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Effect of III-nitride polarization on V_{OC} in p–i–n and MQW solar cells

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We performed detailed studies of the effect of polarization on III-nitride solar cells. Spontaneous and piezoelectric polarizations were assessed to determine their impacts upon the open circuit voltages (V_{OC}) in p–i(InGaN)–n and multi-quantum well (MQW) solar cells. We found that the spontaneous polarization in Ga-polar p–i–n solar cells strongly modifies energy band structures and corresponding electric fields in a way that degrades V_{OC} compared to non-polar p–i–n structures. In contrast, we found that piezoelectric polarization in Ga-polar MQW structures does not have a large influence on V_{OC} compared to non-polar MQW structures.

1 Introduction Recently, InGaN alloys have attracted much attention for use in the development of III-nitride based solar cells with the potential for achieving energy conversion efficiencies exceeding 50% [1]. Even with these theoretically high values, there are several technical challenges to be overcome; achieving high crystallinity, p-type doping in indium-rich InGaN, and control of indium phase segregation with higher indium composition. These challenges have prompted the development of solar cell structures where InGaN/GaN multi-quantum well (MQW) or intrinsic InGaN are inserted between GaN p–n junctions [2–10]. These devices produce large open circuit voltages (V_{OC}) due to their inherently wide bandgap and V_{OC} values reported in the literature are plotted in Fig. 1(a). To ensure a fair comparison, only V_{OC} measured under the standard air mass 1.5 global (AM 1.5G) illumination is shown. The V_{OC} of both structures decreases almost linearly with an increase in indium composition. Interestingly, p–i–n-based III-nitride solar cells have much lower V_{OC} compared to that of MQW structures and the value reduces abruptly with higher indium content. Such conspicuous reduction of V_{OC} in p–i–n structures is partially explained by increased defect densities in the indium-rich InGaN layer that lead to increased leakage current [2, 3]. However, we also found that polarization effects play a significant role in the reduction of V_{OC} in p–i–n structures with higher indium composition and lower V_{OC} when compared to that of MQW structures. III-nitride materials have non-centrosymmetry of the wurzite structures and large ionicity between the covalent metal and nitrogen bond. As a result, large spontaneous and piezoelectric polarizations [11] should be taken into account when calculating the V_{OC} of nitride-based solar cells. In this letter, we detail our study of the effect of polarization upon the V_{OC} by comparing Ga-polar and non-polar conformations to explain the behaviour of V_{OC} in p–i–n and MQW structures.

2 InGaN p–i–n and MQW solar cells The solar cell structures were grown on GaN/sapphire templates with a 2 μm Si-doped n-type GaN layer, an intrinsic absorption region, and a 100 nm Mg-doped p-type GaN layer. The intrinsic absorption region in the two cells was composed of

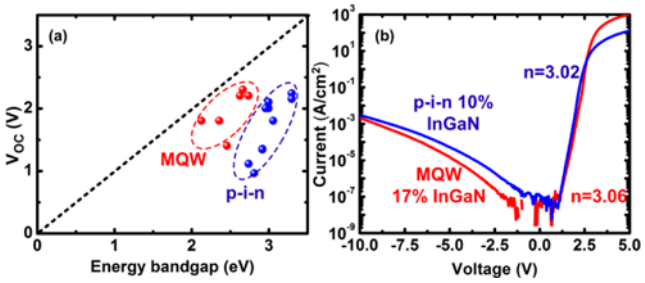

Figure 1 (online colour at: www.pss-rapid.com) (a) Open circuit voltages for MQW (red) and p–i–n (blue) structures [2–10] and (b) dark J–V characteristics of MQW $In_{0.17}Ga_{0.83}N$/GaN and p–i ($In_{0.1}Ga_{0.9}N$)–n solar cells.

200 nm thick $In_xGa_{1-x}N$ for p–i–n structures or 7-period $In_xGa_{1-x}N$/GaN (3/8 nm) for MQW structures. Photovoltaic parameters for our devices are listed in Table 1. It should be noted that higher short circuit current (J_{SC}) for $In_{0.17}Ga_{0.83}N$/GaN MQW structure is observed due to back-side reflection that increases light absorption. Peak values of external quantum efficiency (EQE) in MQW solar cells are much lower than those of p–i–n structures due to enhanced recombination in the quantum wells. Even with similar J_{SC}, lower EQE, and higher indium compositions in MQW structures, higher V_{OC} is observed. One speculation for such enhanced V_{OC} is the improved crystalline quality where the leakage current related to defects in InGaN is much reduced [2, 3]. To assess this, we compared dark J–V characteristics of both structures in Fig. 1(b) and found similar ideality factors of $n \sim 3.0$ in addition to reverse dark current of about mid 10^{-8} A/cm^2 at 0 V bias. While slightly reduced leakage current in MQW structures was observed at higher reverse bias, the dark J–V characteristics indicate that significantly higher V_{OC} cannot be attributed to these slightly smaller leakage currents.

