Phys. Status Solidi RRL **4**, No. 3–4, 88–90 (2010) / **DOI** 10.1002/pssr.201004044

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Investigation on the conversion efficiency of InGaN solar cells fabricated on GaN and ZnO substrates

S. Inoue[1], M. Katoh[1], A. Kobayashi[2], J. Ohta[1], and H. Fujioka[*, 1, 3]

[1] Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba Meguro-ku, Tokyo 153-8505, Japan
[2] Department of Applied Chemistry, The University of Tokyo, 7-3-1 Hongo, Tokyo 113-8656, Japan
[3] Core Research for Evolutional Science and Technology of Japan Science and Technology Corporation (JST-CREST), 5 Sanban-cho, Chiyoda-ku, Tokyo 102-0075, Japan

Received 17 February 2010, revised 2 March 2010, accepted 2 March 2010
Published online 5 March 2010

Keywords solar cells, InGaN, ZnO, device simulation

[*] Corresponding author: e-mail hfujioka@iis.u-tokyo.ac.jp, Phone: +81-3-5452-6342, Fax: +81-3-5452-6343

By the use of a device simulator that takes the quantum effect into account, we have investigated the characteristics of InGaN solar cells stacked coherently on GaN or ZnO substrates. We have found that it is necessary to fabricate nonpolar cells, N-polar cells with p–i–n structures, or III-polar cells with n–i–p structures in order to achieve high conversion efficiency. InGaN solar cells grown on GaN substrates and on ZnO substrates exhibit almost the same conversion efficiencies, in spite of the difference in the intensities of the strains in the InGaN films. Taking the smaller lattice mismatch between InGaN and ZnO into account, we conclude that the use of ZnO substrates, which makes the growth of thick InGaN films with high In concentrations simpler to achieve, is advantageous in the fabrication of high conversion efficiency InGaN solar cells.

Recently, solar cells based on group-III nitride layers have attracted much attention [1–5] because the bandgaps of InGaN alloys can cover almost the whole solar spectrum, from 0.65 eV to 3.4 eV. However, many research groups have found that the fabrication of nitride-based solar cells is quite difficult to achieve because of several unique features of nitride materials. The most serious problem that is encountered in the fabrication of a nitride-based cell structure is the lack of suitable substrates that are lattice matched to InGaN. For the fabrication of InGaN cells, the growth of thick InGaN layers with high In concentrations to absorb a large fraction of the available light is necessary. Conventional substrates for the growth of group-III nitrides, such as sapphire or SiC, have large lattice mismatches with respect to InGaN, and therefore, the use of these substrates leads to a high density of crystalline defects in the InGaN films. On the contrary, ZnO is an ideal substrate material for these devices because it shares the same crystalline symmetry and a-axis lattice constant as $In_{0.18}Ga_{0.82}N$ [6, 7], although the use of ZnO as a substrate material for nitride-based devices has previously been regarded as problematic because of its high reactivity with nitrides. Recently, we have found that the use of a low-temperature growth technique such as pulsed excitation deposition (PXD) [8] helps to suppress the interfacial reactions between ZnO and nitrides and to make the use of ZnO as substrate for the growth of nitrides possible. In fact, we have reported the successful low-temperature growth of high-quality InGaN on ZnO by the use of PXD [9, 10]. In this letter, we will discuss the characteristics of InGaN solar cells grown on ZnO substrates based on data derived from two-dimensional device simulations, putting special emphasis on the effects of polarization.

We have investigated the characteristics of p-GaN/i-InGaN/n-GaN solar cells coherently grown on GaN{0001} or ZnO{0001} by using the two-dimensional device simulator ATLAS, which is based on a self-consistent solution of the Poisson equation, and the current continuity equation.

We have calculated the I–V characteristics for nitride solar cells that consist of an $In_xGa_{1-x}N$ layer sandwiched by p-type and n-type GaN layers, assuming light illumination of AM1.5 at 100 mW/cm^2. The bandgap of $In_xGa_{1-x}N$ was calculated with a bowing parameter of 1.43 eV [11]. The recombination parameters such as radiative recombination coefficients, Shockley–Read–Hall non-radiative recombination coefficients, and Auger non-radiative recombination coefficients are reported in Refs. [12–14]. The In composition dependence of the carrier mobility and the dielectric function for the InGaN layers are based on Refs. [15, 16]. The thicknesses of the p-GaN and the i-InGaN were set to 150 nm or 200 nm, respectively. The carrier concentrations in the p-GaN and the n-GaN layers were 5×10^{17} cm^{-3} and 1×10^{18} cm^{-3}, respectively.

