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Phys. Status Solidi C **10**, No. 3, 437–440 (2013) / **DOI** 10.1002/pssc.201200649

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MOVPE growth of $In_xGa_{1-x}N$ (x~0.5) on Si(111) substrates with a pn junction on the surface

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Received 4 September 2012, revised 8 December 2012, accepted 10 December 2012
Published online 5 February 2013

Keywords InGaN, heteroepitaxy, Si(111), MOVPE, pn junction

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This paper reports the MOVPE growth of $In_xGa_{1-x}N$ (x~0.5) on Si(111) with a pn junction on the surface. By optimizing growth temperature and TMI/(TMI+TEG) molar ratio, InGaN films with In content up to 0.5 are successfully grown without phase separation and metallic In incorporation. No significant differences in tilt fluctuation in grown InGaN are found among three different substrates; GaN/α-Al_2O_3(0001) template, p-Si(111) and n-Si(111) with a p-type layer on the surface. The tilt fluctuation increases with increasing In content in InGaN and shows the maximum at around In composition 0.5. The n-InGaN/p-Si structures show good ohmic characteristics and the resistance obtained from the slope of I-V curves is markedly reduced with increasing In content in InGaN. The Si pn junction beneath the $In_{0.42}Ga_{0.58}N$ layer behaves well as a solar cell with an InGaN filter. For both n-InGaN/p-Si and n-InGaN/pn-Si structures, the presence of an AlN interlayer between the epilayer and the substrate does not have a significant contribution to the series resistance.

1 Introduction The growth of a nitride semiconductor on a semiconducting Si can open up new device applications and widen the possibility of utilization of the individual material. For example, the growth of InGaN with an energy gap E_g~1.8 eV on Si is expected to provide a high efficiency 2-junction tandem solar cell, because photocurrents generated in the InGaN top cell and the Si bottom cell coincide each other (current matching). Such current matching will result in a power conversion efficiency higher than 30% [1]. For the combination of n-$In_{0.45}Ga_{0.55}N$ and p-Si, Ager et al. [2] have calculated the band alignment at the interface and predicted that there is little band bending at the interface and efficient electron-hole recombination (ohmic behavior). This is another advantage for the InGaN/Si system, suggesting that no additional tunnel junction is necessary to connect the InGaN top cell with the Si bottom cell.

Although GaN and InN layers have been grown on Si substrate, the growth of $In_xGa_{1-x}N$ with x > 0.1 on Si remains a challenging task. Recently, MBE growth of $In_xGa_{1-x}N$ with x up to ~0.3 has been reported on Si (111) [3]. However, there have been no reports on the MOVPE growth of InGaN on Si especially with an intermediate In content suitable to be paired with Si in tandem cell. In this work, we report the MOVPE growth of $In_xGa_{1-x}N$ (x~0.5) on Si(111) substrates with a pn junction on the surface. The electrical and optical properties have been also measured for n-InGaN/pn-Si structures.

2 Experimental procedures The growth of InGaN has been carried out using an MOVPE system with a horizontal reactor in the temperature range of 600~800 °C at the pressure of 150 Torr. As sources, trimethyle-indium (TMI), triethyle-gallium (TEG) and NH_3 are used. Two types of Si substrate are used; one is p-type Si(111) and the other is n-type Si(111) with a p layer on the surface. The p layer is formed by the B ion implantation (50~10 keV, 7~1x10^{12}/cm^2) into n-type Si(111) substrate followed by the RTA at 1000 °C. To suppress the nitridation and melt-back of Si substrates during InGaN growth, a 100 nm thick

AlN layer is used as an interlayer. A GaN/α-Al_2O_3(0001) template is also employed as a substrate for comparison. The composition of grown films is determined by using X-ray diffraction (2θ/ω) patterns. Full width at half maximum (FWHM) of (0002) X-ray rocking curve, tilt fluctuation, is also measured to evaluate crystalline quality of grown InGaN. Current I-voltage V characteristics for n-InGaN/p-Si and n-InGaN/pn-Si structures are measured. For n-InGaN/pn-Si structures, I-V curves under AM1.5 100mW/cm^2 illumination are also measured. As ohmic contacts to the n-InGaN, the p-Si and the n-Si, Au (60nm thick), Al (50nm thick) and Au (50nm thick)/Ni (20nm thick) are vacuum-evaporated, respectively, and then annealed in N_2 atmosphere at 500°C for 5 min.

