Evolution of AlN buffer layers on Silicon and the effect on the property of the expitaxial GaN film

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Abstract— **The morphology evolution of high-temperature grown AlN nucleation layers on (111) silicon has been studied using atomic force microscopy (AFM). The structure and morphology of subsequently grown GaN film were characterized by optical microscopy, scanning electron microscopy, x-ray diffraction, and photoluminescence measurement. It was found that a thicker AlN buffer layer resulted in a higher crystalline quality of subsequently grown GaN films. The GaN with a thicker buffer layer has a narrower PL peak. Cracks were found in the GaN film which might be due to the formation of amorphous SiN_x at the AlN and Si interface.**

Index Terms— **Metal-organic Chemical Vapour Deposition, III-V Nitrides**

I. INTRODUCTION

Gallium-nitride-semiconductor offers good potential for application in a wide range of electro-optical [1, 2] and high-power microelectronic devices [3, 4] due to its wide band gap characteristics. However it is very difficult to grow sufficiently large bulk single GaN substrates and GaN films are usually grown hetero-epitaxially on a variety of alternative substrates, such as silicon, silicon carbide and sapphire.

Growth of GaN onto silicon substrate offers very attractive potential for incorporating GaN devices onto silicon-based very large-scale integrated circuits (Table 1). However, due to the large difference in lattice constant, crystal structure, and thermal expansion coefficient, it is rather difficult to epitaxially grow GaN on Si substrate. This problem is approached by the use of buffer layers which are meant to minimize the considerable mismatch between film and substrate so as to allow growth of GaN films of equal quality. Various types of buffer layer were attempted to grow GaN on Si until now, such as SiC [5], AlN [6, 7], GaAs [8] and Si_3N_4 [9]. AlN buffer layer is one of the most promising ways to achieve high quality GaN on Si [10]. Nikiskin [11] reported high quality GaN on Si (111) with AlN buffer layer in gas-source molecular beam epitaxy (GSMBE). The crack-free thin GaN film with good structural characteristics can be achieved. However, such high quality GaN film on Si was mostly grown by MBE. The GaN on Si with AlN buffer layer, the evolution of AlN nucleation layer and the effect on the subsequent GaN growth by metalorganic chemical vapor deposition (MOCVD) were seldom reported.

In this paper, we studied the evolution of AlN buffer layer on Si (111) substrates and the effect on the subsequent expitaxial GaN film using MOCVD.

II. EXPERIMENTAL DETAILS

Boron doped Si (111) wafer with resistivity of 1-4 Ω·cm were used as the substrates. The substrates were cleaned using the RCA recipe followed by dipping into HF solution to form a hydrogen-terminated surface. The growth was carried out in a vertical rotating disk low pressure (200Torr)-MOCVD system. Hydrogen was used as the carrier gas. Trimethylaluminum (TMA), trimethylgallium (TMG), and ammonia (NH3) were used as the precursors for Al, Ga, and N sources respectively. Before growing AlN, the substrate was baked under H2 atmosphere at 1000ºC for 15min to remove the native oxide. AlN buffer layers were grown at 1030ºC for 10min, 46min and 80min respectively. The flow rates of TMA and NH3 for AlN growth were 200µmol/min and 0.45mol/min, respectively. The reactor pressure is 50Torr After AlN growth, the temperature was increased to 1020ºC. The flow rate of TMG and NH3 for the GaN growth was 335µmol/min and 0.40mol/min, respectively. The reactor pressure is 200Torr. The AlN layer was characterized by atomic force microscopy (AFM). X-ray diffraction (XRD), Micro PL, and scanning electron microscopy (SEM) were used to characterize the GaN film.

III. RESULTS AND DISCUSSION

A. Morphology and structure of AlN buffer layer

The morphological evolution of AlN for 10min, 46min and 80min is illustrated in the AFM images of Fig. 1 a, b and c. During this nucleation/growth step, the grains underwent substantial growth, resulting in an increase of the average grain size, from 20-30nm to 80-160nm. Furthermore, the RMS surface roughness increased from 0.749nm to 3.923nm.

