Epitaxial lateral overgrowth of GaN over AlO$_x$ surface formed on Si substrate

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An approach by which single crystal $\alpha$-GaN can be grown laterally over oxidized AlAs (AlO$_x$) formed on Si substrates is demonstrated. Regular $\alpha$-Ga$_2$O$_3$ stripe templates, spatially separated by AlO$_x$, on which subsequent GaN growth is selectively seeded are formed. Since the boundary between the stripe template and AlO$_x$ is nominally planar, two pyramidal planes on separated GaN can merge by growing laterally over the AlO$_x$ (referred to as planar epitaxial lateral overgrowth). Transmission electron microscopy reveals that the number of structural defects in GaN laterally grown over the AlO$_x$ is remarkably reduced compared to that in GaN grown on the stripe templates, and accordingly cathodoluminescence reveals a strong band edge emission from GaN laterally grown over the AlO$_x$, suggesting that this approach allows us to grow GaN on Si substrates with fewer defects. © 1999 American Institute of Physics. [S0003-6951(99)03019-3]

It has been more than 30 years since epitaxial lateral overgrowth (ELO) of GaAs over SiO$_2$ masks was demonstrated.1–3 Recently ELO has gained considerable attention as an approach to reduce the defect density of GaN grown on sapphire4,5 or SiC6 substrates using hydride vapor phase epitaxy (HVPE) or metalorganic chemical vapor deposition (MOCVD). ELO growth occurs by lateral homoepitaxy over the dielectric mask. In conventional ELO of GaN,4–6 the SiO$_2$ mask is predominantly used for defining an opening on a substrate where GaN growth has already been initiated. The necessity of using a GaN layer to initiate the ELO increases the cost of the process and creates potential current leakage paths and capacitive coupling between devices.

In this letter, we present an ELO technique for the growth of “defect free” GaN that is entirely different than conventional ELO of GaN in terms of its geometrical structure and the materials involved. It is based on recent discoveries in which we have demonstrated epitaxial growth of GaN on AlO$_x$/Si substrates.7 Here we further develop this technique for ELO of GaN on Si.

Samples studied were prepared as shown in Fig. 1 (see also Ref. 7). First, undoped AlAs (3500 Å) and undoped GaAs (300 Å) were grown on $p$-type ($N_p\sim1\times10^{18}$ cm$^{-3}$) Si(111) substrates by atmospheric MOCVD as shown in (a). A two-step growth technique,8 optimized especially for Si(111), was employed for the AlAs growth, which involves a low-temperature (460 °C) grown AlAs buffer layer (350 Å thick) followed by a high-temperature (760 °C) grown AlAs overlayer. The surface of the GaAs/AlAs/Si(111) is specular when viewed with an optical microscope. Then, as seen in (b), regular GaAs stripe patterns were formed by conventional photolithography followed by the oxidation process that selectively converts AlAs to AlO$_x$ by heating in H$_2$O/N$_2$ ambient at 425 °C.9 The stripe patterns (4 μm wide on 10 μm centers) were aligned parallel to the [110]$_{Si}$ direction. As described earlier and shown schematically in (c), during the oxidation, the region covered with GaAs forms a template layer consisting of oriented single crystal islands of $\alpha$-Ga$_2$O$_3$ at the interface between the GaAs and AlO$_x$,10 while the region not covered with GaAs forms no template layer, i.e., only AlO$_x$. This allows us to initiate the growth of GaN only on the region that has the template.9 After the GaAs is removed, in (d), the whole sample was annealed at 1000 °C in dry O$_2$ for 1 h. Finally, GaN was grown by atmospheric MOCVD using a multi-step growth approach11 on the surface where we have $\alpha$-Ga$_2$O$_3$ stripe templates spatially separated by AlO$_x$ as displayed in (e). Although GaN growth is seeded only on the stripe templates, two pyramidal planes on separated GaN stripes grow laterally over the AlO$_x$ and eventually merge to form a continuous layer of GaN as shown in (f).

In Fig. 2, cross-sectional scanning electron microscopy

FIG. 1. Sample preparation for epitaxial lateral overgrowth of GaN over AlO$_x$: (a) GaAs and AlAs are grown. (b), (c) After patterning GaAs stripes, AlAs is wet oxidized to convert to AlO$_x$. During oxidation $\alpha$-Ga$_2$O$_3$ stripe templates are formed. (d) GaAs is removed to expose the surface of the templates. (e) GaN growth is initiated only on the templates. (f) GaN grows laterally over AlO$_x$.
(XSEM) shows an image corresponding to the growth stage displayed in Fig. 1(f) in which a continuous layer of GaN has been formed. As seen here, the thickness of AlO$_x$ over which GaN grows laterally appears to be slightly thicker than the template/AlO$_x$ region. This is more obvious in cross-sectional transmission electron microscopy (XTEM) shown later. The inset displays an image taken at a lower magnification, indicating the area, surrounded by a rectangle, from which Fig. 2 was taken.