3 Results and discussion Figure 1 shows X-ray diffraction (XRD) 2θ/ω profiles for InGaN films with a different In composition grown on p-Si(111) substrates. A nondoped 100 nm-thick AlN layer is used as an interlayer. One can see that InGaN films with In content 0-0.5 and InN are successfully grown without phase separation and metallic In incorporation. The In composition is controlled by both growth temperature and TMI/(TMI+TEG) molar ratio, as the case for the InGaN growth on GaN/α-Al_2O_3(0001) template [4]. As can be seen in Fig. 1, FWHM of the InGaN(0002) peaks is gradually increased with increasing In content. This is due to the compositional fluctuations in the films, as many researchers have discussed. The fluctuation can be described in term of a spinodal decomposition model [5]. Figure 2 shows the XRD 2θ/ω profiles for InGaN films grown on n-Si(111) substrates with a p layer on the surface. Two films with a different In composition are grown with a constant TMI/(TMI+TEG) molar ratio 0.5 at a different temperature T_g. The film grown at 600 °C has an In content of 0.46, which is close to the TMI/(TMI+TEG) molar ratio, while that grown at 750 °C has an In content of 0.24. Such a reduced In content for the 750 °C-grown film is due to the decomposition of InN component and the consequent

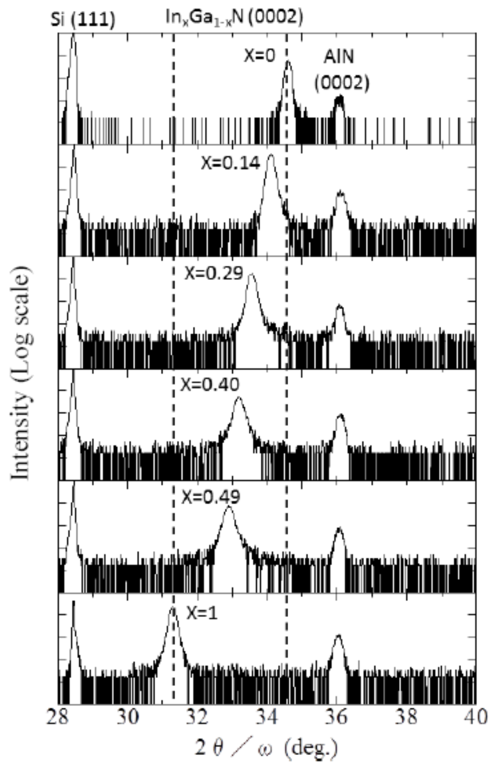

Figure 1 X-ray diffraction (XRD) 2θ/ω profiles for InGaN films with a different In composition grown on Si(111) substrates. A 100 nm-thick AlN is used as an interlayer.

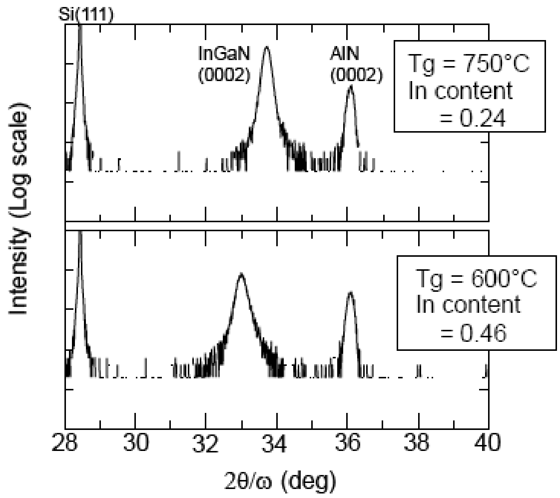

Figure 2 XRD 2θ/ω profiles for InGaN films grown on n-Si(111) substrates with a p layer on the surface. Two films with a different In composition are grown with a constant TMI/(TMI+TEG) molar ratio 0.5 at a different temperature T_g.

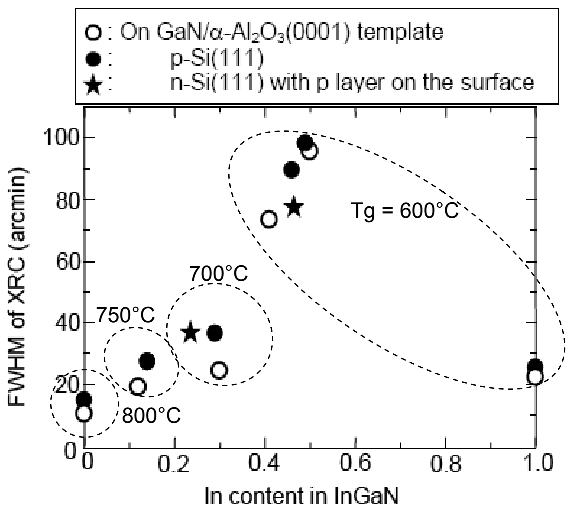

Figure 3 In composition dependence of FWHM of X-ray rocking curve, tilt fluctuation, for InGaN films grown on different substrates at a different temperature T_g.

evaporation of metallic In from the growing surface. The results shown in Fig. 2 clearly show that the junction formation in the n-Si by the B-ion implantation does not become the hindrance of the InGaN growth.

