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Low thermal resistance of a GaN-on-SiC transistor structure with improved structural properties at the interface

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ABSTRACT

The crystalline quality of AlGaIn/GaN heterostructures was improved by optimization of surface pretreatment of the SiC substrate in a hot-wall metal-organic chemical vapor deposition reactor. X-ray photoelectron spectroscopy measurements revealed that oxygen- and carbon-related contaminants were still present on the SiC surface treated at 1200 °C in H₂ ambience, which hinders growth of thin AlN nucleation layers with high crystalline quality. As the H₂ pretreatment temperature increased to 1240 °C, the crystalline quality of the 105 nm thick AlN nucleation layers in the studied series reached an optimal value in terms of full width at half maximum of the rocking curves of the (002) and (105) peaks of 64 and 447 arcsec, respectively. The improvement of the AlN growth also consequently facilitated a growth of the GaN buffer layers with high crystalline quality. The rocking curves of the GaN (002) and (102) peaks were thus improved from 209 and 276 arcsec to 149 and 194 arcsec, respectively. In addition to a correlation between the thermal resistance and the structural quality of an AlN nucleation layer, we found that the microstructural disorder of the SiC surface and the morphological defects of the AlN nucleation layers to be responsible for a substantial thermal resistance. Moreover, in order to decrease the thermal resistance in the

GaN/SiC interfacial region, the thickness of the AlN nucleation layer was then reduced to 35 nm, which was shown sufficient to grow AlGaN/GaN heterostructures with high crystalline quality. Finally, with the 35 nm thick high-quality AlN nucleation layer a record low thermal boundary resistance of $1.3 \times 10^{-8} \text{ m}^2\text{K/W}$, measured at an elevated temperature of 160 °C, in a GaN-on-SiC transistor structure was achieved.

FOOTNOTES

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THE BODY OF THE PAPER

I. INTRODUCTION

GaN-on-SiC based transistors have been intensively developed for the next-generation of high-power and high-frequency electronics, because of several promising advantages that this wide-bandgap semiconductor material system can bring. Firstly, SiC has a very high thermal conductivity, and thus can inherently serve as a heat sink in the devices, when used as substrate. Moreover, the low lattice mismatch between GaN and SiC ($\sim 3.4\%$) enables that good crystalline quality of GaN-based high electron mobility transistor (HEMT) structures can be obtained without the need for many interlayers for strain accommodation. Such interlayers can largely increase the local thermal boundary resistance (TBR) causing high device channel temperature [1,2], resulting in limited device performance, poor reliability or short device life time due to severe self-heating [3]. Nevertheless, at least one interlayer is still required in the GaN-on-SiC system in order to wet the SiC surface facilitating GaN two-dimensional growth. For this an AlN nucleation layer (NL) is commonly used [4,5].

Previously, substantial effort has been made to establish the correlation between the *effective* TBR (TBR_{eff} ; the total thermal resistance contributed from the AlN NL and its interfacial regions) and the properties of AlN NLs through structural investigations using transmission electron microscopy (TEM) [6-8]. However, no detailed attention was paid to the interfacial conditions, particularly, the AlN/SiC interface, i.e. the SiC surface, which is of significance for the subsequent growth. In this work, we systematically studied the impact of SiC substrate surface pretreatment on the crystalline quality of subsequently grown AlN NLs and GaN buffer layers (BLs) in a HEMT structure. Furthermore, we investigated the influence of the structural properties in the GaN/AlN/SiC region on the TBR_{eff} , here referred to as the GaN/SiC interface, including the surface of SiC substrate as well as the crystalline quality, morphology and thickness of the AlN NLs.

