

Thermal Annealing Effects on the Properties of MBE-GaN p-n Junction

Ezzah Azimah Alias,¹ Norzaini Zainal,^{1*} Ahmad Shuhaimi² and Zainuriah Hassan¹

¹Nano-optoelectronics Research and Technology, School of Physics, Universiti Sains Malaysia, 11800 USM Pulau Pinang, Malaysia

²Department of Physics, Faculty of Science, Universiti Malaya, Lembah Pantai, 50603 Kuala Lumpur, Malaysia

*Corresponding author: norzaini@usm.my

Abstract: *This paper presents the properties of GaN p-n junction grown on a Si substrate by molecular beam epitaxy (MBE) at different annealing temperatures. The samples were annealed using conventional furnace annealing. The effects of thermal annealing on the samples were observed via X-ray diffraction (XRD), atomic force microscopy (AFM), photoluminescence (PL), current-voltage (I-V) and energy dispersive X-ray (EDX) measurements. From the measurements, the optimum annealing temperature was found to be 1,000°C, which gave the sample the best crystal quality. However, the optimum sample showed poor electrical characteristics due to the diffusion of Si atoms from the substrate towards the p-GaN layer. This effect was more significant for the samples annealed above 1,000°C.*

Keywords: GaN p-n junction, thermal annealing, conventional furnace, molecular beam epitaxy, atomic force microscopy

1. INTRODUCTION

GaN and its related alloys have been amongst the most popular materials for developing high power and high frequency applications. Fabricating GaN in a p-n junction is a basic structure for GaN-based devices such as light emitting diodes (LEDs), laser diodes and solar cells. Hence, improving the quality of GaN-based p-n junctions at their initial stages is considered essential so that the fabrication of high quality devices is possible.

Thermal annealing has been identified as a preferable approach to reduce the density of defects in GaN and hence improve the crystal structure of the epitaxial layers.¹⁻³ Thus far, rapid thermal annealing (RTA) is a thermal treatment technique that has been widely used in numerous research studies and industrial processes. Despite its widespread use, RTA has the limitation that it does not supply uniform heat to a wafer even though it offers fast heat treatment. Alternatively, conventional furnace annealing can provide a more uniform temperature distribution across the wafer and allows atoms to have enough time

to acquire sufficient kinetic energy, which subsequently could minimise the lattice strain, dislocations and other structural defects.³ Until now, studies on the annealing of GaN have only been devoted to the RTA treatment.¹⁻³ Hence, there are limited reports demonstrating the use of conventional furnace annealing for producing GaN with better properties, especially for GaN p-n junctions. If this technology is established, further improvement of GaN-based devices can be achieved.

In this study, the authors present the effect of using various annealing temperatures on the properties of the GaN p-n junction on a Si substrate by means of conventional furnace annealing. The annealed samples were characterised for their structural, surface morphological and optical aspects. An optimum temperature that promoted a better crystalline structure of the GaN p-n junction was proposed. Finally, the electrical properties of the optimum sample were observed and compared to the as-grown sample.

2. EXPERIMENTAL

A GaN p-n junction was grown on (111)-oriented Si substrate by a molecular beam epitaxy (MBE) system. Initially, the surface of the Si substrate was cleaned by exposing it to Ga flux at a temperature of 900°C. This step is required to remove SiO₂ on the surface, thus providing a clean growth surface for the nitride epitaxy. Next, an AlN buffer layer was deposited at 870°C in which both the Al and N shutters were opened simultaneously for 15 min. Subsequently, an n-GaN epilayer was grown on top of the buffer layer and was followed by the growth of a p-GaN epilayer at a growth temperature of 870°C. The thicknesses of the n-GaN and p-GaN layers were approximately 0.4 μm and 0.3 μm, respectively. From Hall-Effect measurements, the electron concentration in the n-GaN layer was $1 \times 10^{17} \text{ cm}^{-3}$, while in the p-GaN, the electron concentration was $1 \times 10^{18} \text{ cm}^{-3}$. The structure of the GaN p-n junction sample is shown in Figure 1.