Fig. 1a shows high density of AlN grains on the surface of Si as 3-dimensional islands, and the average size of the grains is about 20-30nm. In general, GaN was grown on

sapphire using 2-step growth procedure [12, 13]. The first step consists of AlN or GaN growth at lower temperatures (~600ºC) in order to achieve a smooth, fine-grained film; the second step consists of GaN growth at higher temperature (~1100ºC). However, studies found that the SiNx tended to form below 900ºC on Si substrate due to the strong bonding of Si-N [14]. But even at high temperatures, SiNx tends to form when TMA and ammonia was introduced into the chamber. This will be explained later. In our growth, high temperature (1100ºC) was used for the AlN layer. A high density of AlN nuclei ($2.2\times10^{11}/cm^2$) was observed and these nuclei grew in size and at 10min the average height of these grains was about 2-4nm as shown in Fig. 1a.

Fig. 1b shows the morphology of AlN at 46min growth. The grain size has increased to 80-160nm, which shows the rapid and continuous growth of the grains. From Fig. 1b, we notice the grains form triangular islands on the surface of Si substrate. This might be explained by the competition of surface energy vs. the strain energy. At shorter time, surface energy minimization dominates, in which certain crystallographic planes confined the shape of the islands.

Comparing Fig. 1b and 1c, we found that grain size did not change much, but the RMS surface roughness increased from 3.923nm to 8.069nm, and the average height of the AlN grains increased to 10-30nm at 80min. With longer time evolution of AlN buffer layer, the film grew thicker, but is confined by the shape of the grains as deposited by strain energy minimization. The top of the islands was relatively flat as seen from the AFM figure.

In the growth condition used, conversion from 3D to 2D growth was observed which was proposed by other paper [11, 15]. The possible reason might be the SiNx form at the interface of AlN and Si even at the high temperatures. Due to the strength of Si-N bonds, SiNx islands would form on the surface of Si when TMA and ammonia were introduced into the chamber. Suppressing the formation of SiNx would be an effective way to acquire high quality of GaN film.

B. *Characteristics of GaN epilayer*

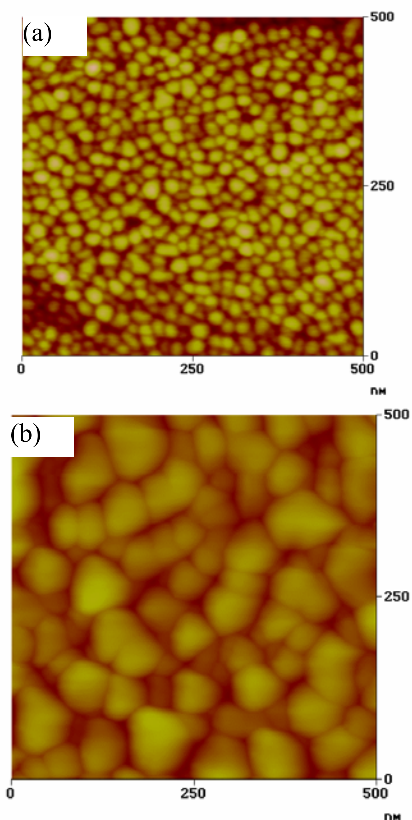
Fig. 2 shows the optical microscope pictures of GaN grown for 60min on 46min-AlN buffer layer (Fig. 2a) and on 80min-AlN buffer layer (Fig. 2b). Fig. 3 shows the SEM diagrams of GaN films on 46min-AlN buffer layer (Fig. 3a) and on 80min AlN buffer layer (Fig. 3b). From Fig. 2a and 3a, the surface of GaN film was rough and obvious islands were observed on the surface. Fig. 2b and 3b shows that the surface is smooth, but cracks were observed in the GaN film. Despite the rough morphology of the buffer layer (80min-AlN), the epitaxial GaN above showed a smooth surface. The cracks were produced due to the difference in thermal expansion coefficient during cooling from the growth. Comparing these two samples, we found that the thicker buffer layer gave better surface morphology of the subsequently grown epitaxial GaN film. This might due to the relatively flat islands, which offer better templates for the subsequent growth of GaN.