II. EXPERIMENTAL DETAILS

All samples were grown on on-axis n-type 4H SiC (0001) chemical-mechanical polished substrates from Cree using a horizontal hot-wall metal organic chemical vapor deposition (MOCVD) reactor working at the pressure of 50 mbar. The process temperature was measured in a hole at the upstream part of the susceptor. The surface morphology of the as-received SiC substrates exhibits typically one-bilayer-height (0.25 nm) atomic steps. Before loaded into the reactor, the substrates were cleaned in acetone, methanol, and a solution of $\text{NH}_4\text{OH} + \text{H}_2\text{O}_2 + \text{H}_2\text{O}$ (1:1:5) at 80 °C, and $\text{HCl} + \text{H}_2\text{O}_2 + \text{H}_2\text{O}$ (1:1:5) at 80 °C, each solution for 5 min, followed by D.I. water rinsing and N_2 purging. Five samples were pre-treated in H_2 at different temperatures varying from 1200 °C to 1280 °C prior to growth, and then a complete $\text{Al}_{0.28}\text{Ga}_{0.72}\text{N}/\text{GaN}$ HEMT structure was grown starting with a 105-nm-thick AlN NL layer. Ammonia, TMAI, and TMGa were used as precursors for N, Al, and Ga diluted in a mixture of H_2 and N_2 as process gases. A constant NH_3 flow (2 l/min) was used for the whole growth process. The AlN nucleation layers were grown with a V/III ratio of 1043, at temperatures 100 °C below the H_2 etching temperatures for each sample. The GaN buffer layers (1.6 μm) were grown with a V/III ratio of 625 at relatively low temperature of 1020 °C to increase the residual carbon incorporation [9], while the GaN spacer layer (100 nm) and the AlGaN barrier layer (25 nm) were grown at 1080 °C. An additional sample was treated by the optimal H_2 etching process before the growth, and then the growth of the HEMT structure started with an AlN NL with reduced thickness (35 nm).

The structure quality of the epilayers was evaluated by the symmetric and asymmetric rocking curves (ω -scans) in high-resolution X-ray diffraction measurements (HR-XRD). Thermal conductivity of the SiC substrates (κ_{SiC}) and the TBReff of the AlN NLs were

characterized by using a combined Raman thermography measurement and 3D finite element thermal simulation approach. The κ_{SiC} was measured to be 420 W/mK for the SiC substrates used in this study. TBR_{eff} was measured by the transient GaN temperature response at the centre of pulse-operated (pulse width 300 ns) ungated transistors with an active area of $5 \times 100 \mu\text{m}$, using time resolved Raman thermography. Further details of the TBR measurement technique, the TBR extraction and design and processing of the transistor can be found in Refs. [1, 6, 7]. Also, atomic force microscopy (AFM) was used to characterize the morphology of SiC surfaces and AlN NLs. To identify the chemical composition of the SiC surface, the X-ray photoelectron spectroscopy (XPS) technique was utilized at beamline I311 at the MAX national synchrotron laboratory, Lund, Sweden. High energy resolution of less than 100 and 300 meV at photon energy of 140 and 750 eV, respectively, was utilized to collect the surface core levels spectra.

III. RESULTS AND DISCUSSION

A. Influence of H₂ pretreatment on the crystalline quality of AlN NLs and GaN BLs

Full width at half maximum values (FWHM) of the symmetric and asymmetric rocking curves for the AlN NLs and the GaN BLs in the HEMT samples are shown in Fig. 1. (a). The peak widths of the (002) and (105) reflections of the AlN NLs gradually decrease and reach a minimum when the H₂ pretreatment temperature increased from 1200 to 1240 °C, and then broadened when the H₂ pretreatment temperature was higher than 1240 °C. The narrowest FWHMs of AlN (002) and (105) reflections obtained are 64 and 447 arcsec, respectively, indicating that the thin 105-nm-thick AlN NL grown on SiC pre-treated at 1240 °C has the highest crystalline quality. The crystalline quality of the GaN BLs showed a similar dependence on the pretreatment temperature as that of the AlN NLs. The best crystalline quality of the GaN BL with FWHMs of 149 and 194 arcsec for the (002) and (102) peaks, was also obtained for 1240 °C pretreatment. This result reveals that the growth of AlN NL and GaN BL can be simply improved by the SiC pretreatment temperature. The optimal pretreatment temperature 1240 °C was later implemented in the growth process for the sample with a reduced thickness of the AlN NL. We found that the peak widths of both the (002) and (105) rocking curves for the AlN NLs with 35 nm and 105 nm thickness are very similar, as shown by a representative rocking curve plotted in Fig. 1. (b). Moreover, the quality of the GaN BL remains excellent, as shown in Fig. 1. (c), when reducing the thickness of the AlN NL down to 35 nm. In this case, we can reasonably assume that the HEMT samples, having 35-nm-thick and 105-nm-thick AlN NLs grown on SiC substrates pre-treated at 1240 °C, possess similar structural properties. This helps later to highlight the effect of AlN NL thickness on the corresponding TBR_{eff} .