A unique feature of the ELO GaN demonstrated here is that the starting surface, the surface consisting of $\alpha$-Ga$_2$O$_3$ stripe templates and AlO$_x$, is nominally planar. This planar surface allows GaN to grow beyond the boundary between the template and the AlO$_x$ and to grow laterally over the AlO$_x$ from the beginning of the growth (accordingly our ELO approach is referred as planar epitaxial lateral overgrowth (PELO) below). By contrast, in conventional ELO, the starting surface has abrupt steps at the edge along the boundary between the SiO$_x$ mask and the opening on GaN. Thus, the GaN can start growing laterally over SiO$_x$ only after the GaN surface is level with the SiO$_x$ surface.

More importantly, in PELO, two separated GaN stripes merge by creating a common region formed by two pyramidal planes that merge. Generally in conventional ELO, voids or cracks are observed in GaN where two approaching ELO segments, originally seeded on different openings on a substrate, meet. However, in Fig. 2, no apparent voids or cracks are observed within the resolution of the picture. In fact, a similar case for ELO of Si has been studied and shown similar results.

It is also worth mentioning that in PELO-grown GaN, both the part seeded on the template and the part laterally grown over AlO$_x$ is electrically isolated from the substrate. In conventional ELO, the grown GaN is connected via the GaN pre-layer on which GaN is seeded through SiO$_x$ openings.

A bright field XTEM image taken from the region containing both GaN grown on the template and PELO GaN over AlO$_x$ is shown in Fig. 3. A gradual transition in thickness, as mentioned earlier, apparently exists between AlO$_x$ and the template. In analogy to conventional ELO of GaN, PELO GaN over AlO$_x$ is expected to have fewer structural defects than GaN seeded on the template. In fact, a significant reduction in the number of structural defects is clearly seen in Fig. 3, as one moves from GaN on the template to the PELO region. A large number of defects including defects running almost parallel and perpendicular to the growth direction can be seen in GaN grown on the template denoted as (i). However, the number of structural defects, in particular the defects nearly running parallel to the growth direction, dramatically drops in GaN above the transition region denoted as (ii). Eventually in PELO GaN over AlO$_x$ as denoted as (ii), the defects almost completely disappear.

The XTEM contrast in PELO GaN over AlO$_x$ appears to be uniform within the layer while in GaN on the template, the dark contrast associated with defects, is stronger near the interface between AlO$_x$ and Si substrate. This suggests that PELO GaN over AlO$_x$ is not seeded on the surface of the AlO$_x$. Consequently, the only defects seen in PELO GaN over AlO$_x$ are those that propagate laterally from the GaN grown on the template. Moreover, some of the defects seen in GaN on the template appear to bend over, resulting in a segment of a defect running perpendicular to the [111]$_{Si}$ direction. It should also be noted, as reported earlier, that the type of defects seen in GaN on the template differ from the type of defects generally observed in GaN on sapphire(0001). The defects seen in GaN on the template predominantly create line contrast perpendicular to the [111]$_{Si}$ direction, while typical threading dislocations that run parallel to the [111]$_{Si}$ direction are rarely seen.

Finally, in Fig. 4 is shown the cathodoluminescence (CL) spectrum taken from (a) PELO GaN over AlO$_x$, and (b) GaN grown on the stripe template. As can be seen clearly, the intensity of the band edge emission at 359 nm from PELO GaN is approximately nine times higher than that from the GaN on the stripe template. This most likely reflects the reduction in the defect density in PELO GaN as observed in XTEM (detailed discussion on other features seen in Fig. 4 can be found in Ref. 7).

For practical objectives, thicker PELO layers where the...
two pyramidal planes merge are desirable. One simple way to accomplish this is to implement a growth technique such as HVPE that has a much higher growth rate, particularly on the pyramidal plane of GaN. Conventional ELO GaN using HVPE has been investigated, proving that pyramidal planes that grow laterally over SiO$_2$ eventually merge to form a continuous film. 4

There is also the possibility to adjust the growth conditions for MOCVD such that either the growth rate on the pyramidal plane of GaN is further enhanced or that it is greatly suppressed on the basal plane while maintaining a reasonable growth rate on the pyramidal plane. As indicated in an earlier report on InP ELO, the growth temperature is expected to play an important role that significantly influences the kinetics of growth on a particular low index plane. Thus choosing appropriate growth temperature may allow us to have a higher growth rate on a pyramidal plane than on a basal plane of GaN.

In summary, we have demonstrated a technique by which GaN can be laterally grown over a planar surface consisting of $\alpha$-Ga$_2$O$_3$ stripe templates and AlO$_x$ formed on Si substrates. GaN stripes are selectively grown on the stripe templates spatially separated by AlO$_x$, then pyramidal planes on separated GaN stripes seeded on different stripe templates merge by growing laterally over AlO$_x$. XTEM reveals that the number of structural defects in PELO GaN over AlO$_x$ is remarkably small in comparison with that in GaN grown directly on the templates. Accordingly, CL shows a strong band edge emission from PELO GaN. The PELO approach seems to be a feasible technique to grow GaN on Si substrates, the commercial size of which can be up to 12 in. in diameter, with less structural defects, voids, and cracks. Detailed optical properties of PELO GaN are currently being studied.

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FIG. 4. CL spectrum taken from (a) PELO GaN over AlO$_x$ and (b) GaN grown on the stripe template.