The conversion efficiency of p-GaN/i-InGaN/n-GaN double-hetero solar cells depends strongly upon the charge distribution at the heterointerfaces, since the band discontinuity can work as an energy barrier to the photo-generated carriers in the i-InGaN layer. Therefore, we estimated the charge distribution near the heterojunction of the p-GaN/i-InGaN/n-GaN cell taking the quantum effect into account by the use of the Bohm quantum potential method [17]. The Bohm quantum potentials are expressed as

$$Q_n = -\frac{\hbar^2}{2m_n}\frac{\nabla^2\sqrt{n}}{\sqrt{n}} \quad \text{and} \quad Q_p = \frac{\hbar^2}{2m_p}\frac{\nabla^2\sqrt{p}}{\sqrt{p}},$$

where Q_n and Q_p are the Bohm quantum potentials for electrons and holes, respectively, $\hbar$ is Planck's constant, m_n and m_p are the effective masses for electrons and holes, respectively, and n and p are the electron and hole concentrations, respectively.

To investigate the intrinsic characteristics of the nitride cells, we first calculated the I–V curves of the GaN/InGaN/GaN cells without taking the effect of the piezoelectric or spontaneous polarizations into account, which corresponds to the case of nonpolar solar cells grown coherently on substrates that are lattice matched to InGaN. The hole concentration profile at the p-GaN/i-InGaN interface and the electron concentration profile at the i-InGaN/n-GaN interface are shown in Fig. 1. One can see that the carrier profiles at the heterointerfaces as estimated by classical calculations are significantly different

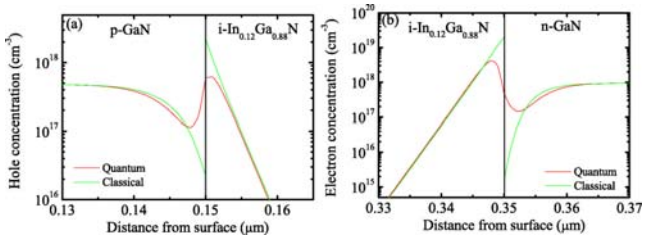

Figure 1 (online colour at: www.pss-rapid.com) (a) Hole concentration profile at the p-GaN/i-$In_{0.12}Ga_{0.88}N$ heterointerface and (b) electron concentration profile at the i-$In_{0.12}Ga_{0.88}N$/n-GaN heterointerface calculated by the use of classical and quantum methods.

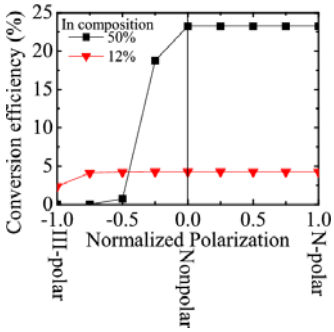

Figure 2 (online colour at: www.pss-rapid.com) Polarity dependence of conversion efficiency for nitride cells with In compositions of 12% and 50%.

from those derived from the quantum calculations. This result indicates that it is necessary to take the quantum effect into account in order to simulate the internal state of solar cells correctly.

Since it is well known that the piezoelectric and spontaneous polarizations in group-III nitride films seriously affect the performance of nitride devices, we have investigated the polarity dependence of the conversion efficiency. Figure 2 shows the conversion efficiency for InGaN cells with In compositions of 12% and 50% as a function of normalized polarization, P_n, caused by the crystalline orientation. In this figure, the values of –1, 0, and 1 for the horizontal axis, P_n, correspond to III-polar, nonpolar, and N-polar cells, respectively. In Fig. 2, the conversion efficiency for cells with an In composition of 50% is larger than that for cells with an In composition of 12%, since the amount of light absorption primarily determines the efficiency. In the case of nonpolar cells, the polarization charge is not induced at the heterointerface, and hence, the energy band diagram in the i-InGaN layer is determined by the band discontinuity at the heterointerface, as shown in Fig. 3(b) and (e). In the case of III-polar cells, the holes (electrons) in the p-GaN (n-GaN) layer are depleted, since a positive (negative) total polarization charge is induced at the heterointerface of the p-GaN/i-InGaN (i-InGaN/n-GaN). Therefore, the internal fields in the i-InGaN layers are reduced or their direction is inverted, as shown in Fig. 3(a) and (d). This leads to dramatically reduced conversion efficiencies, because the confinement effect of carriers increases the recombination rate. On the other hand, in the case of N-polar cells, the holes (electrons) in the p-GaN (n-GaN) layer can screen the polarization charge, although a negative (positive) total polarization charge is induced at the heterointerface of p-GaN/i-InGaN (i-InGaN/n-GaN). Therefore, the internal electric fields in the i-InGaN layers remain almost the same with those for nonpolar cells, as shown in Fig. 3(c) and (f), and the conversion efficiencies exhibited by the N-polar cells are as high as those for nonpolar cells. These results indicate that it is necessary to utilize nonpolar cells, N-polar cells with p-GaN/i-InGaN/n-GaN structures, or III-polar cells with n-GaN/i-InGaN/p-GaN structures in order to achieve high conversion efficiency.