It is understandable that the crystalline quality of the GaN BLs can be improved by refining the growth of the AlN NLs, so that less misfit dislocations generated in the AlN NLs

would propagate into the GaN BLs. In order to understand why the crystalline quality of AlN NLs showed a considerable dependence on the pretreatment temperature, further investigation of the effect of high-temperature H₂ treatment on the SiC substrate was carried out using the XPS technique. Core levels spectra of the SiC substrates, Fig. 2, were collected at photon energy of 750 eV for the treatment performed at 1200 °C and 1320 °C. The SiC surface treated at 1200 °C clearly showed a strong signal of O 1s (~532 eV) indicating an oxidized SiC surface. This was also illustrated by a high energy resolution of the Si 2p spectrum collected at a photon energy of 140 eV, see Fig. 2 inset, which shows an additional oxide component located at the higher binding energy side of the bulk SiC substrate. Moreover, the C 1s core level shows not only a carbon signal from the SiC substrate but also graphite-like carbon at the higher binding energy side (~285 eV). These extra components were removed efficiently after H₂ treatment at 1320 °C. This can be an explanation for the observed improvement of AlN NLs crystalline quality when the pretreatment temperature is increased above 1200 °C, as shown in Fig. 1(a). While we cannot rule out the possibility that the improved crystalline quality of the thin AlN nucleation layer was due to the increased AlN growth temperature, it is still reasonable to expect that the impact of the substrate surface condition is larger on the crystalline quality of the thin nucleation layers than the growth temperature effect. This argument is well supported by Ref. [10]. Furthermore, the surface morphology of SiC substrates after H₂ etching at the temperatures 1200 ~ 1240 °C was also investigated as shown in Fig. 3. Clearly, no morphological defects were observed in the case of the treatment at 1200 °C, but some pit-like defects along the step edges appeared as the treatment temperature increased to 1220 °C, indicating that a more effective/aggressive H₂ etching process was taking place at the elevated temperature. As the H₂ treatment temperature further increased to 1240 °C, the surface showed more destruction. Therefore, the results obtained from both XPS and AFM suggest that the pretreatment at 1240 °C is the

transition pretreatment temperature for the SiC surface condition, where the H₂ was not only removing the surface contaminants but also started to dissociate the SiC atomic steps. Thus, the improvement of AlN NL crystalline quality in the series is likely because of an effective removal of the surface oxide and the graphite-like carbon contaminant. The degradation of the AlN NL crystalline quality as the pretreatment temperature increased above 1240 °C could be related to the degraded surface morphology of the SiC substrates.

B. TBR_{eff} of the AlN nucleation layer

The time-revolved Raman thermography was performed to extract the TBR_{eff} of the AlN NLs. Since the TBR_{eff} is temperature-dependent [7], it should be noted that the all measurements were done at an interface temperature of GaN-SiC around 160 °C, which was controlled by a heating backplate. As shown in Fig. 4, the TBR_{eff} first reduced from 2.0×10^{-8} to 1.45×10^{-8} m²K/W as the pretreatment temperature increased from 1200 °C to 1220 °C, and then increases up to 3.3×10^{-8} m²K/W as the pretreatment temperature reached 1240 °C. Surprisingly, the highest TBR_{eff} value was measured from the sample containing the best crystalline quality of the AlN NL in the series. However, the measured TBR_{eff} value not only results from the AlN NL, but is also affected by the interfacial regions. This reveals the significance of the interfacial quality in the regions of AlN-SiC and AlN-GaN to the TBR_{eff}. The AlN-SiC interface condition was assessed earlier by measuring the SiC surface morphology after H₂ pretreatments. The AFM results suggest that the remarkable increase of TBR_{eff} in Fig. 4 is likely associated with the severe surface decomposition of the SiC substrate, which can greatly enhance phonon scattering due to structural disorder. Nevertheless, as the pretreatment temperature increased further from 1240 °C to 1280 °C, the corresponding TBR_{eff} decreased again. In order to gain more insight into this phenomenon,

the growth of HEMT samples pre-treated at 1240 °C and 1280 °C was aborted after the AlN NL to facilitate structural characterization. As shown in Fig. 5, we observed that high-density hollow pit-like defects appear in the AlN NL grown at 1140 °C, and more complete coalescence is obtained in the AlN NL grown at 1180 °C. The reason for the difference in the defect density is not completely clear, but higher AlN growth temperature, which enhances lateral growth, partly accounts for the reduction of the number of pit-like defects. More importantly, the results indicate that the high TBR_{eff} measured in the HEMT sample pre-treated at 1240 °C may not only be caused from the destructed AlN-SiC interface but also by the high-density voids in the AlN NL initial growth stage due to the fact that the growth took place on a decomposed SiC surface. Summarizing the results obtained above could lead to a valuable scheme how to reduce TBR_{eff} . Firstly, the pretreatment process needs to be optimized in a way that provides a contaminant-free and ordered surfaces of the SiC substrates to obtain a low AlN/SiC interface resistance and leads to high crystalline quality of the AlN NL. Thus, less structural defects like misfit dislocations, pits, voids are present in the AlN NL, which in turn, improves its thermal conductivity.