3 Effect of III-nitride polarization upon p–i–n solar cells The V_{OC} in p–i–n structures is closely related to the potential difference across the i-InGaN layer; $qV_{bi} = qV_{bij,n} - \Delta E_{C,n} + qV_{biw} + qV_{bij,p} + \Delta E_{C,p}$ where $V_{bij,n}$, $V_{bij,p}$ and V_{biw} are the built-in voltages at the junction interface and inside i-InGaN and $\Delta E_{C,n}$ and $\Delta E_{C,p}$ are the conduction band offsets as shown in Fig. 2(a). In this case, V_{bi} provides the theoretical upper limit of V_{OC} in ideal devices ignoring other voltage limitations such as material defects and Auger recombination which typically set a limit of $V_{OC} \approx E_g/q - (nkT) \ln (J_0/J_{SC})$ where J_0 is the saturation current density, q is the unit charge, n is the ideality factor, and T is the temperature [3]. Since the V_{OC} balances built-in electric field (F_{bi}) across a cell and leads to zero net current, the investigation of electric field and energy band structures can provide insight into polarization effects on the V_{OC}. Therefore, we simulated energy band structures for Ga-polar and non-polar p–i–n structures using SILENSe – a software tool that accounts for specific features of III-nitride epitaxial layers including strong III-nitride polarization. For V_{OC}, forward bias was simulated to yield current density equal to the measured J_{SC} for p–i–n and MQW solar cells as shown in Table 1, resulting in a net current equal to zero; $J = J_0(\exp(qV_{OC}/nkT) - 1) - J_{SC} = 0$. For the non-polar solar cells, the AMPS-1D solar simulation tool is also used to confirm V_{OC} using the parameters of III-nitride materials from Ref. [10]. Figures 2(a) and (b) show the simulated energy bandgaps and corresponding electric fields for Ga-polar and non-polar p–i–n structures. With very thick 200 nm InGaN, it is expected that piezoelectric polarization can be neglected due to fully relaxed InGaN films, but spontaneous polarization (SP) is dominant. The SP, which is in the opposite direction of the c-plane as shown in Fig. 3, induces a sheet charge density at the InGaN/GaN interface. These strong SP charges enhance the space charges and, as a result, lead to the modification of the built-in voltage in Ga-polar p–i–n structures as shown in Fig. 2(a). Even though net V_{bi} remains constant for Ga-polar and non-polar structures, V_{bij} is substantially increased and V_{biw} is reduced for Ga-polar structures. Corresponding electric fields are also modified accordingly as shown in Fig. 2(b). Further modification of V_{bij} and V_{biw} in Ga-polar structures is observed with increased indium

Table 1 Photovoltaic parameters of p–i–n and MQW cells.

	In (%)	V_{OC} (V)	FF (%)	J_{SC} (mA/cm^2)	peak EQE (%)	η (%)	Reference
p–i–n	10	2.0	79.7	0.76	67	1.2	[13]
	10.7	2.0	79.5	0.64	75	1	[7]
MQW	17	2.2	80.0	1.3	37	2.3	[13]
	19	2.3	77.6	0.77	25	1.4	[13]

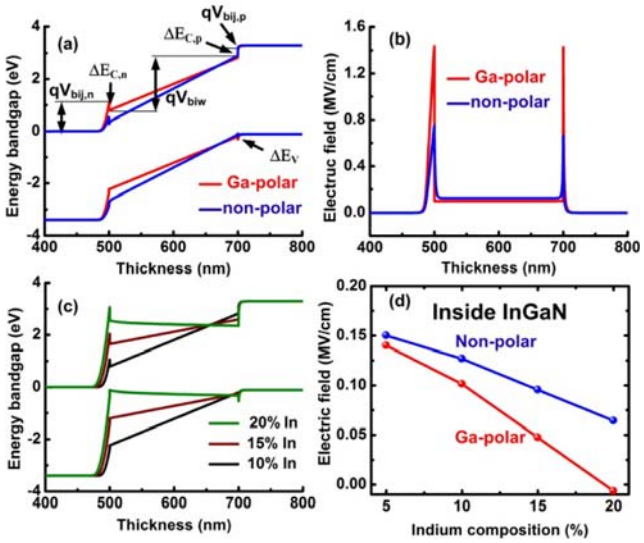

Figure 2 (online colour at: www.pss-rapid.com) (a) Energy bandgap of Ga-polar and non-polar $In_{0.1}Ga_{0.9}N$ p–i–n, (b) corresponding electric field, (c) energy bandgap, and (d) electric field inside InGaN layer as a function of indium compositions. Electron and hole concentrations were 5×10^{18} and 5×10^{17} cm^{-3} for n-and p-GaN layers, respectively.

