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Optimization of semibulk InGaN-based solar cell using realistic modeling

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Due to its high absorption coefficient and variable bandgap, InGaN is being intensively studied for photovoltaic applications. Growth of thick homogenous InGaN absorbers is challenging due to relaxation, clustering, and transition from 2D to 3D growth. These issues can be avoided by a semibulk multilayer structure. In this work, we analyze InGaN-based semibulk-structured solar cells in detail. We show that for indium content lower than 15%, GaN interlayers' thickness has no influence on carrier transport due to the low barrier height. A conversion efficiency of 2.4% can be expected for this indium content. However, for higher indium content (15–30%), we show that the thinner the GaN interlayers, the better the conversion efficiency. Beyond 30% of indium, the conversion efficiency is hindered by the barriers' important height even for very thin thicknesses of GaN in-terlayers. We show also that, for semibulk structure, both growth direction (N-face and metal-face) have similar impact on efficiency. This theoretical study gives the guidelines for the fabrication of InGaN-based solar cells that can be used as a wide-bandgap top cell in multijunction solar cells.

1. Introduction

InGaN alloys have a direct bandgap that is variable from 0.76 eV to 3.42 eV (Vurgaftman and Meyer, 2003) which covers the totality of the solar spectrum. They have a very high absorption coefficient ($\sim 10^5 \text{ cm}^{-1}$ near bandgap) so that a few hundred nanometers of thickness are sufficient to absorb the majority of incident light (Wu et al., 2002). These advantages, among others such as good high temperature performance, make this material a potential candidate for high efficiency solar cells.

However, InGaN photovoltaic (PV) performance has been hindered by poor crystalline quality (Bhuiyan et al., 2012). The growth of high quality InGaN layers with more than 20% of indium is difficult mainly due to the formation of extensive crystal defects and phase separation within the layer (El Gmili et al., 2013). The critical layer thickness for a fully strained high quality InGaN with high In content is only a few nanometers (Zhao et al., 2011; Holec et al., 2007). A new approach has been proposed recently to grow a relatively-thick high-quality InGaN layer, which is called a semibulk structure (Pantzas et al., 2013), due to the insertion of thin GaN interlayers that absorb excess In that accumulates at the heterojunction surface and

contribute to InGaN phase separation. We have demonstrated higher crystalline quality compared to a bulk layer (El Gmili et al., 2013). We have also demonstrated high external quantum efficiency (EQE) with a peak of 85% for InGaN-based semibulk-structured solar cell (Arif et al., 2017), and with a state-of-art current density of 0.57 mA/cm^2 for 8% of indium.

It is important to understand the effect of semibulk structures on the efficiency of InGaN solar cells. In this work, we study the influence of structural parameters on the power conversion efficiency (PCE) of InGaN-based semibulk-structured solar cells with SILVACO TCAD software.

2. Model description

Our model is calibrated to the multilayered solar cell experimentally achieved by Young et al. (2013), which shown a high PV performance. As there is no information about the free carrier concentrations, we have considered complete ionization for dopants with n-type concentration of $2 \cdot 10^{19} \text{ cm}^{-3}$ and p-type average concentration of $5 \cdot 10^{19} \text{ cm}^{-3}$. Similar level of hole concentrations have been already demonstrated experimentally (Gunning et al., 2012). For intrinsic

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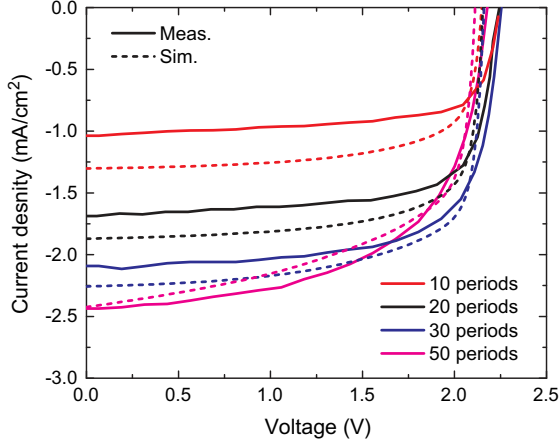


Fig. 1. Simulation vs. measurements: $J(V)$ curves of InGaN-based semibulk-structured solar cell with 10, 20, 30 and 50 periods.

