Analysis on the dislocation of GaN on different substrate

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Abstract. Though there are still disputes on whether the threading dislocation density (TDD), to produce high quality Gallium Nitride (GaN) with low TDD is needed. In this passage, we would first show the impact of dislocation and review the latest methods to reduce dislocation on Si, GaN, and sapphire. The Si substrating with serpentine channels could produce GaN by using Si substrate with low density dislocations. The method that use the markless-3D provides a new way to reduce the dislocation from big off-angle. The multiple-step growth technique controls the conditions of crystallization and use two steps of crystallizing to grow with both low dislocation density and 2D growth shape. The last method is to use the Na-flux method to exclude cracks with sapphire in crystal.

1. Introduction

Nowadays, the third generation semiconductor is widely used because of its wide bandgap, high electron mobility, and high electron saturation velocity, especially for GaN which is used for light-emitting diodes (LEDS), laser diodes (LDs) and high-power transistors. However, GaN could not normally grow on normal substrate we usually use such as sapphire, Si and SiC. Hence, there is high density of dislocations approximately $10^8$ to $10^{10}$ cm$^2$. In recent years, there are a lot of methods to overcome these issues in order to get a high-quality, low -curvature, low-cost, and large-diameter GaN substrate. However, it is very difficult to meet all these requirement in one method. So how to meet as many requirements as possible is one big issue.

It would seriously affect the performance of semiconductor devices, so in this work, we reported the harm of dislocation and ways to reduce dislocation on both foreign substrates and GaN substrate. Despite there are a lot of dislocations, the efficiency of GaN-based light emitting diodes could still be up to 80%. But it does not mean that such high densities of dislocation have no link with the efficiency. In early studies, it is considered by some scholars that there are some kinds of dislocations that do not have radiative active and there are other studies shows that certain defect emission lines in GaN is because of dislocation.
2. Impact of dislocations

It is hard to give an exact answer on how the dislocations in GaN would impact the performance of a device, because there are more than one device that are affected by the high density of dislocation which is difficult to evaluate the impact of each device. But there is no deny that the dislocation have some effect on transistors. The study shows very differently, some reported that mainly threading screw dislocations (TSDs) are responsible for the leakage currents, but others elaborated that both the TSDs and threading mixed type dislocations (TMDs) play important roles on this, there are also some researches shows that these two kinds of dislocations may have no effect. In general, we now do not known what the link between one specific kind of dislocation and the current. [1]

For any dislocations, there are chances to create the deep states in the gap which could act as nonradiative centers because of the dangling bonds. However, inside the GaN, the core of the dislocation may reconstruct, and the dangling bonds would be remover. Although there are great amount of core structures, there are two kinds of type. The first type conjecture to create the nonradiative centers, but the second type proposed not. Except the direct effect from the dislocation, the long-range direct impact would also have an impact on the attraction of impurities and native point defects. However, based on recent study, the sample surface constitutes a stress-free boundary that leads a complex three-dimensional strain. Because of this phenomenon, if the probe of the experiment is smaller than 140nm, there will be a high possibility to give a wrong conclusion about the nonradiative decay. These are always used in cathodoluminescence (CL) and photoluminescence (PL) map taken from the GaN layers surface. fig1 shows the configuration of the top-view CL experiment at the GaN(0001) surface (upper plane) with the electron beam scanning across the outcrop of a dislocation (vertical line), surrounded by a piezoelectric field (mushroom-like shape representing an isosurface of the field) induced by the strain relaxation near the surface. The QW (bottom plane) is buried at a depth of 650 nm.[2]Because of this new discovery, there would be a lot of studies showing the nonradiative decay need to be re-experiment and now there is nearly no direct evidence shows that nonradiative activity links with GaN.

![Figure 1. Configuration of the top-view CL experiment](image)

3. Methods for dislocation in GaN

(1) GaN epitaxially grown on Si substrate with serpentine channels
Nowadays there are some efficient ways to achieve low dislocation density of GaN such as epitaxial lateral overgrowth (ELOG) and its derivatives. However, these methods need more than one growth steps and more than one regions with high density of dislocation per mask opening. The new way to further reduce the dislocation density uses serpentine channel patterned mask which needs only one opening and has one high-dislocation region every mask opening and this way could be used in sapphire substrates and Si substrate. It means that this way could be widely used because of the mature silicon substrate technology.

The experiment firstly used the standard photolithography and reactive-ion etching (RIE) to obtain the 2μm and 12μm width stripe-shape windows. Then created the serpentine cross-sectional channels. Finally used the buffered oxide etchant (BOE) to remove the SiO2 until AlN was exposed in the bottom of the window.

Using this method, the GaN firstly grew at the bottom of the window then grew up to the channels and finally grew out of the top windows. Because the using of serpentine, GaN is lateral growth and finally merged with each other. In this way, the density of dislocation in the wind area would be significant drop compared to the conventional ELOG. The density of dislocations of wing at window regions are decrease to 2.4×10⁷ cm⁻² which would have been a great contribution to the performance of device. Although it is complex for the mask preparation, it is still a good way to make GaN on Si. If it could mass manufacture, there would be a great upgrade on efficiency of transistors, LDs, LEDs and so on[3].