Figure 3 shows In composition dependence of FWHM of X-ray rocking curve, tilt fluctuation, for InGaN films grown on a different substrate at a different temperature. As seen in this figure, no significant differences in tilt fluctuation are found among three different substrates. The junction formation in the n-Si by the B-ion implantation followed by the annealing at 1000 °C is found to scarcely affect the quality grown InGaN. The results in Fig. 3 also indicate that the crystalline quality of the epilayer is not only a function of lattice mismatch between epilayer and-substrate. As a general trend, tilt fluctuation seems to show the maximum value at around intermediate In composition (~0.5), suggesting the deterioration of the crystalline quality due to the solid phase miscibility gap [5, 6]. Figure 3 seems to show that growth temperature is also one of important parameters to govern the crystalline quality. Since the films with In content 0.4-0.5 are grown at 600 °C, such low temperature growth may also contribute to the large tilt fluctuations 70-100 arcmin.

The electrical properties have been measured for n-InGaN/p-Si structures with an AlN interlayer. Figure 4 shows the I-V curves (a) and resistance (b) for n-InGaN/p-Si structures. The inset in (a) shows the schematic cross-sectional view of the sample. The In content in InGaN layer is varied from 0.14 to 0.49. All the samples show good ohmic characteristics in spite of the presence of the AlN interlayer, as seen in Fig. 4(a). The resistances obtained from a slope of the I-V curves are found to be markedly reduced with increasing In content, as shown in Fig. 4(b). Such results are very interesting and useful for the device application of the InGaN/p-Si structure. For example, a resistance as low as 1 Ω cm^2 for In content 0.5 will give no significant effects to the series resistance of InGaN/Si tandem cell. However, the results shown in Fig. 4 cannot be easily understood, because a 100 nm-thick AlN interlayer exists between the epilayer and the substrate and the AlN layer seems to be insulating. In this case, however, there is quite little possibility that the upper contact (60 nm-thick Au) to the n-InGaN layer penetrates through the 400 nm-thick InGaN and 100 nm-thick AlN layers directly to p-Si. Gherasoiu et al. [3] have reported a similar result. They found that the presence of AlN interlayer did not have a significant contribution to the series resistance. Thus, further investigation will be needed to clarify the current flow mechanism of InGaN/AlN/Si structures.

The electrical and optical properties have been also measured for n-InGaN/pn-Si structures. Figure 5 shows the I-V characteristics (a) and spectral response (b) for an n-$In_{0.42}Ga_{0.58}N$/pn-Si structure. The inset in (a) shows the schematic cross-sectional view of the sample. The sample shows a rectifying property in the dark and a photocurrent of about 10 mA/cm^2 under AM1.5 100 mW/cm^2 illumination, as can be seen in Fig. 5(a). In the spectral

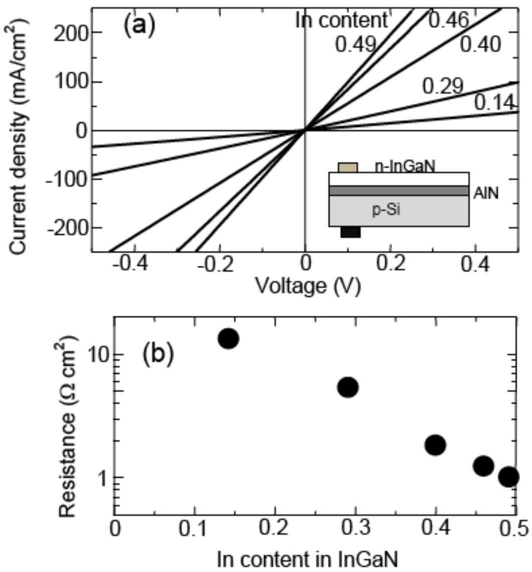

Figure 4 I-V characteristics (a) and resistance (b) between n-InGaN and p-Si. The inset in (a) shows the schematic cross-sectional view of the measured sample.