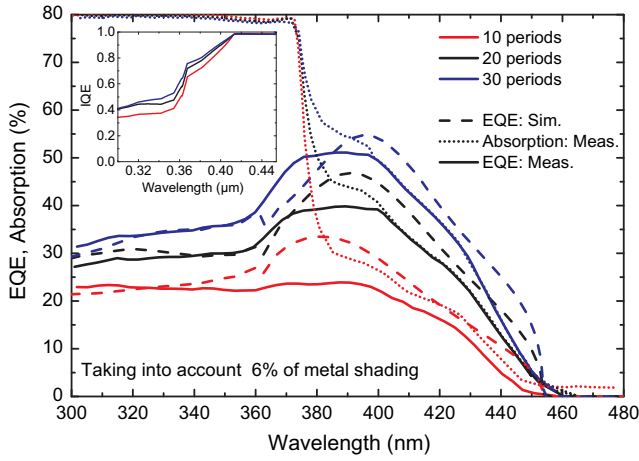


Fig. 2. Simulation vs. measurements: EQE and absorption curves of InGaN-based semibulk-structured solar cell with 10, 20 and 30 periods. Inset: Simulation IQE curve.

Table 1

Comparison between measured and modeled short circuit current J_{sc} . An absolute difference of about 0.2 mA/cm^2 is observed.

Periods	Meas. (mA/cm^2)	Sim. (mA/cm^2)	Error (%)	Absolute diff. (mA/cm^2)
10	1.04	1.30	25	0.26
20	1.69	1.87	10.6	0.18
30	2.09	2.26	8.1	0.17

concentration, we have used a value of $8.10^{16} \text{ cm}^{-3}$ by fitting to experimental results. We have used the Transfer Matrix Method (TMM) in order to calculate the photogeneration rate through the structure. More details about physical models used in our simulations can be found in reference [El-Huni et al. \(2016\)](#).

In order to validate the used model in our simulations, we have reproduced experimental results obtained by [Young et al. \(2013\)](#). Fig. 1 shows the comparison between simulation and measurements for $J(V)$ curves for 10, 20, 30 and 50 periods of InGaN/GaN. In these simulations we have taken into account the attenuation of polarization effect as the number of periods increases as demonstrated experimentally by [Bai et al. \(2001\)](#). We have also lowered the carrier lifetime to 1 ns instead of 5 ns in InGaN at 50 periods as it has shown a lower material quality in their structure. A bowing parameter of 1 has been used for bandgap calculation. This value was based on from EQE curves and also based on Ref. ([Moses and Van De Walle, 2010](#)). We have used the same

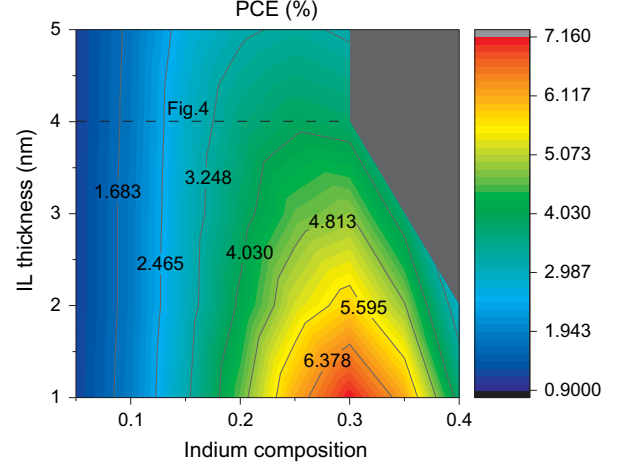


Fig. 3. Map of PCE in function of indium content and IL thickness.

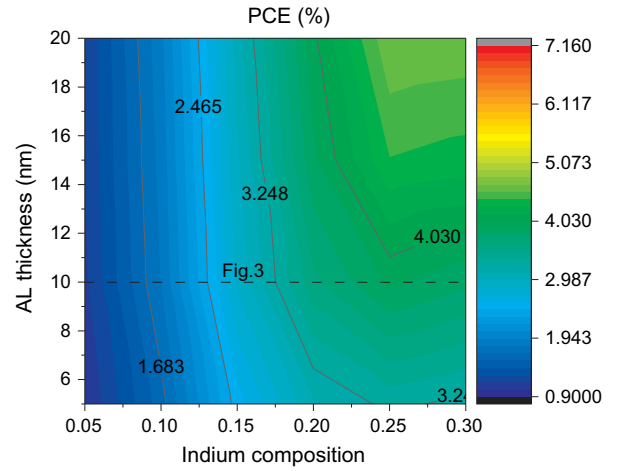


Fig. 4. Map of PCE in function of indium content and AL thickness.

value to calculate electron affinity for InGaN, while the maximum valence band varies linearly ([Moses and Van De Walle, 2010](#)).

