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Cambridge University Press
978-1-107-40825-8 - Compound Semiconductors for Energy Applications and Environmental Sustainability: Materials Research Society Symposium Proceedings: Volume 1167
Editors: F. Shahedipour-Sandvik, E. Fred Schubert, L. Douglas Bell, Vinayak Tilak and Andreas W. Bett
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Compound Semiconductors for PV Applications

Mater. Res. Soc. Symp. Proc. Vol. 1167 © 2009 Materials Research Society **1167-O01-04**

Utilizing Polarization Induced Band Bending for InGaN Solar Cell Design

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ABSTRACT

Strong polarization effects observed in III-nitride materials can invert the surface carrier type. The corresponding band bending can be used to design InGaN solar cells. Similar surface inversion was observed in the past with silicon-based Schottky-barrier solar cells, but was limited by Fermi level pinning. The formation of two-dimensional electron gas by polarization fields in III-nitrides has been reported. Using a similar idea, the growth of a thin AlN capping layer on p-InGaN has resulted in band bending, hence depletion region, under the surface that can be used to separate any generated photo-carriers. Hall measurements at different depths on these structures confirm the inversion of surface carrier type. Solar cells based on this concept have resulted in an open circuit voltage of 2.15 V and short circuit current of 21.8 µA.

INTRODUCTION

Schottky-barrier solar cells invert the surface type of the semiconductors and are formed by metal deposition on semiconductors. The Schottky barrier height depends on the difference between metal work function and the semiconductor Fermi level. Silicon-based Schottky solar cells have been studied in the past [1]. The main limitation of these devices was Fermi level pinning to mid-band gap, limiting the open circuit voltage to half the band gap. Photo-response from III-nitrides Schottky devices were studied on GaN using several metal contacts. InGaN based Schottky devices have not yet been reported. Alternate approaches to invert the surface in other semiconductors have not been possible, but in III-nitride materials there is the inherent polarization which can be used to invert surfaces.

InGaN materials with their wide band gap range (0.7 to 3.4 eV) are ideal for solar cells to span most of the solar spectrum [2]. InGaN-based solar cells using quantum wells and p-i-n structures have been reported [3, 4]. A unique property of the III-nitrides is their inherent polarization property [5]. Strong polarization fields with formation of two-dimensional electron gas (2DEG) have been reported in III-nitrides and are used in high-electron mobility transistors [6]. The photo-response from surface inversion caused by the polarization property has not been explored in the past.

In this paper a study of surface inversion caused by thin AlN on InGaN is presented. The theoretically calculated band diagrams are presented followed by experimental evidence showing the formation of 2DEG and finally the photo-voltaic response from a p-InGaN/AlN structure. The III-nitride solar cells formed by polarization are not formed by inversion from a Schottky metal, however, these in principle demonstrate a similar behavior with an advantage of an optically transparent capping layer.

THEORY

Polarization is present in III-nitrides (0001) as a consequence of the non-centrosymmetry of the wurtzite structure and the large ionicity of the covalent metal-nitrogen bonds. The net polarization is composed of spontaneous and piezoelectric polarization [7]. The direction of piezoelectric polarization is dependent on the polarity of the material as well as on the strain. The spontaneous polarization in each epi-layer is calculated using the equations 1 below.

$$P_{sp}(In_xGa_{1-x}N) = -0.042x - 0.034(1-x) + 0.037x(1-x)\,(C/m^2) \tag{1}$$

$$P_{sp}(AlN) = -0.09\,(C/m^2)$$

The piezoelectric polarization is dependent on the strain introduced by lattice-mismatch and is calculated using equation 2:

$$P_{pz} = 2\varepsilon_x\left[e_{31} - e_{33}\frac{C_{13}}{C_{33}}\right] \tag{2}$$

Where, ε_x is strain at the InGaN-AlN interface, e_{31} (-0.58) and e_{33} (1.55) the elastic constants for AlN layer and C_{13} (115 GPa) and C_{33} (385 GPa) piezoelectric constant for AlN epi-layer.

The growth of pseudomorphic epi-layers results in formation of two-dimensional electron gas (2DEG) or two-dimensional hole gas at the interface, induced by polarization. 2DEG formation has been well studied, and using the above mentioned values as input into the "Silense" simulation program, the thermal equilibrium band diagrams are presented.

To study the extreme case AlN epi-layer on InGaN is selected. The band diagram of 100 nm p-InGaN with 5 nm AlN capping layer is shown in Figure 1. The formation of 2DEG can be clearly noticed in the band diagram. Solar cell operation requires a depletion region i.e. band bending. The formation of 2DEG in the III-nitrides introduces the required band bending for use as a solar cell and this is the study presented in this paper.

