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Structural Properties Studies of GaN on 6H-SiC by Means of X-ray Diffraction Technique

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Abstract — Epitaxial growth of GaN has become an interest topic in term of light emitting device fabrication. Most of the commercial GaN based device is normally grown on sapphire substrate. For power device application, SiC has been found to be a desirable candidate for GaN epilayer due to their high thermal conductivity, small lattice mismatch, and hexagonal lattice mismatch with cleaved facet for the laser cavity. In this paper, X-ray diffraction (XRD) technique is employed to study the structural properties of GaN thin film grown on 6H-SiC substrate. For conventional XRD ω-2θ scan, only diffraction peaks from GaN(002) and its multiple reflections were observed, along with reflections from SiC(006) peak. These results suggest that the GaN film is in wurtzite phase. For XRD rocking curve of omega scan of (002) diffraction plane of the GaN, a full width at half maximum of about 259 arcsec is obtained.

***Keywords*: X-ray diffraction, GaN, 6H-SiC, mismatch**

I. Introduction

Epitaxial growth of gallium nitride (GaN) has become an interest to many researchers due to its wide application on light emitting devices fabrication [1], [2] and limitations in achieving high crystal quality in epitaxial materials[3]. In recent development of GaN related material, many of the GaN based devices was grown on sapphire substrate. Silicon carbide (SiC) has been found as a desirable candidate for GaN epilayer, especially on the power devices application [4] due to their high thermal conductivity, small

lattice mismatch and hexagonal lattice mismatch with cleaved facet for the laser cavity [5]. GaN grown on hexagonal SiC (6H-SiC) substrate was reported to have small lattice mismatch as low as +3.5% to +4.0% [3], [4] compared to sapphire (Al_2O_3) substrate which is having around -13% [3].

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The objective of this work is to evaluate the crystalline quality of the GaN grown on 6H-SiC sample and to identify
the mismatch density within the epilayer and the substrate. We employed high resolution X-ray diffraction (HRXRD) technique to characterize the structural properties of sample.

II. Experiment

Hydride vapor phase epitaxial growth GaN wafer from Technologies and Devices International Inc., USA, was used in this study. The wurtzite structure GaN epilayer was unintentionally doped n-type with carrier concentration of about 3×10^{17} cm^{-3} and its thickness was about 0.34 μm.

In this work, conventional 2theta-omega (2θ-ω) scan or also known as phase analysis (PA) method and HRXRD rocking curve (RC) were employed to examine the crystalline structure and quality of the GaN epilayer. All the XRD measurements were carried out by using PANalytical X'Pert Pro MRD system with CuK_α X-ray source. The data from the experiment was collected by using PANalytical X'Pert Data Collector software while PANalytical X'Pert Epitaxy software was employed to further analyze the data collected to identify the lattice mismatch, examine the crystalline quality of the sample and also to conduct fitting of the experimental data with the theoretical data.

For the PA measurements, the accessories used were the fixed slit unit and programmable receiving slit unit. Absolute scan in 2theta-omega (2θ-ω) scan mode and with the range of 30° to 80° was employed. Through this scan mode the crystalline structure/phase of the sample can be assessed. Under this scan mode, the sample and detector are rotated simultaneously to maintain the detector at the same angle from the scattering plane as the incident angle. Thus the diffracted beams that are detected are only from crystalline planes parallel to the surface of the sample.

For the symmetric RC measurements, a Ge220 4-crystal monochromator and triple axis optic were used. Relative scan in omega-2theta (ω-2θ) scan and omega (ω) scan modes were performed. The ω symmetric RC scan of (002) plane is performed both to evaluate crystalline quality of the sample. Under this scan mode, the sample is moved around the scan range while the

position of the detector is always fixed at 2θ.

III. Results & Discussions

Figure 1 shows the result of the PA measurement carried out on the GaN grown on 6H-SiC sample. Two high intense peaks at the 34.58^o and 35.58^o are clearly seen. The origin of this peak is the GaN(002) and the 6H-SiC(006), respectively. Apart from that, the second order reflection peaks from the GaN layer and 6H-SiC substrate are also observed around 72.5^o and 77.5^o, respectively. These peaks are corresponding to the GaN(004) and the 6H-SiC(012), respectively. Since only diffraction peaks from GaN(002), SiC(006) and their multiple reflections are observed, it is suggested that the GaN epilayer is in good crystalline quality and with wurtzite phase.

Besides the main diffraction peaks, it is interesting to note that there are sub-peaks located just beside these main peaks, as shown in the inset of figure 1. These sub peaks are actually resulted from the diffraction of $CuK\alpha_2$ radiation. As in the PA measurement, the X-ray tube used is in the line focus mode. In this case, both the $CuK\alpha_1$ (wavelength 1.5406Å) and $CuK\alpha_2$ (wave length 1.5444Å) radiations are incident on the sample. Subsequently, there are two diffraction peaks resulted from a crystalline plane. The presence of these sub-peaks also an indication of the well defined of the crystallinity of the epilayer. From the figure 1 (inset), it can be found that the peak from $CuK\alpha_2$ is relatively lower than peaks from $CuK\alpha_1$. This is due to the intensity of $CuK\alpha_2$ is comparatively lower than that of the $CuK\alpha_1$. Note that the peak position of the first order and second order reflection is comparable with those reported by Wetzel et al. [6].

