

Theory Research on the Solar Cell Material of GaN by a Novel Method

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Abstract— Solar cell material GaN films were grown on 6H-SiC by metalorganic chemical vapor deposition (MOCVD). An in situ SiNx interlayer was employed during the growth process, which acted as a nano-mask to promote epitaxial lateral overgrowth. The threading dislocations (TDs) density in the films may be reduced to $1.7 \times 10^8 \text{ cm}^{-2}$ by the SiNx interlayer. The TD reduction method relies on the formation of faceted islands on the SiNx-treated GaN surface. Some TDs bend to the facets of GaN islands, some TDs with an opposite Burgers vector could be annihilated when bending over by 90° and forming half-loops after reacting with each other at the interface. The improvement of surface morphology, optical quality and strain relaxation were achieved by the SiNx interlayer also. The GaN films reported here will provide various opportunities for the development of high efficiency and high performance semiconductor devices based on GaN material. Subsequent research has laid a theoretical foundation.

Keywords- Solar cell; GaN; Strain; optical; SiNx

I. INTRODUCTION

Study and Application of GaN materials is currently the forefront of global semiconductor research and focus is to develop microelectronic devices, optoelectronic devices in new semiconductor materials, and with the SiC, diamond and other semiconductor materials together, known as following the first generation of Ge, Si semiconductor material, the second generation GaAs, InP third generation of semiconductor material after the compound semiconductor material. It has a wide direct band gap of a strong bond, and high thermal conductivity, good chemical stability (corrosion is hardly any acid) and other properties, and a strong ability of anti-radiation, in optoelectronics and high temperature and high power

devices frequency microwave devices application has broad prospects.

Indium nitride (InN) is probably the most important semiconductor since silicon and Gallium nitride (GaN). By virtue of its wide band gap and some other excellent properties such as high breakdown voltage, high saturated drift velocity, high mechanical and thermal stability; it has potential for a wide range of solid-state optoelectronic and electronic applications. Actually, high quality GaN films have already been exploited commercially for solar cells, and the GaN/InGaN solar cells with internal quantum efficiencies as high as 60 % were also fabricated on sapphire substrates using MOCVD method [6]. Therefore, more and more efforts are made to efficiently grow GaN films of better quality due to the practical application.

At present, the deposition of GaN films have been reported by using different methods, such as metal organic vapor-phase epitaxy (MOVPE), molecular beam epitaxy (MBE) and hydride vapor-phase epitaxy (HVPE), Pulsed laser deposition (PLD) as well as sputtering. However, the grown of high quality GaN films is limited to the small deposition temperature. This is mainly because of the decomposition of the GaN films under the high temperature. It is worthwhile to mention here that there have been limited reports on high quality GaN films deposited at low temperature. In this study, the high quality InN films are successfully achieved at the low temperature by electron cyclotron resonance plasma enhanced metal organic chemical vapour deposition (ECR-PEMOCVD) system. The ECR-PEMOCVD system combines advanced features of MBE and MOCVD, which is a new type of as-grown film deposition technology, and this method can produce high-density charge and

stimulated particles by using microwave electron cyclotron resonance discharge at low pressure. Since the multicusp cavity-coupling ECR plasma source was adopted to provide active precursors, the growth temperatures were effectively decreased and the N_2 reactivity can be remarkably enhanced by the ECR process, this method was necessary for the formation of GaN films under the low temperature.

GaN material series having a low heat generating rate and a high breakdown field, high-power electronic devices is the development of high-temperature and high-frequency microwave devices the important material. Now, with advances in technology breakthroughs MBE GaN material applications and critical film growth techniques, successfully grown a variety of GaN heterostructures. GaN material prepared by a metal field effect transistor (MESFET), heterojunction field effect transistor (HFET), modulation doped field effect transistor (MODFET) and other new devices. The modulation-doped AlGaN / GaN structure with high electron mobility ($2000\text{cm}^2 / \text{v} \cdot \text{s}$), a high saturation velocity ($1 \times 10^7\text{cm} / \text{s}$), a lower dielectric constant, is the production of microwave devices priority materials; GaN wide band gap (3.4eV) and sapphire and other materials as the substrate, thermal performance, is conducive to the device operating at high power conditions.

In this study, GaN films were prepared by ECR-PEMOCVD system at the low temperature for different TMIn fluxes. The results demonstrate that the dense and uniform GaN films with highly c-axis preferred orientation are successfully achieved on the sapphire substrates under optimized TMIn flux, and the RHEED and XRD results of the optimized GaN film show the high quality with the high c-orientation along the substrates. The AFM images show that the uniform and dense GaN is of the smooth surface. The obtained GaN/Sapphire structure will be used as a wide range of high-power semiconductor devices and the solar cells.