The difference in the short current density (J_{sc}) between simulation and measurement is due to the difference between measured absorption and absorption model for long wavelengths, as shown in EQE curves in Fig. 2. However, the absorption model used in our simulations was obtained empirically for high indium concentrations and interpolated for low indium concentrations ([Brown et al., 2010](#)). Furthermore, the difference is an absolute value of about 0.2 mA/cm^2 and not relative, as shown in Table 1. In addition, in the inset of Fig. 2, we show simulated internal quantum efficiency (IQE), showing strong similarity to measurements. Experimental IQE can be deduced from the ratio between the measured EQE and absorption.

The structure achieved by [Young et al. \(2013\)](#) has an InGaN sublayers of 3 nm while GaN interlayers can be reduced to 2 nm as demonstrated in a previous work ([Pantzas et al., 2013](#)). In this study we propose an optimization of semibulk structure in terms of structural parameters while taking into account growth limits.

3. Results and discussion

We studied the dependency of PCE in terms of structural parameters (indium content, InGaN sublayers' thickness, GaN interlayers' thickness and polarization). We should note that for the following simulations, we have used an anti-reflective coating that has the same reflectance as reported by [Young et al. \(2014\)](#). Hereafter, we will refer to InGaN absorber sublayer as AL, and GaN interlayer as IL.

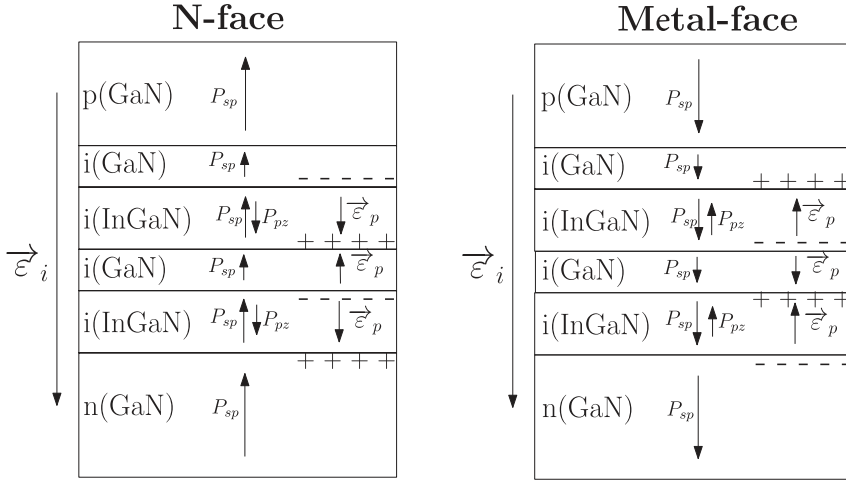


Fig. 5. Schematic representation of polarization-induced charges and fields in semibulk structure with N-face and metal-face growth direction.

3.1. IL thickness influence

We change the thickness of high-bandgap IL from 1 to 5 nm, while keeping the AL thickness fixed at 10 nm. In order to understand the effect of IL thickness only, we have considered zero polarization-induced charges for this part. We have fixed the number of periods to 30 as it has shown to be the optimum for the structure achieved by Young et al. (2013), and also at this number of periods the polarization-induced charge can be neglected. Fig. 3 shows the map of PCE as a function of indium content and IL thickness. For low indium content, the IL thickness has no influence on PCE due to the fact that the barriers' height is so low that the photogenerated carriers can pass by thermionic emission. While for high indium content, the barriers' height becomes more important and the tunneling effect becomes predominant where the tunneling probability is exponentially dependent on the barrier's thickness. Beyond 30% of indium content, the PCE decreases even for thin IL. This is due to the fact that the barriers' height becomes so important that the tunneling probability decreases. For this reason, in AL-thickness dependency of PCE we have varied the indium content from 5 to 30% only.

3.2. AL thickness influence

As in the previous study, we have not considered the polarization-induced charge in order to have a pure influence of AL thickness. We have varied the thickness of AL from 5 nm to 20 nm, while keeping the IL thickness at 4 nm. Even though the optimum is reached with thinner

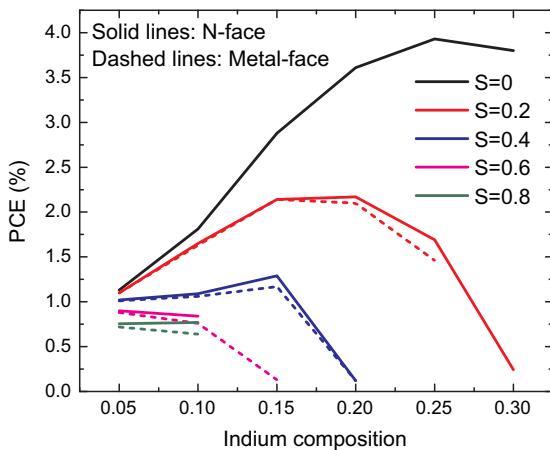


Fig. 6. PCE in function of In content for different values of screening factor S , with N-face and Metal-face growth direction.

