GaN MOCVD on Si via single crystal rare-earth oxide buffer layer

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Keywords: GaN-on-Si, rare-earth oxides, rare-earth nitrides, MOCVD, MBE

Abstract
GaN layers were grown on Si (111) by MOCVD using epitaxial single crystal rare-earth oxide buffer which helps to solve mechanical strain related problems arising due to lattice and thermal expansion mismatch between the III-N layer and the substrate. Chemical stability of the rare-earth oxide in contact with silicon as well with GaN is analyzed. Transformation of rare-earth oxide to rare earth nitride during GaN MOCVD process is studied. It is demonstrated that the oxide layer serves as Si diffusion barrier to GaN thus preventing back-etching effect.

INTRODUCTION

Efforts to grow GaN on large diameter Si wafers are driven by lower substrate price compared to native GaN or other foreign substrates like sapphire, SiC, as well as possibility to use depreciated Si fabs and thus reduction of cost of GaN wafer. The technology is already adopted by some major companies for fabrication of GaN power devices and, in some less extend, for light emitting diodes (LED) on 150 nm Si wafers and recently on 200mm wafers, as for example it was advertised by IMEC [1]. Generally, the GaN-on-Si epitaxy requires AlN buffer layer which serves for strain management and prevention of Si diffusion to GaN. Still, AlN is not ideal material for either of the tasks. For example, Si diffusion which results in unintentional doping of a GaN layer still remains an issue because of Si solubility in AlN at eutectic point of 577°C. Application of other types of the buffer layers are considered [2] [3]. We introduce new material engineering solutions for the GaN-on-Si process by utilization of an epitaxial grown single crystal rare-earth oxide buffer on Si. It offers flexibility to the epitaxy process by opening up possibility to use approaches typical for GaN epitaxy either on sapphire or Si: GaN or AlN first, respectively. In this work we study advantages of the oxide buffer as well as its chemical and structural properties that influence process at interface oxide/silicon and oxide/III-N.

EXPERIMENT

The erbium oxide was grown in a custom-made solid source epitaxy (SOE) system capable to handle up to 200 mm diameter wafers. HF dipped Si(111) wafers were loaded into the reactor and heated up there for 20 min at 750 °C in a low silicon flux in order to remove residual silicon dioxide from the surface and to obtain a flat 7x7 reconstructed silicon surface. The erbium oxide layers were grown at a growth rate of 1 μm/hour by the evaporation of the metal from an effusion cell, and molecular oxygen was delivered from a gas manifold. Oxygen partial pressure in the chamber was approximately 5.2 x10⁻⁶ mbar during oxide growth. The substrate temperature was 720 °C during growth of the oxides. Thomas Swan close shower head reactor capable to process up to 200 mm wafers was used for GaN metal organic chemical vapour deposition (MOCVD). Trimethylgallium (TMG) and NH₃ were used as gallium and nitrogen sources, respectively.

RESULTS AND DISCUSSION

Under optimized SOE growth conditions as described in earlier works [4] [5], rare-earth oxide interface with silicon is abrupt with no silicon dioxide or silicide interlayer detectable (Fig 1a). However, during GaN MOCVD growth with temperatures above 1050°C, chemical reaction between silicon and the oxide takes place at the very interface between the layer and the substrate forming erbium silicate as can be identified from scanning transmission electron microscopy (STEM) (Fig. 1b) in combination with X-ray dispersion spectroscopy (EDX) (Fig. 2) and X-ray diffraction (XRD) peak at (Fig. 3).

![Figure 1. High resolution TEM image of Er₂O₃ layer on Si(111) before GaN MOCVD (a), and scanning TEM image of Er₂O₃ interface with Si(111) substrate after GaN MOCVD at 1150°C (b).](image)

Two peaks marked as (A) and (B) at Θ = 15.03° and Θ = 15.62°, respectively, could be attributed to polycrystalline erbium silicate as can be concluded from composition of the
interlayer (Fig. 2). However, we were not able to identify exact composition of the silicate. No silicate peaks were detected in XRD measurements of samples with GaN grown at temperature below 1050ºC temperature (not shown here). Because the formation of the silicate interlayer is self-limiting process, silicon diffusion is stopped at the interface between the oxide and the silicon. No silicon detected was in III-N layer grown on top of the oxide (Fig. 4). There is also no trace of erbium or oxygen detected in the GaN layer.

![Figure 2. EDX elements concentration profile of erbium oxide and silicon interface.](image2)

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![Figure 3. XRD scan of a III-N HEMT structure growth on Si(111) via rare-earth oxide buffer layer.](image3)

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An additional peak at $\Theta = 16.03^\circ$ is attributed to ErN(111) with rocksalt structure. Interface between the rare-earth nitride and the GaN layer is well distinguishable on TEM images (Fig. 5). Intensity of the nitride XRD peak correlates with temperature and time of the process, as it was confirmed from results of earlier experiments. We speculate, that the path of the diffusion of nitrogen atoms is through oxygen vacancies in bixbyte structure of erbium oxide. AlN interlayers were grown in the GaN layer for additional mitigation of tensile strains. They are detected by XRD measurements. Full width half maxima (FWHM) of XRD GaN <002> and <102> peaks respectively, 563 arcsec and 1464 arcsec reveals good quality of the GaN layer. Two dimensional electron gas (2DEG) structure with 26 nm Al$_{0.25}$Ga$_{0.75}$N barrier layer on top of 1.5μm GaN formed on erbium oxide buffer on Si(111) demonstrates electron density of $5 \times 10^{12}$ cm$^{-2}$.

![Figure 4. EDX spectra of GaN layer close to interface with Er$_2$O$_3$.](image4)

CONCLUSIONS
A novel combined solid source epitaxy and MOCVD process approach is introduced for growth 2DEG structure with GaN layer on rare-earth oxides buffer on Si(111) substrate. REO layer serves as a barrier for Si diffusion to GaN and prevents back-etching of the later.

![Figure 5. TEM image of MOCVD grown GaN on Er$_2$O$_3$.](image5)

REFERENCES