Three samples of GaN films with different SiNx depositing time were grown on Si-terminal (0001) 6H-SiC substrates (n-type) using MOCVD in a Thomas Swan 3x2 close-coupled showerhead reactor. The substrates used here were commercial wafers with on-axis direction. The samples were first ramped to 1100 °C for hydrogen (H₂) baking, to remove the surface damage induced by mechanical polish. Then an AlGaIn buffer layer was deposited at 1040 °C: TMGa and TMAI flow kept on 21.99 $\mu\text{mol}/\text{min}$ and 4.68 $\mu\text{mol}/\text{min}$, respectively, while NH₃ flow was 3 slm. Then a 1 μm GaN template was prepared at the same temperature. In this time, a 6 nm SiNx nano-mask was induced by the same temperature, After SiNx time, a 4 μm GaN were sequentially grown with the same condition as the former GaN. The high-resolution X-ray diffraction (XRD), Photoluminescence (PL), Raman, scanning electron microscopy (SEM) is carried out to characterize the quality of GaN films.

II. EXPERIMENTS

In this study, the samples were prepared on sapphire substrates using an electron cyclotron resonance plasma enhanced metal organic chemical vapour deposition (ECR-PEMOCVD) system at various TMIn fluxes. The experimental device of ECR-PEMOCVD is a new type of thin film deposition technology, because this technology combines advanced features of MBE with MOCVD and uses microwave electron cyclotron resonance discharge at low pressure to produce high-density charge and stimulated particles. In this case, the gas is very easy to achieve chemical reaction and then deposit the films. So compared to the conventional plasma enhanced chemical deposition (PECVD), the ECR plasma conditions has more advantages.

First, the substrate will be using an ultrasonic cleaning in acetone for 5 minutes, then for 10 minutes using an ultrasonic washing in ethanol, and finally with demonized water, ultrasonically cleaned for 12 minutes and finally dried with nitrogen.

Prior to the growth, the substrate surface was thermally cleaned by pure H₂ at 600°C for 20 min with the H₂ flux of 50sccm added 10sccm N₂. The next process is the surface of sapphire substrate was nitridation using the plasma with the N₂ flux of at 450 °C for 5 min. The purpose of the nitridation procedure are to form AlN buffer layer, which can help lowering the mismatch between sapphire and InN down to 12%, and the ways are dramatically improving the surface morphology and crystalline quality of GaN film.

III. RESULTS AND DISCUSSION

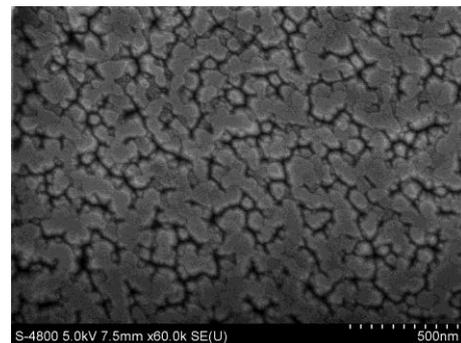


Figure SEM image of GaN surface after 20 min SiNx deposition

Fig .1 provides the SEM image of GaN surface after 20 min SiNx growth. It can be seen obviously that the grown SiNx covers the surface partially, making a porous structure. The purpose of taking a long SiNx growth time (20 min) is to clearly show the porous structure.

The FWHM of three samples as a function of SiNx interlayer time is shown in Fig .2. The full width at half maximum (FWHM) of (002) diffraction is correlated with the density of screw dislocations, while asymmetric (102) is sensitive to the pure edge and mixed dislocations [4]. The TD density can be calculated by the equation [5].

Where ρ_s is the screw dislocation density, ρ_e is the edge dislocation density, $\beta(002)$ and $\beta(102)$ are the full width at half maximum (FWHM) of (002) and (102) diffraction, while B_s and B_e are Burger vector sizes of the screw ($c = 0.5185$ nm) and edge ($a = 0.3188$ nm) components. The screw dislocation densities are calculated as 7.9×10^7 cm⁻², 4.2×10^7 cm⁻² for two samples, and the edge dislocation densities are 5.7×10^8 cm⁻² and 1.7×10^8 cm⁻². There are two mechanisms responsible for the TD termination. First, the nano-SiN_x mask is preferentially formed at the TD cores because of the presence of N-dangling bonds for Si-N formation to terminate TD [6]. Second, due to Fig .1, the in situ SiN_x interlayer incompletely covers the underlying GaN template which acts as a nano-scale mask. Then the subsequent growth is similar to ELO [7], lots of TDs were terminated, and the quality of GaN was improved.