A correlation between the nucleation layer thickness and the thermal resistance was also observed. TBR_{eff} values of 3.3×10^{-8} for 105 nm and 1.3×10^{-8} W/m²K for 35-nm-thick AlN nucleation layers demonstrate that reduction of the thermal resistance by reducing the AlN thickness is very efficient if a high-quality AlN layer can be obtained. Even though both samples were pretreated at 1240 °C, which is slightly above the optimum temperature from the TBR perspective, the thermal resistance contributed from the layer itself can be minimized by reducing the thickness. A further TBR_{eff} reduction is expected if the 35-nm AlN nucleation layer was grown on the SiC surface pretreated at 1220 °C. Nevertheless, the 35 nm thick AlN NL has the lowest thermal resistance to date, lower than any previously reported TBR values for standard GaN/SiC device structures [7]. Since the crystalline quality

and the thermal conductivity of an AlN layer were shown to improve considerably along with increased thickness [8, 11]. An intriguing question arises: shall the thickness of an AlN NL be increased to reduce TBR_{eff} ? The TBR_{eff} region acts as series thermal resistance between the GaN layer and SiC substrate. The crystalline property of the AlN NL vary within the layer, containing an initial region of higher defect density and lower thermal conductivity close to the AlN/SiC interface, improving through the layer thickness. Nevertheless, because the thermal conductivity of the AlN thin film is lower than that of the GaN and SiC [12], increasing the total layer thickness will increase the effective thermal resistance between these layers. Therefore, increasing the NL thickness would not be an effective solution to reduce TBR_{eff} . A thin AlN NL with high crystalline quality and low interfacial disorder should be the best choice from the thermal management aspect, although it poses a severe challenge from the growth point of view. Recently, Hironori Okumura et al. have demonstrated very high crystalline quality of an AlN layer coherently grown on SiC [13]. It is promising to further reduce TBR_{eff} with this type of AlN growth scheme. Combining thickness reduction with an improved thermal conductivity, the thermal resistance of an AlN NL would be effectively reduced.

CONCLUSION

High crystalline quality of a very thin AlN NL and a subsequently grown GaN BL was obtained by optimizing the SiC surface pretreatment temperature, allowing for effective surface contamination removal. The microstructural disorder of the SiC surface and the morphological defects of AlN NLs were found to be of significance for the thermal resistance in the GaN-SiC region. Finally, by decreasing the AlN NL thickness we demonstrated a record low AlN TBR_{eff} of $1.3 \times 10^{-8} \text{ m}^2\text{K/W}$ in a GaN HEMT structure measured at 160 °C

by the Raman thermography technique. These results are very essential for development of a high heat-transfer interlayer for GaN-on-SiC technologies.

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VII. FIGURES

FIG. 1. FWHM of symmetric and asymmetric X-ray rocking curves showing the (a) dependence of crystalline quality of AlN NLs and GaN BLs on pretreatment temperature. (b) (002) rocking curve for the AlN NLs with thickness of 35 nm and 105 nm. (c) (002) and (102) rocking curves of the GaN BL grown on the 35 nm-thick AlN NL.

FIG. 2. Core levels spectra collected using a photon energy of 750 eV from SiC substrate after H₂ treatment at 1200 °C and 1320 °C. The high energy resolution Si 2p spectrum recorded using photon energy of 140 eV indicating a surface oxide component is shown in the inset.

FIG. 3. AFM images of SiC surface morphology after 15 min H₂ treatment at (a) 1200 °C (b) 1220 °C and (c) 1240 °C.

FIG. 4. TBR_{eff} measured at the GaN-SiC interface temperature of 160 °C for the AlN NLs in the HEMT samples grown on the SiC substrates pre-treated at different temperatures.

FIG. 5. AFM images of the AlN NLs grown at (a) 1140 °C (b) 1180 °C on the SiC substrates pre-treated at 1240 °C for (a) and 1280 °C for (b).