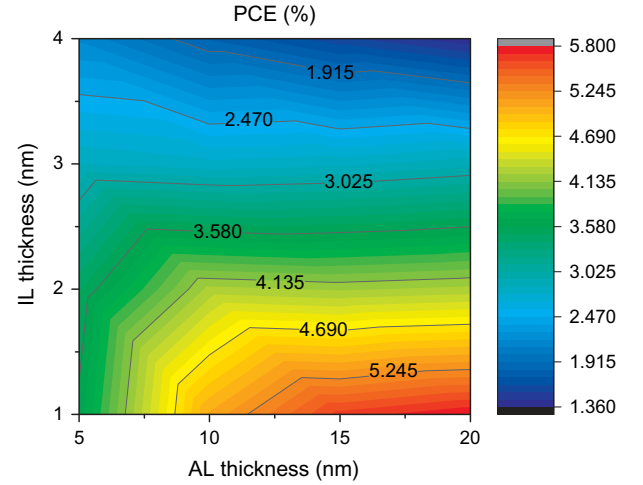


Fig. 7. PCE in function of the IL and AL thicknesses. Screening factor has been fixed at 0.2. Indium composition was fixed to 25% with 15 periods.

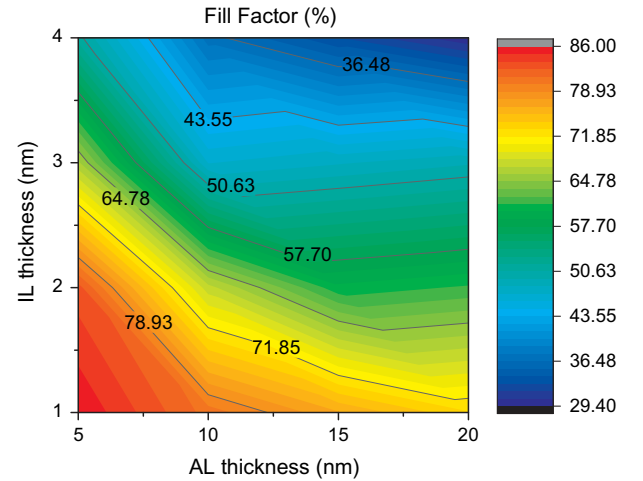


Fig. 8. Fill factor in function of the IL and AL thicknesses. Screening factor has been fixed at 0.2. Indium composition was fixed to 25% with 15 periods.

IL, we prefer to start from values currently demonstrated in experiments. We have fixed the number of periods to 30 as in the previous study. Fig. 4 shows the map of PCE as a function of indium composition and AL thickness. For low indium content, the AL thickness has almost

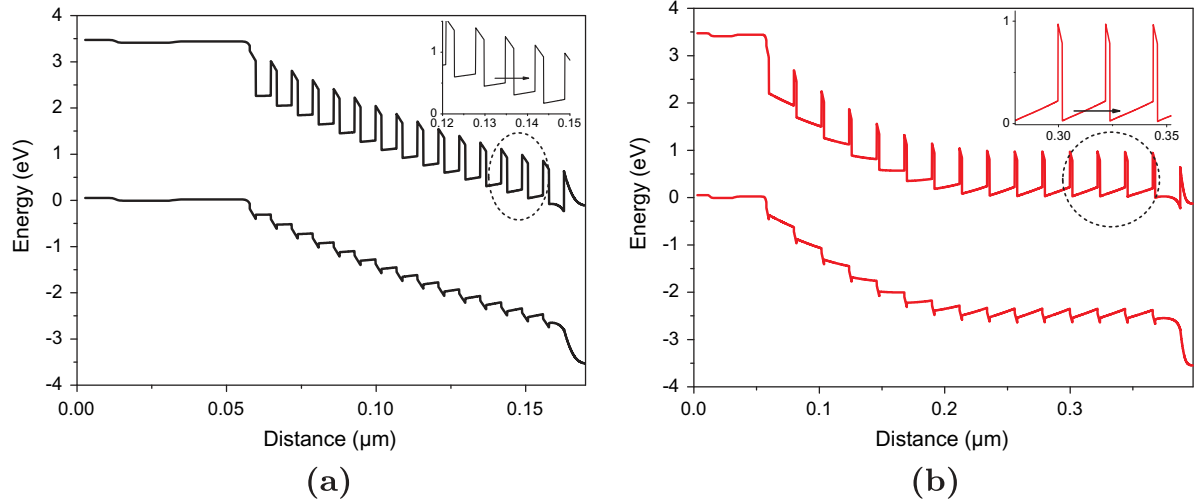


Fig. 9. Band diagram for semibulk structure with 15 periods and AL thickness of (a) 5 nm and (b) 20 nm. $S = 0.2$ and $In = 25\%$.