XRD was performed to investigate the crystal phase of the GaN films. Fig 4a and 4b show the XRD pattern of GaN film deposited on 46min-AlN and 80min-AlN buffer layer, respectively. From Fig. 4b, besides a (111) peak of Si (2θ=28.5º), and (0002) peak of AlN (2θ=36.1º), there is a pronounced (0002) peak of the GaN with the c-plane spacing for the (0002) at 0.5167nm, which is consistent with the hexagonal lattice. Compared with that of Fig. 4b, the (0002) peak of GaN in Fig. 4a has a slightly different 2 θ=34.6º, which has different c-plane spacing of 0.5186nm. In Fig. 4a, AlN is thinner than that of Fig. 4b resulting in a weaker AlN peak.

The double-crystal X-ray rocking curve (DCXRD) of the (0002) diffraction of GaN film deposited on 46min-AlN and 80min-AlN respectively (shown as Fig 5 a, b), showed full width at half maximum (FWHM) of 1.8213º and 0.4551º respectively. GaN film deposited on the thicker AlN buffer layer shows higher crystallity, which means higher quality, compared to that of the thinner buffer layer.

The optical properties of the GaN samples were characterized by photoluminescence measurement (PL). The PL spectrum of the GaN samples is shown in Fig. 6a and 6b. From Fig. 6, we found that GaN grew on the thicker buffer layer has a narrower peak, but weaker in intensity.

C. Figures



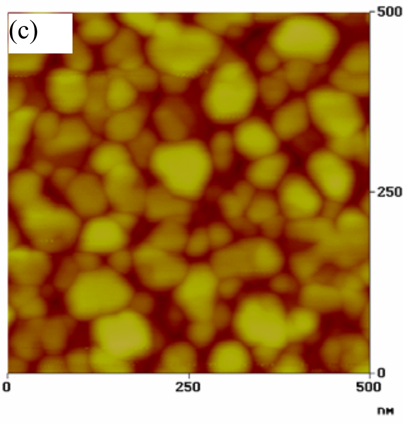
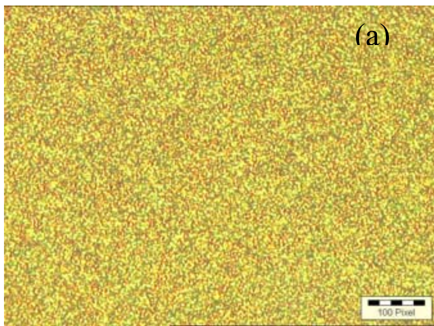
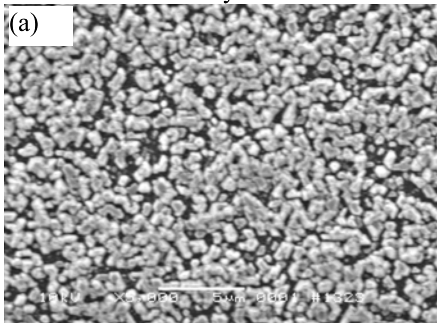


Fig. 1 The surface of AlN buffer layers on Si (111) substrate with different duration time (a) 10min, (b) 46min, (c) 80min



(b)

Fig 2 Optical Microscope image of GaN film a) GaN film grown on 46min AlN buffer layer b) GaN film grown on 80min AlN buffer layer