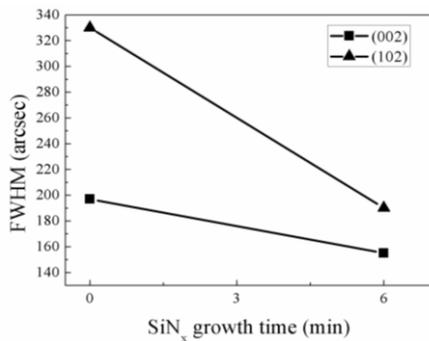


Figure 2. Relationship between SiN_x time and FWHM of (002) and (102) diffraction

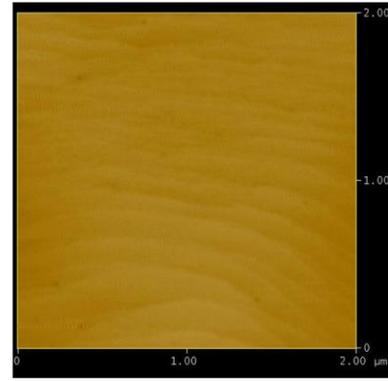
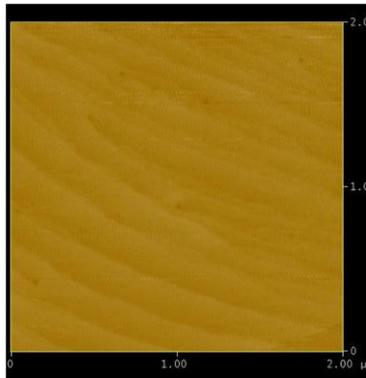


Figure 3. Atomic force microscopy of two samples

Fig .3 shows the AFM images of the samples. Step terminations combined with some dark dots can be clearly observed. The step terminations indicate that a step-flow mode is formed in the samples. The dark dots in the surfaces are related to edge dislocations or mix dislocations [8]. The RMSs are 0.25 and 0.17 nm respectively. The surface of SiN_x sample is smoother than the conventional one.

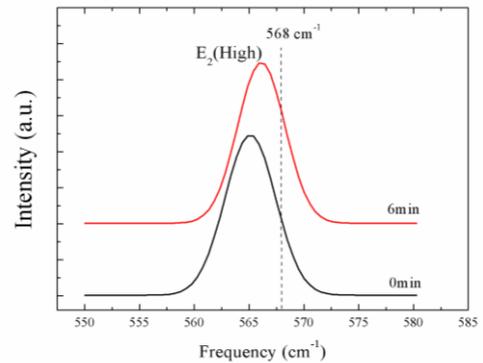


Figure 4. The room temperature of Raman spectra of two samples

Fig .4 displays the Raman spectra near E₂ mode. In the Raman scattering geometry, the GaN E₂ photon peak is a convenient indicator of strain, however, a tensile stress will result in a photon frequency redshift while a compress stress must be responsible for a photon frequency blueshift. The E₂ phonon lines of GaN layers in this study all subjected to a low-frequency shift is indicative of the existence of a biaxial tensile strain in GaN layers.

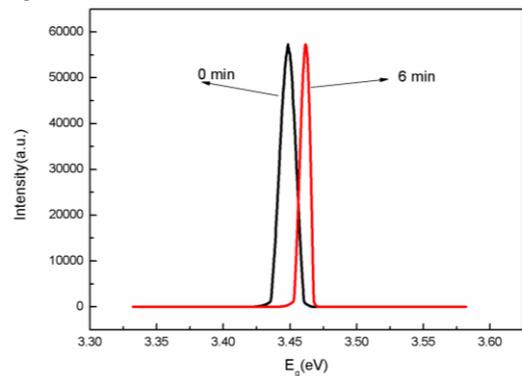


Figure 5. Low temperature PL of two samples at 10K,

Fig. 5 shows the near-band edge low temperature PL spectra of samples at 10K. The dominant line emission in these spectra is related to recombination of donor bound excitons (D0X). As SiNx interlayer induced, there is an obvious blueshift of D0X peaks. It is well known that the residual stress can affect the energy band gap and a tensile stress will result in a decrease of energy band gap while a compress stress cause an increase of band gap. The two samples subject to a lower photon energy compared to 3.472 eV of a strain-free bulk GaN [9]. Thus, the samples in this study suffered tensile strain. The FWHM of standard process was 10.5 meV, and rapidly decrease to 5.1 meV with a 6 min nano-SiNx interlayer. This decrease indicates the SiNx interlayer considerably improved the optical properties of GaN [10].

IV. CONCLUSION

In the letter, we employ an in situ SiNx as mask during GaN process to promote lateral growth. TDs were terminated effectively by bending to the facets of GaN islands, or annihilated by reacting with each other of opposite Burgers vector, while nano-SiNx mask preferentially forming at the TD cores may be another mechanism responsible for the TD termination. Also, the optical quality is improved with the increasing SiNx time. Finally, the improvement of quality and strain relaxation of GaN epilayer is achieved by the in situ SiNx interlayer.

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