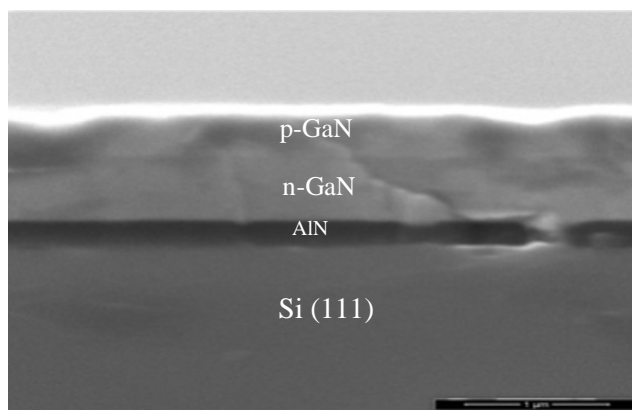


Figure 1: A cross-section image from FE-SEM of GaN p-n junction on Si substrate.

After growth, the samples were sliced into several pieces and then annealed at 500°C, 700°C, 1,000°C, 1,100°C and 1,200°C under ambient nitrogen in a conventional furnace. All of the samples were characterised to study their structural, morphological, optical and electrical properties. The compositional information including the properties of the defects, which indicates the crystalline quality of the samples, was investigated by XRD (PANalyticalX'Pert Pro MRD) analysis with a Cu-K α 1 radiation source ($\lambda = 1.5406 \text{ \AA}$). Meanwhile, the surfaces of the samples were observed to evaluate their roughness via atomic force microscopy (AFM) measurements. Photoluminescence (PL) measurements were performed at room temperature to study the optical properties of the samples. In these experiments, a HeCd laser with a wavelength of 325 nm was used for exciting the samples. Subsequently, the current-voltage (*I-V*) characteristic allowed the authors to study the electrical properties of the optimum sample and then to compare the results with the as-grown sample. Prior to the electrical measurements, Ni/Au was deposited onto the samples using a thermal evaporator system. A forward bias was applied to the samples at room temperature.

3. RESULTS AND DISCUSSION

Figure 2(a) shows the data of the XRD phase analysis for the as-grown sample. Diffraction peaks were observed at 28.4°, 34.5° and 36.1°, and they corresponded to Si (111), GaN (002) and AlN (002), respectively. Apparently, this result indicates that the sample has been grown as a single crystal structure. A similar result was also observed in all of the annealed samples. On the other hand, Figure 2(b) shows the dependence of the full-width at half maximum (FWHM) of the samples (taken from the XRD [002] rocking curve scans) on the

different annealing temperatures. It can be observed that the crystal structure of the samples improved as the temperature increased to 1,000°C. The annealing process allowed the disordered atoms to be more active and subsequently rearrange to form a better structure on the perfect crystal grains. Hence, the annealing process reduced the defects inside of the samples. Such behaviour has also been previously observed.⁴ However, a further increase in the temperature above 1,000°C causes severe degradation to the samples because the out-diffusion of Ga atoms from the surface becomes more significant, creating a non-stoichiometric region on the surface, as previously reported.⁵ Therefore, the FWHM increases dramatically when the temperature exceeds 1,000°C, and therefore, data for the 1,200°C annealed sample cannot be measured.

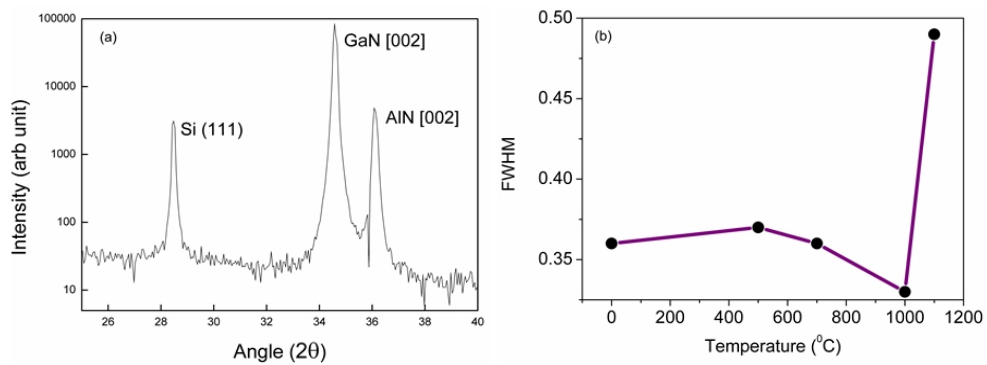


Figure 2: Illustration of (a) XRD phase analysis of GaN p-n junction on Si substrate, and (b) FWHM of the samples annealed at different temperature, taken from XRD rocking curve (002) scan.