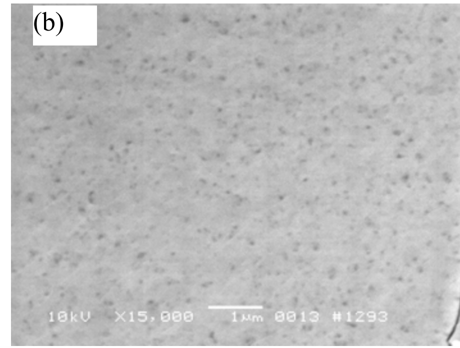
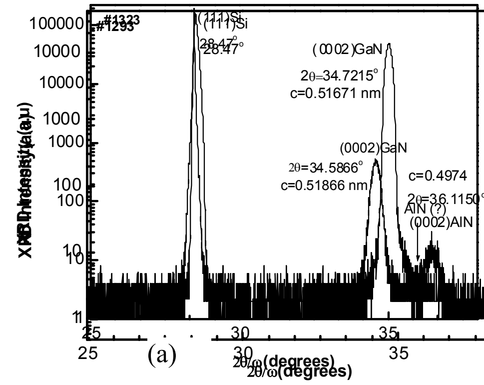
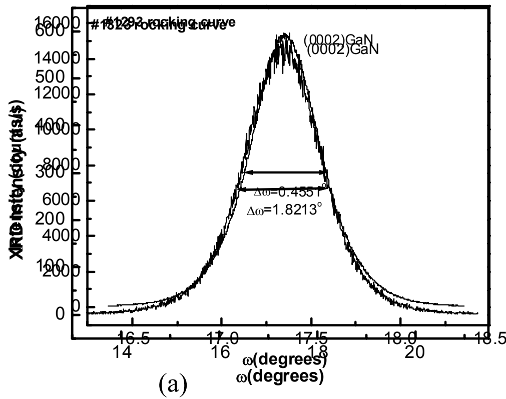


Fig 3 SEM photography of GaN film a) GaN film grown on 46min AlN buffer layer b) GaN film grown on 80min AlN buffer layer



(b)

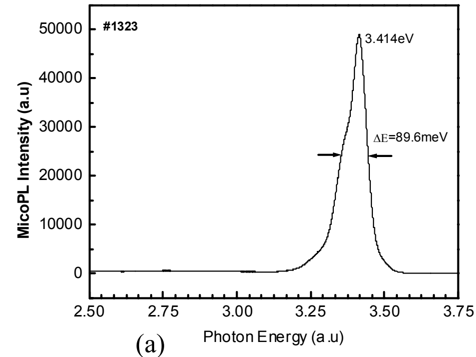
Fig. 4 XRD Curves of samples a) GaN grown on 46min AlN b) GaN grown on 80min AlN



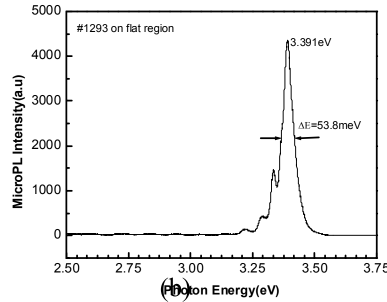
(a)

(b)

Fig. 5 Rocking curve of (0002) diffraction of GaN film a) on 46min-AlN b) on 80min-AlN



(a)



(b)

Fig .6 PL spectrum of GaN film a) grown on 46min-AlN b) grown on 80min-AlN

Table 1 Different substrate for GaN growth

Substrate	*Sapphire*	*SiC/ZnO*	*Si*
Disadvantage	Not conductive; electrodes for devices are not readily fabricated	difficult to obtain	Lattice mismatch (17%); difference in thermal expansion coefficient
Advantage	Has been widely studied, less lattice mismatch	Conductive; relatively good lattice match with GaN	Available in large size; high quality at low cost; integration with silicon microelectronics and optoelectronics

C. CONCLUSIONS

In summary, we studied the evolution of AlN buffer layer grown at a high temperature using MOCVD, and examined the quality of the subsequent epitaxial GaN film. The properties were characterized using AFM, XRD, SEM, optical microscope, and PL. We found that a thicker buffer layer resulted in a better quality of the GaN film. But there were still cracks in the GaN film, which might be due to the formation of SiN_x at the AlN and Si interface.

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