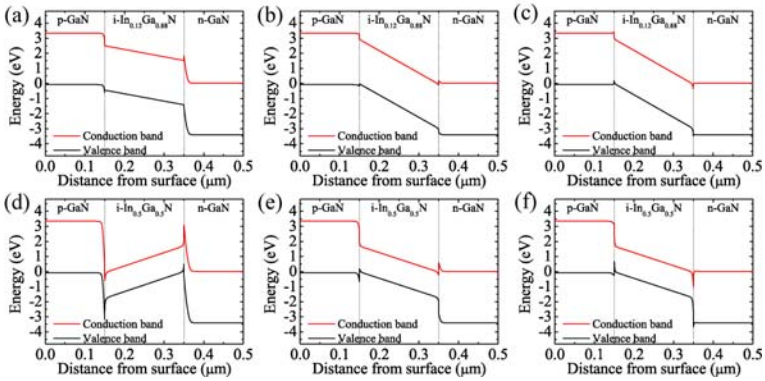

Figure 3 (online colour at: www.pss-rapid.com) Energy band diagrams for (a), (d) III-polar cells, (b), (e) nonpolar cells, and (c), (f) N-polar cells with In compositions of (a)–(c) 12% and (d)–(f) 50%.

The dependence of conversion efficiency on In composition was then calculated for III-polar cells with n–i–p structures stacked coherently on GaN or ZnO substrates. As shown in Fig. 4, the conversion efficiencies peaked at In compositions of around 50%, due to the balance between increasing light absorption and decreasing open-circuit voltage with increasing In composition. The difference in the conversion efficiency between the cells on GaN substrates and on the ZnO substrates is negligibly small, although the intensities of the strain in the InGaN films on the ZnO substrates are much smaller. This phenomenon can be attributed to the tensile strain in the GaN films coherently grown on the ZnO substrates, which makes the total polarization charge at the heterointerfaces for the cells on the two substrate types almost the same. From the viewpoint of process technology, the crystal growth of thick InGaN films with high In compositions on GaN substrates is extremely difficult, due to the large strain in the InGaN films. Therefore, the use of ZnO substrates, which enables us to reduce the strain in the i-InGaN layers, is advantageous for the fabrication of high conversion-efficiency nitride solar cells. In fact, we have found that a 400 nm thick $In_{0.33}Ga_{0.67}N$ film can be successfully grown on a ZnO substrate by the use of a PXD low-temperature growth technique [10]. We have also found that lattice relaxation was not very serious in this $In_{0.33}Ga_{0.67}N$ film, in spite of the large thickness and the high In concentration [8].

In summary, we have investigated the characteristics of InGaN solar cells coherently grown on GaN or ZnO substrates by the use of a device simulator that takes the quantum effect into account. Investigating the dependence on polarity of the conversion efficiency has revealed that it is necessary to fabricate nonpolar cells, N-polar cells with p-GaN/i-InGaN/n-GaN structures, or III-polar cells with n-GaN/i-InGaN/p-GaN structures to achieve high conversion efficiencies. The InGaN cells on both GaN substrates and ZnO substrates exhibit almost the same conversion efficiencies, in spite of the difference in the intensities of the strains in the respective InGaN films. Taking the smaller lattice mismatch between InGaN and ZnO into account, we conclude that the use of ZnO substrates, which makes the growth of thick InGaN films with high In concentrations much simpler, is advantageous in the fabrication of high conversion-efficiency InGaN solar cells.

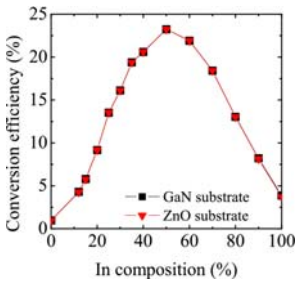

Figure 4 (online colour at: www.pss-rapid.com) Dependence of conversion efficiency on In composition as evaluated for III-polar cells with n–i–p structures or N-polar cells with p–i–n structures stacked coherently on GaN and ZnO substrates.

Acknowledgements This work was partially supported by the "R&D on Innovative PV Power Generation Technology" project contracted by The University of Tokyo with the New Energy and Industrial Technology Development Organization (NEDO).

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