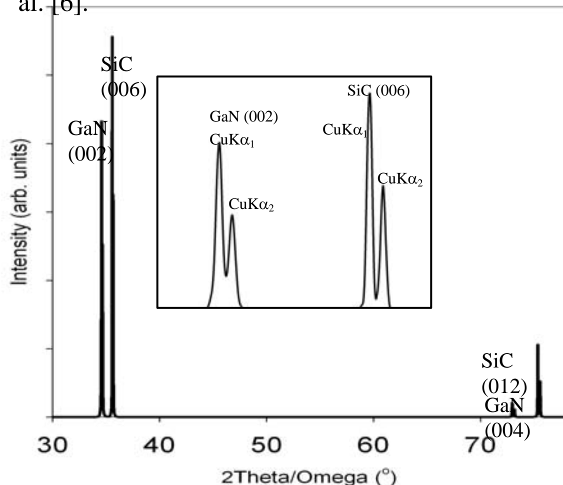

Figure 1: Phase analysis of GaN(002) grown on SiC(006). The inset figure shows the magnified peaks of the first order diffraction peaks of GaN(002) on SiC(006).

Figure 2 shows the XRD RC spectra of the sample in ω-2θ scan mode together with its theoretical fitting. It is found that two peaks located at omega = 17.29^o (2θ = 34.5^o) and 17.79^o (2θ = 35.5^o) can be clearly observed. This confirmed the result found in the PA measurement as discussed earlier and both peaks represent the GaN(002) layer and 6H-SiC(006) substrate, respectively. From figure 2, it can be seen that the experimental and theoretical XRD RC curves are in good agreement with each other.

Through the RC analysis, information on the lattice mismatch of the studied sample can be obtained. Apart from that relaxation of the epilayer can also be determined. In this work, we used the PANalytical X'pert Epitaxy software to analyze the lattice mismatch of the sample. Based on the analysis, it is found that the GaN epilayer is in the fully relaxed state. In addition, the lattice mismatch between GaN epilayer and SiC substrate obtained from this analysis is 3.53%. This result is comparable to the results reported by Ding et al. and Wetzel et al. [4, 6].

Figure 3 illustrates the symmetric RC spectra of (002) plane for the wurtzite structure GaN epilayer measured with ω scan mode. The full width half maximum (FHWM) of the GaN(002) diffraction peak is about 259 arcsec. This result implied that the sample studied is having good crystalline quality.

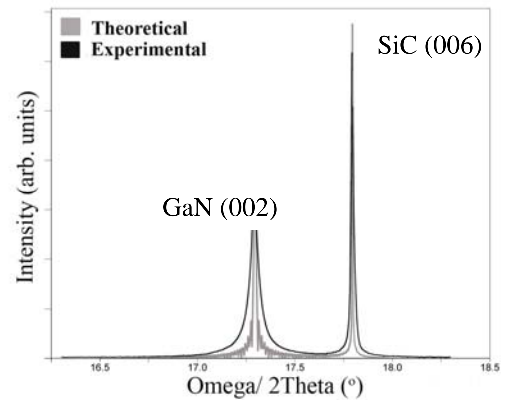

Figure 2: High resolution X-ray rocking curve of GaN(002) grown on SiC(006) in ω-2θ scan mode and its theoretical fitting.

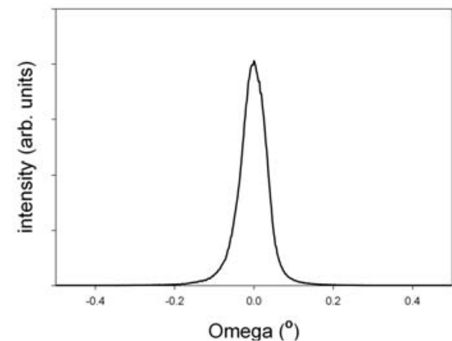

Figure 3: Symmetric RC XRD spectrum of (002) plane for the wurtzite structure GaN grown on SiC(006).

The XRD PA and RC have been carried out on the GaN epilayer on 6H-SiC substrate grown by MBE. The results showed that only GaN(002) diffraction peaks are found along with SiC(006) with their reflection. This suggested that the GaN epilayer on the sample was in wurtzite structure. Relative small FWHM of the GaN(002) diffraction peak from ω-scan (259 arcsec) shown that the studied sample has good crystalline quality. Calculation by PANalytical X'pert Epitaxy

software revealed that the lattice mismatch between GaN(002) epilayer and SiC(006) substrate is 3.53%, where the GaN epilayer is at fully relaxed state. With the observations and results discussed, we can conclude that the 6H-SiC could be a potential choice of substrate for GaN epitixal growth to produce good crystalline quality material for its application.

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