![Figure 2. the steps to deposit GaN by using the Si substrate with serpentine channels[3]](image)

(2) *GaN prepared by hydride vapor phase epitaxy and maskless-3D*

Because nowadays most of currently available GaN (0001) substrates are made by hydride vapor phase epitaxy (HVPE) and they are boules, which means that these boules are curved and have internal stress gradient. According to existing studies, the density of the inclined TDs is relative to the curvature and it could be solved by reduced the TDD.

It is necessary that TDs meet each other, because the main mechanisms for TDD reduction is fusion or annihilation reactions of TDs. In GaN crystals, TDD would be significantly reduced by increasing the growth thickness. However, according to today’s technology, it is difficult to grow thick enough to decline TDD to a very low level. There are also other ways to decline TDDs but they are usually with low productivity and high cost. So producing a 3D growth shape without masks on a normal seed substrate is needed.
Just like normal technology, it first uses the GaN (0001) substrates as seed substrate and uses GaCl and NH₃ for the source of gallium and nitrogen. The growth temperature is between 990 °C and 1050 °C. The biggest challenge is to control the growth shape, so it is necessary to control the atmosphere, temperature and pressure of growth and V/III ratio. Then use the HVPE at 1050°C, because in this temperature it could proceed with the 2D growth shape.

By using the maskless-3D method, we could get a better GaN substrate with low TDD and a small off-angle variation and furthermore, and this method is also easy for achieve because it would not require the complex mask or and 3D structures. This method is also very flexible, if it is just required for a relatively low density of TDD and use the maskless-3D method, but if it is required for a lower density of TDD, we could grow GaN with a double markless-3D structure and in this way, and the TDD is decreased to 10⁴ cm⁻² [4].

(3) multiple-step growth technique based on facet and flattening growth
In the experiment, they firstly use the comparative experiment to test how the temperature and V/III ratio effect on hydride vapor phase epitaxy (HVPE). As the result, the experiment shows that a lower growth temperature and higher V/III ratio would get the best quality. But a higher growth temperature and lower V/III ratio is more likely to get a 2D growth. So they use the two step of growth. Firstly use the low growth temperature and high V/III ratio to get the relative a low density of dislocation, then use high growth temperature and low V/III ratio to promote planar growth. In this way, the density of dislocation decreased significantly and if there are needs for lower dislocation density, it can be done by repeating this method over times.[5]

(4) crack-free GaN substrates grown by Na-flux method with sapphire dissolution technique
Because GaN is usually grown on the foreign substrate. One of the source of dislocation is produced because of the thermal stress that used to separate the GaN from the foreign substrate. It would be a big challenge for the production of large-diameter GaN wafer.

In this method they first experiment the sapphire in Na-Ga-Li-C flux and determine the best dissolution temperature, flux composition and so on. The sapphire was first used to be the substrate of GaN, then the HVPE was used to grow the GaN. This new method to suppress do not need very complex steps and it could produce a relative large diameter GaN substrate with low density of dislocation. Furthermore, this method could also be used in fabrication of crack-free freestanding GaN substrates by the Na-flux coalescence growth technique, because using the large point seed would make the large contact interface, and as the result, there would be cracks. But combine the Na-flux coalescence growth and the sapphire dissolution techniques. In this way, it could exclude all the cracks in GaN crystals.

4. Suggestion
Although device based on low density of TDD GaN is efficient, there are still a lot of problems for mass production. For example, the studies are always very complex, and the factory is not as precise as laboratory, so how to reduce both steps and the environmental impact on material growth such as environment temperature simultaneously is important for industrial production.
Though the methods above, there is a big room for improvement. We could use the maskless-3D growing to grow a GaN substrate and then use the serpentine to grow a more perfect GaN crystal. Use the combine method could further reduce the density of dislocation but also would be more complex. However, it could be foreseen that these methods could be widely use in the future.

Table 1. The substrate and density of dislocation of all methods

| method          | Density of dislocation       | substrate  |
|-----------------|-------------------------------|------------|
| serpentine      | 2.4×10^7 cm^2 (window region)| Si         |
| Markless-3D     | 4×10^5 cm^2                  | GaN        |
| Multiple-step   | 8.4×10^5 cm^2                | sapphire   |
| Na-flux method  | 10^6 cm^2                    | sapphire   |

5. Conclusion

There is still no method that could produce large and high quality GaN with low density of dislocation, but there are some new methods to produce high quality GaN in wide-used substrate such as Si and sapphire, and it gives us new methods to decrease the density of dislocation. The serpentine channels and markless-3D method are going to decrease the density of dislocation caused by mask. The multiple-step growth use two steps or more steps to produce high quality GaN substrate. The Na-flux method is to decrease the cracks caused by sapphire.

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