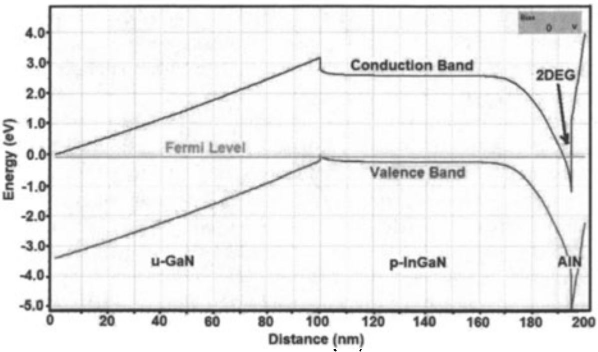

Figure 1. Equilibrium band diagram of p-InGaN with AlN capping layer under no bias

GROWTH and CHARACTERIZATION

Epitaxial Growth

The 100 nm thick p-InGaN layer with 5 nm AlN capping layer structure described above, and a 100 nm thick n-InGaN with 5 nm AlN capping layer, were grown on standard undoped-

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GaN/sapphire templates in an Emcore MOCVD reactor. Trimethylgallium (TMG), trimethylaluminum (TMAl) and trimethylindium (TMI) were the precursors used to introduce gallium, aluminum and indium, respectively, into the reactor using hydrogen as the carrier gas; Ammonia (NH3) was used as the nitrogen source. Cp_2Mg was used for p-type doping and SiH_4 was used for n-type doping of InGaN. The u-GaN layer was grown using a two step process, where typically a 20-40 nm thin GaN buffer layer growth at 550°C was followed by the epitaxy of high-quality 2 μm thick GaN template at 1030°C. The growth temperature for the InGaN layer was set to 740°C, and the AlN was grown at the same temperature to avoid the decomposition of InGaN.

Material and Device Characterization

High-resolution X-ray Diffraction (HRXRD) studies were performed with an X'Pert diffractometer featuring Ge(220) hybrid four bounce monochromator in double-crystal mode with $CuK_{\alpha 1}$ monochromatic radiation. The samples were characterized for optical reflection and transmission using PerkinElmer Lambda 1050 UV/Vis/NIR system in the 250 to 700 nm range. The p-InGaN was thermally treated at 650°C in N_2 ambient for 20 min to activate the p-type material. Time-integrated photoluminescence (PL) measurements on the InGaN samples were conducted in the temperature range of 8K to 120K. The excitation source was a 325 nm, 45 mW He-Cd continuous wave laser. Hall measurements were performed with an HMS-3000 system at room temperature using Van der Pauw arrangement. The Hall measurements were done on the surface of AlN and at a depth of 40 nm from surface after etching AlN epi-layer using inductively coupled plasma. The current-voltage (I-V) measurements were performed at room temperature under no illumination (dark) and AM 1.5 (1 sun) conditions using a custom built and calibrated system having an AM 1.5 filter from Newport-Oriel. The ohmic contacts were formed using In-Ga metal on the surface and at a depth of 40 nm from the surface.

RESULTS and DISCUSSION

The observed crystalline quality of the epitaxial layers is shown in Figure 2. The InGaN composition is determined to be around 15% for p-InGaN and 13.5% for n-InGaN layers. The fringes around the 15% p-InGaN layer indicate the absence of extended crystalline defects in the volume of InGaN layer that could affect the performance [9]. A broad AlN peak is also observed, and this thin layer is probably amorphous or poly crystalline due to the low growth temperature of AlN.

The PL at 8 K is shown in Figure 3(a) with multiple peaks around 3 eV. The band gap of the material is 3 eV and the peaks observed above 3 eV are related to the donor-acceptor pair transitions. The band gap is also confirmed to be 3 eV by the optical absorption shown in Figure 3(b). The optical absorption band edge, shown in Figure 3(b), is sharp, indicating absence of extended crystalline defects or phase separation in the InGaN epi-layers [10]. The solar cells studied here are wide band gap and hence the sharp band edge is required to transmit all the energy not absorbed by this active layer.

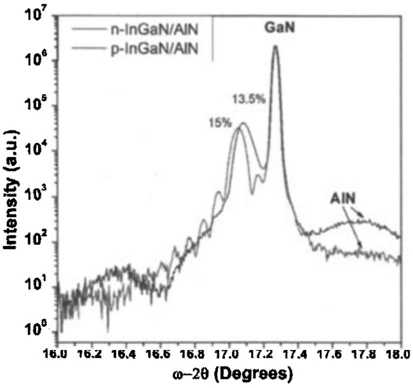

Figure 2. ω-2θ (0002) rocking curve for p-InGaN with AlN capping layer and n-InGaN with AlN capping layer