Figure 3 shows the roughness of the surfaces of the samples at different annealing temperatures. Overall, the surface roughness decreases as the temperature increases to 1,000°C. This behaviour contributes to an improved crystal structure, especially by the removal of grain boundaries on the surface at higher temperatures. Because the annealing process has allowed the rearrangement of disordered atoms that are to be grown on the perfect crystal structure, the average size of the grains on the surface becomes larger, leading to a more uniform and smoother surface. As expected, a temperature above 1,000°C gives severe roughness to the surface due to the formation of a non-stoichiometric region. We also suspect that there is a tendency of background impurities, such as oxygen, to be incorporated into the surface layer.

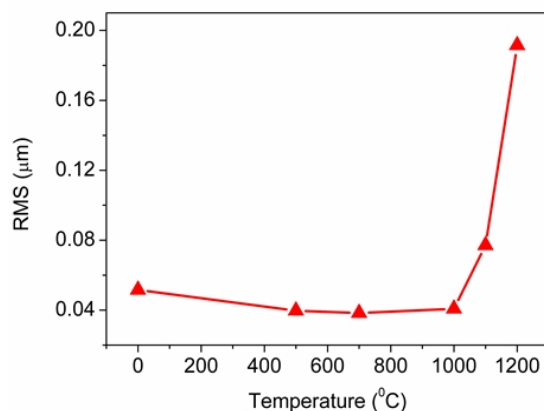


Figure 3: Surface roughness of GaN p-n junction on Si substrate at different annealing temperature.

Figure 4(a) shows the PL spectra of the GaN p-n junction at various annealing temperatures. A dominant peak appears at approximately 3.37 eV in most samples. This peak may correspond to the transition of free electrons to the acceptor level in GaN. A peak near to the bandgap emission is also detected at approximately 3.40 eV. Figure 4(b) clearly shows that the PL intensity (in magnitude) of the dominant peak increases as the temperature increases to 1,000°C. Such behaviour is related to the formation of better crystallised GaN structure with reduction of defect density at higher annealing temperature. However, the samples that are annealed beyond 1,000°C exhibit poor optical properties. It is worth noting that there is a shift of the dominant peak towards a lower energy as the annealing temperature increases. This red-shift behaviour is not clearly understood. Nevertheless, many reports attribute this behaviour to the increase of a Si impurity in the GaN films.^{6,7}

In this work, the electrical properties of the samples of GaN p-n junction annealed at 1,000°C were investigated via *I-V* measurement. The as-grown sample was also measured for comparison. The results are shown in Figure 5. Evidently, the diode characteristic of the annealed sample has nearly disappeared, a result that can most likely be attributed to the out diffusion of Si from the Si (111) substrate, increasing the Si dopant impurity in the p-GaN layer and at the same time increasing the electron carrier density in the p-GaN. Similar behaviour has also been previously reported.^{4,8} At a certain level, the electron becomes a major carrier in the layer, inverting it from p-type to n-type conductivity. As a result, this inversion destroys the effect of the p-n junction of the sample.

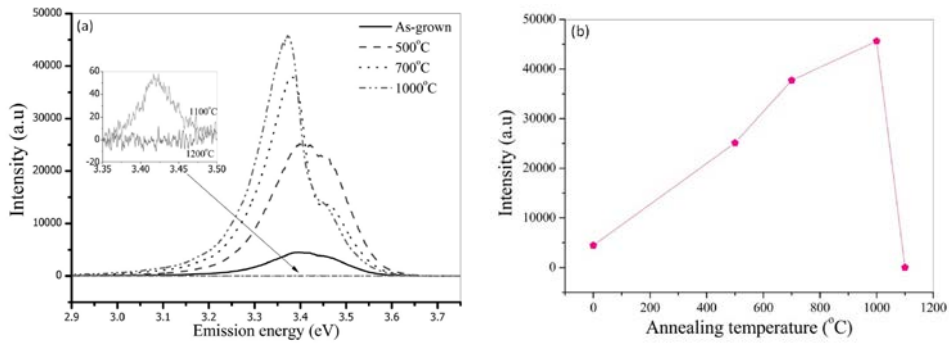


Figure 4: Illustration of (a) PL spectra of GaN p-n junction on Si substrate at different annealing temperature, and (b) dependence of PL intensity (in magnitude) for the peak emission at 3.37eV on different annealing temperature.