no influence on PCE. This is due to the fact that with low indium content we obtain high bandgap, and the photon with energies higher than bandgap will be absorbed in p-GaN and in the first few nanometers of InGaN. However, for higher indium composition (hence lower bandgap), the incident photons with energies higher than bandgap needs more distance to be absorbed, and for this reason PCE increase with increasing AL thickness. However, we should note that the impact of AL thickness is not the same when the polarization effect is taken into account, as will be shown.

3.3. Polarization influence

In terms of polarization effect, some studies have shown that N-face growth direction is favorable for p-on-n InGaN-based solar cell (Chang and Kuo, 2012). However, because of the succession of layers in semibulk structure, the polarization does not have the same effect as in the bulk structure. In the semibulk structure even with the N-face polarity, there would be an electric field (ϵ) opposed to the collection of photogenerated carriers in IL. Fig. 5 shows the distribution of charges as well as the direction of the electric fields in semibulk structure for both N-face and metal-face polarities. In order to study the influence of polarization, we have introduced a screening factor (S) for the polarization-induced charge (PIC) so that when $S = 0$ means the PIC is totally screened, and when $S = 1$ means that theoretical value of PIC is taken as 100%. We have fixed the AL thickness to 10 nm and IL thickness to 4 nm. We have varied the indium content from 5% to 30%. The number of periods is fixed to 30. As shown in Fig. 6, the growth direction is indifferent in semibulk structure, since the behavior is the same regardless of the polarity of PIC.

3.4. Structure optimization

After having studied each parameter separately, we have proceeded to the optimization of semibulk structure in terms of AL and IL thicknesses for 25% of indium and with taking into account polarization. We have chosen this indium level because it has shown to be suitable for 4-terminal InGaN/Silicon tandem cell (El-Huni et al., 2016). Fig. 7 shows the map of PCE as a function of AL and IL thicknesses using 15 periods with 0.2 screening factor. One can see that the optimum is obtained at an IL thickness of 1 nm and AL thickness between 15 and 20 nm, with a PCE of 5.8%. However, for semibulk structure with indium of 25% we expect the IL thickness to be 2 nm or higher in order to maintain the strain in the structure. For 2 nm of IL thickness, the optimal AL thickness is 9 nm, where beyond this thickness the PCE does not change. This is due to the decrease of fill factor that compensates the gain in

photogenerated current. As shown in Fig. 8, fill factor decreases with the increase of IL and AL thicknesses. This is because for thicker AL the conduction band bending in AL, caused by electric field discontinuity, will behave as a higher and thicker barrier than in the case with thinner AL, which hinders the tunneling probability. Fig. 9 shows the difference in band diagrams for 15 periods with AL thickness of 5 and 20 nm. In addition, as the AL thickness increases, the active region exceeds the depletion region. For IL thickness beyond 3 nm, the AL thickness should be lower than 10 nm.

4. Conclusion

We have carried out in this work a theoretical study, using realistic simulations, on InGaN-based semibulk-structured solar cell. We have first validated our model using experimental results. Then, we have shown that for semibulk structure, beyond 30% of indium the PCE deteriorates due to the barriers' height. For low indium composition ($< 15\%$), barriers' thickness has no influence because the photogenerated carriers can pass by thermionic effect. However, for indium compositions between 15% and 30%, the thinner the GaN interlayers' thickness, the better the PCE. We have also shown that both growth directions (N-face and metal-face) have the same impact on PCE. We have also optimized a semibulk-structured InGaN-based solar cell with 25% of indium and we found that for 2 nm of IL thickness, the optimal AL thickness is about 9 nm. Beyond this thickness fill factor decrease compensates the increase in photogenerated current and the PCE keep unchanged. Our work shows the guidelines, while taking into account the technological issues, to achieve InGaN-based semibulk-structured solar cell. Such wide-bandgap solar cell can be combined with other cells in order to achieve a multijunction solar cell.

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