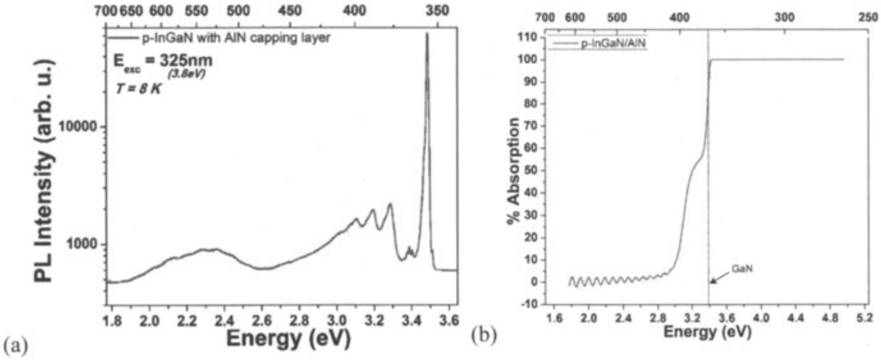

Figure 3. Optical properties of p-InGaN with AlN capping layers (a) Photo-luminescence at 8K (b) Optical absorption

The Hall measurement results for two locations shown in Figure 4 are tabulated in Table 1. The carrier concentration before thermal activation of p-InGaN measured on the AlN surface was 2.671×10^{13} cm^{-3}, while after activation it was measured to be -2.021×10^{17} cm^{-3}, indicating formation of a 2DEG. Under similar conditions with n-InGaN epi-layer, the carrier concentration on the AlN surface was measured to be -1.785×10^{19} cm^{-3}. The carrier concentrations below the AlN surface for p-InGaN and n-InGaN were measured to be 1.027×10^{18} and -3.194×10^{18} cm^{-3}, respectively. Other parameters extracted from Hall measurement, mobility and resistivity, of epi-layers are also tabulated in Table 1. The mobility of p-InGaN and n-InGaN are in the range typically observed with epi-layers without any capping layer [11].

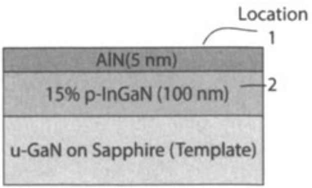

Figure 4. Location of Hall measurement

Table 1. Hall measurement results

Location / Condition	1		2
	Not Activated	Activated	Activated
p-InGaN /AlN capping layer			
Carrier Concentration (cm^{-3})	2.671×10^{13}	-2.021×10^{17}	1.027×10^{18}
Mobility (cm^2/Vs)	2.942	0.6109	5.978
Resistivity (Ω-cm)	7.944×10^{4}	50.55	1.017
n-InGaN /AlN capping layer			
Carrier Concentration (cm^{-3})	-	-1.785×10^{19}	-3.194×10^{18}
Mobility (cm^2/Vs)	-	54.49	18.83
Resistivity (Ω-cm)	-	6.418×10^{-3}	0.1038

The photo-response of the device is shown in Figure 5. The open circuit voltage of 2.15 V and short circuit current of 21.8 μA are observed. A very good diode action is observed under no illumination, but with illumination under AM 1.5 spectrum, a change in series and shunt resistance is observed with fill factor less than 5.

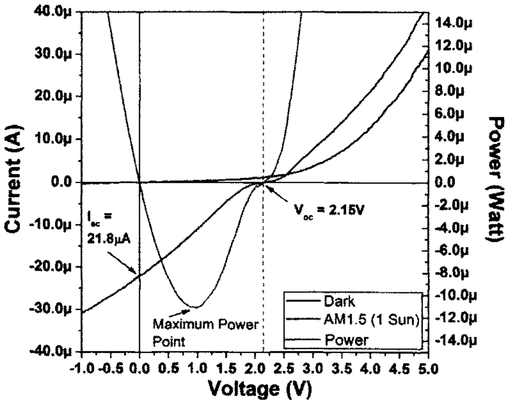

Figure 5. Current-Voltage characteristics under dark and AM1.5 (1 sun) conditions

Conventional Schottky-barrier solar cells are formed by surface inversion using Schottky metal contacts. The limitation with these solar cells lies with the aerial coverage originating from shadowing by metal contacts. The depletion region width in Schottky solar cell structures is formed below and in short range around the Schottky metal contact. The polarization in III-nitrides can be used to invert the surfaces, and this inversion is caused by optically transparent epi-layers. A few drawbacks of the polarization based structures are formation of a potential well at the InGaN/AlN interface and the optimum thickness of AlN epi-layer. The optimum thickness of AlN epi-layer should be thick enough to cause strong band bending and thin enough for photo-carrier to tunnel.

CONCLUSIONS

Schottky-barrier type InGaN solar cells using inherent polarization can be used to design III-nitride solar cells. The simulated band diagrams and the supporting experimental device structures were presented. The band diagrams indicate a clear 2DEG formation and the corresponding band bending can be used to design solar cells. The Hall measurements indicate the surface type inversion and 2DEG formation with AlN capping layer on p-InGaN. The photovoltaic response from the surface inverted device structure was demonstrated, with 2.15 V open circuit voltage and 21.8 μA short circuit current. Although the fill factors are low, these can be improved with improvements in ohmic contacts and by addressing the current spreading issues commonly observed in InGaN solar cells.

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