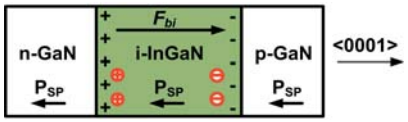

Figure 3 (online colour at: www.pss-rapid.com) Schematic of p–i–n structure with SP.

composition as shown in Fig. 2(c) where V_{bij} continuously increases, leading to flatter energy band structures inside InGaN layers. This is due to increased SP and band offset at the InGaN/GaN interface with increased indium composition where conduction and valence band offsets between InN and GaN are 2.22 and 0.58 eV, respectively [12]. It should be noted that the electric field inside In-rich InGaN abruptly drops and with an indium composition of about 20%, the electric field is equal to zero as shown in Fig. 2(d). In this case, the extraction of electrons and holes occurs only at the ~20 nm thick InGaN/GaN interface, but not inside the i-InGaN layer as shown in Fig. 2(c). Our simulation indicates that Ga-polar p–i($In_{0.1}Ga_{0.9}N$)–n structures yielded V_{OC} of 2.58V while the simulated V_{OC} for non-polar p–i–n structures was 2.73 V. This result clearly indicates that III-nitride polarization in p–i–n structures has a deleterious effect upon the V_{OC}. Since the detrimental effect of polarization upon V_{OC} increases with increased indium composition, conspicuous reduction of V_{OC} in Ga-polar structures in Fig. 1(a) can be attributed to the III-nitride polarization as well as increased leakage current caused by defects resulting from increased indium compositions [2, 3].

4 Effect of polarization of III-nitride upon V_{OC}

In the MQW structures seen in Fig. 4, piezoelectric polarization is much stronger than spontaneous polarization and induces a negative sheet charge at the n-GaN/InGaN interface. This negative sheet charge will cause the reduction of positive space charge at the n-GaN/InGaN interface. Similarly, negative space charges reduce at the p-GaN/InGaN interface. Such a reduction of interfacial space charges minimized the interfacial energy bending which is observed in MQW structures. Resulting energy band structures are shown in Fig. 4(b) and electric fields at the interfaces in Fig. 4(c) are indeed reduced when compared to those of p–i–n structures. Figure 4(b) shows the comparison of energy band structures between Ga-polar and non-polar MQW devices which are similar except for the strong modification at the quantum wells and barriers. The simulated V_{OC} for Ga-polar $In_{0.17}Ga_{0.83}N$/GaN MQW structures was 2.73 V while non-polar MQW yielded V_{OC} of 2.68 V, indicating no significant influence of polarization upon V_{OC}. It can be noted that there is a discrepancy between the measured and simulated V_{OC} for Ga-polar p–i–n and MQW structures. This discrepancy might originate from III-nitride material defects leading to higher leakage current and subsequently degraded V_{OC}.

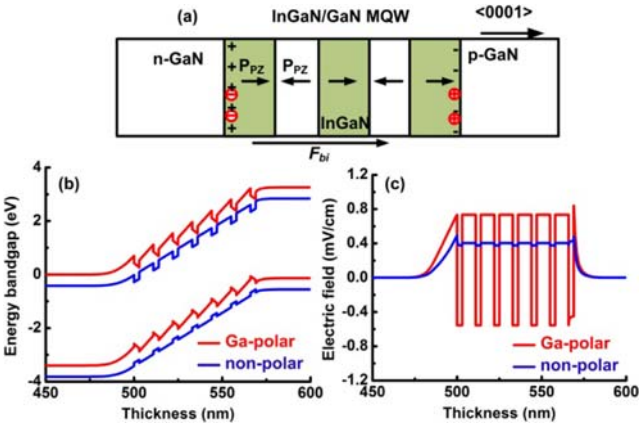

Figure 4 (online colour at: www.pss-rapid.com) (a) Schematic of MQW structure with polarization, (b) energy bandgap of Ga-polar and non-polar $In_{0.1}Ga_{0.9}N$/GaN MQW and (c) corresponding electric field. For clarity, the energy bandgap of the non-polar structure was shifted downward.

5 Conclusion We performed theoretical simulations to study the behaviours of the observed V_{OC} for p–i–n and MQW nitride solar cells. It is found that strong spontaneous and piezoelectric polarizations should be taken into account when estimating the V_{OC}. For p–i–n solar cells, spontaneous polarization has a detrimental effect on V_{OC} while for MQW solar cells, the piezoelectric polarization is dominant and does not have a large influence on the V_{OC}.

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