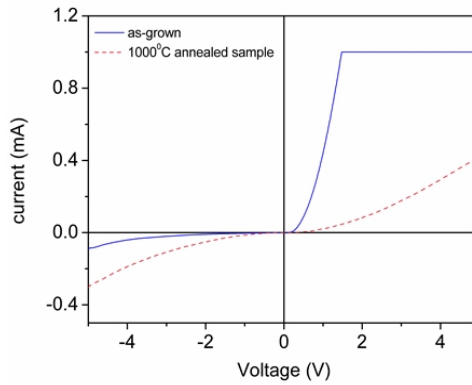


Figure 5: *I-V* characteristics of GaN p-n junction on Si substrate for as-grown sample and annealed at 1,000°C.

On the positive bias, it can be observed that the annealed sample has a lower current than the as-grown sample. We suggest that this result is due to the formation of several SiN_x micro-grains on the surface that resulted from the diffusion of Si atoms. These SiN_x micro-grains have insulator characteristics that could increase resistance to the current flow. Apart from that factor, the formation of the SiN_x could explain the red-shift behaviour in the PL measurement. On the negative bias, a larger leakage current characteristic can be observed for the annealed sample. It is generally reported that the leakage current mechanism relates to defects. However, this seems to not be the case in this study because we have shown that the sample annealed at 1,000°C has the smallest defect density. Hence, this behaviour is not clearly understood, but the authors tentatively suggest that it could be correlated to the reduction of the p-n diode effect.

The behaviour of the auto-doping of Si atoms was also further investigated. Figure 6 shows distribution profiles for Ga and Si atoms at various temperatures using EDX measurements. Apparently, the loss of Ga atoms increases slightly when the sample is annealed at 1,000°C. However, this effect is much more significant at an annealing temperature of 1,100°C. At the same time, Si atoms are diffused considerably towards the surface at the same temperature. This result gives a clear indication that an annealing temperature above 1,000°C leads to severe degradation of the properties of the GaN layer, which is aligned with the results of the XRD, AFM, PL and *I-V* measurements.

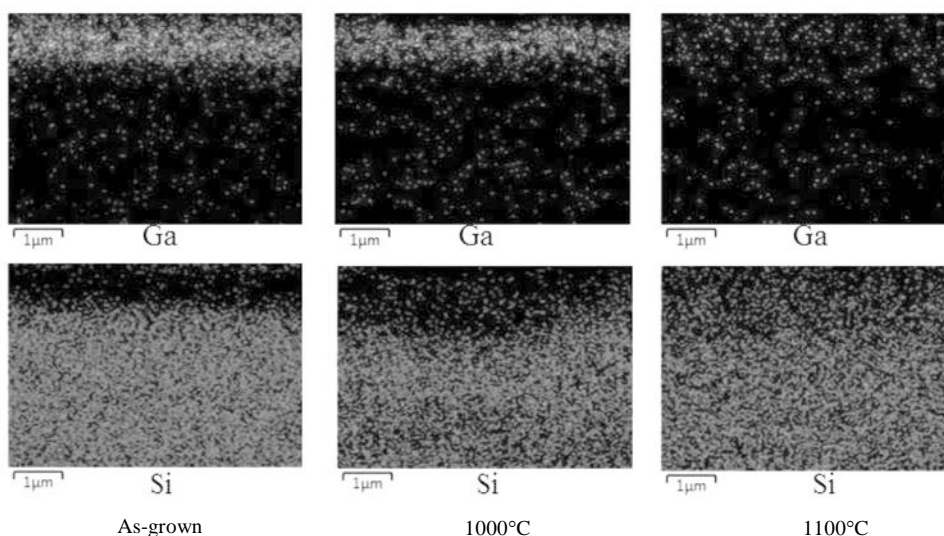


Figure 6: Distribution profiles of Si and Ga atoms from EDX mapping measurement.

4. CONCLUSION

To conclude, we have shown that thermal treatment via a resistance furnace has improved the properties of the GaN p-n junction grown on a Si substrate up to 1,000°C. However, the electrical effect of the p-n junction was degraded in the optimum sample due to the diffusion of Si atoms towards the p-GaN layer. This problem was more significant for temperatures above 1,000°C. At temperatures above 1,000°C, the out-diffusion of Ga atoms also occurred, thus resulting in a non-stoichiometric region on the surface of the sample. Herein, we suggest that an increase in Mg doping in the p-GaN layer as well as fabrication of the sample into a smaller size may overcome this problem.

5. ACKNOWLEDGMENT

This work was supported by Accelerated Program of Excellence (APEX) Delivering Excellence 2012 under account number 1002/PFIZIK/910326 and Short Term Grant 2011 under account number 304/PFIZIK/6311066. The technical support from the Nano-optoelectronics Research and Technology Laboratory staff is gratefully acknowledged.

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