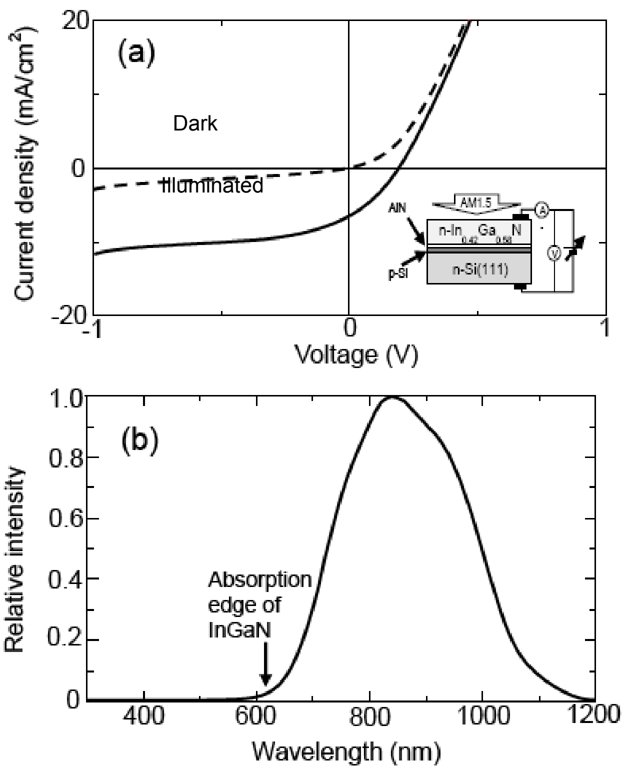

Figure 5 I-V characteristics (a) and spectral response (b) for n-$In_{0.42}Ga_{0.58}N$/pn-Si structure. The inset in (a) shows the schematic cross-sectional view of the sample.

response shown in Fig. 5(b), the absorption edge of the $In_{0.42}Ga_{0.58}N$ layer is clearly seen. Thus, the Si pn junction beneath the $In_{0.42}Ga_{0.58}N$ layer behaves well as a solar cell. Both the low V_{oc} and J_{sc} for the present cell may be due to that the structure and the fabrication process of the Si pn junction have not yet been optimized as a solar cell. It should be pointed out again that there exists an insulating AlN layer between the n-InGaN and the B-implanted p-type Si layer. However, the presence of the AlN interlayer does not have a significant contribution to the series resistance. Thus, we have successfully fabricated the high quality n-$In_{0.42}Ga_{0.58}N$/pn-Si(111) hetero-structures for 2-juction tandem cell. Since we already reported the achievements of p-type conduction in InGaN on α-Al_2O_3(0001) up to an In content of 0.4 [4], these achievements will soon allow us towards the fabrication of InGaN-Si tandem cell.

4 Summary We have studied the MOVPE growth of $In_xGa_{1-x}N$ (x~0.5) on Si(111) substrates. Two types of Si substrate are used; one is p-type Si(111) and the other is n-type Si(111) with a p layer on the surface. By optimizing growth temperature and TMI/(TMI+TEG) molar ratio, InGaN films with In content up to 0.5 are successfully grown without phase separation and metallic In incorporation. No significant differences in tilt fluctuation are found among three different substrates; GaN/α-Al_2O_3(0001) template, p-Si(111) and n-Si(111) with a B-implanted p-type layer on the surface. The junction formation in the n-Si by the B-ion implantation followed by the annealing at 1000 °C is found to scarcely afect the quality of grown InGaN. As a general trend, tilt fluctuation shows the maximum value at around intermediate In composition (~0.5), suggesting the deterioration of the crystalline quality due to the solid phase miscibility gap. The n-InGaN/p-Si structures show good ohmic characteristics and resistances obtained from the slope of the I-V curves is markedly reduced with increasing In content. The Si pn junction beneath the $In_{0.42}Ga_{0.58}N$ layer behaves well as a solar cell with a InGaN filter. For n-InGaN/p-Si and n-InGaN/pn-Si structures, the presence of the AlN interlayer between the epilayer and the substrate does not have a significant contribution to the series resistance. Such results are very interesting and useful for the device application of the InGaN/Si structures.

Acknowledgements This work was supported in part by "Creative research for clean energy generation using solar energy" project in Core Research for Evolutional Science and Technology (CREST) programs of Japan Science and Technology Agency (JST), Japan.

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