit voltage (V_{OC}) increased from 1.45 to 1.53 V, the short-circuit current density (J_{SC}) improved from 0.116 to 0.121 mA/cm^2, and the fill factor increased from 39.7 to 41.5% under the solar simulator, yielding around 13.3% improvement in conversion efficiency after the passivation procedure.

In addition to conversion efficiency, IPCE moderately increased by approximately 13% at around 600 nm wavelength in the visible region after passivation.

7. References

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