Dislocations Analysis in III-V Nitrides - A Cost Effective MOCVD Epitaxy Solution

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To sustain the worldwide high demand of electrical energy, GaN is a strongly emerging material grown on SiC for RF frequency or on Si for power electronic device applications. However, GaN cost-effective hetero-epitaxial growth suffers with high defect densities. The technology improvements require accurate prediction with an understanding of their formation. The qualitative and quantitative extraction of types of defects is very difficult to accomplish from an experimental point of view [1-2].

TNL-EpiGrow™ simulator provides cost effective solution to replicate the epitaxial growth in a similar manner as real time reactor [3-4]. TNL-Chemical kinetics utility package provides facility to simulate and optimize the gas and surface phase chemical reactions to help a user work efficiently with large systems of chemical reactions. The adsorption, hopping and desorption mechanism rates are computed using in-house developed kinetic Monte Carlo (kMC) algorithms with capabilities to reproduce the real MOCVD reactor based epitaxial growth experiments[3-4].

In present work authors report the growth morphology of buffer layers of AlN on Si (111) substrate via MOCVD reactor equivalent to an AIXTRON CRIUS® close-coupled-shower head (CCS) architecture [3-4]. The growth process steps include epitaxy of (i) AlN, (ii) varying Al composition in $Al_xGa_{1-x}N$ buffer layers. The basic aim of present work is to understand the formation of line dislocations layer by layer. The AlN lattice parameter (a) is taken 3.1258A as compared to Si (111) 3.84 A. The lattice mismatch causes the tensile strain. At the Si/AlN interface the strain will be high. It reduces as growth proceeds for upper AlN layers. Due to high strain, the probability of formation of line dislocation at interfacial AlN layers is high as compared to upper AlN monolayers. The density of line dislocations depends upon thickness of AlN layers. Successively, epitaxial buffer layers of $Al_xGa_{1-x}N$ with x=0.8, 0.5 and 0.2 are deposited. The lattice parameters of ternary compound increases with increase of Ga content in $Al_xGa_{1-x}N$ as compared to AlN and generate the compressible strain. The thickness of various $Al_xGa_{1-x}N$ buffer layers are optimized to achieve overall minimum strain within $Si/AlN/Al_{0.8}Ga_{0.2}N/Al_{0.5}Ga_{0.5}N/Al_{0.2}Ga_{0.8}N$ structure, further used for GaN epitaxy. The thickness of each buffer layer is decided by proper optimization of partial pressures (**Table I**) of various input gases and chemical kinetics to achieve high quality GaN film with minimum dislocation defects. The roughness at each interface is shown in **Fig.1a**. **Table II** depicts the dislocation data and lattice parameters of deposited materials. It is found that dislocation density increases with the increase of Ga content (0 - 50%). However, the decrease in dislocation density is observed with the further increase of Ga content beyond 50% (**Table II)**. The dislocation densities data is also justified from the roughness curve where a sudden rise is visible for $Al_{0.8}Ga_{0.2}N$ growth which finally comes down for Ga rich layers. **Fig.1b** and **Fig.1c** shows surface and overall structure respectively. **Fig.1b** reflect the island-based growth and justifies the experimental Stranski–Krastanov (S-K) growth mode.

1. Sven Besendörfer et al., The impact of dislocations on AlGaN/GaN Schottky diodes and on gate failure of high electron mobility transistors, **Scientific Reports** (2020) 10:17252.
2. Abdul Kadir et. al., Influence of substrate nitridation on the threading dislocation density of GaN grown on 200 mm Si (111) substrate, **Thin Solid Films** (2018) 663:73-78
3. P. K. Saxena et. al., An innovative approach for controlled epitaxial growth of GaAs in real MOCVD reactor environment, **Journal of Alloys and Compounds** (2019) 809:15175
4. TNL-EpiGrow Simulator user manual (2023) https://www.technextlab.com/epi_g.html

Table I: input Partial Pressure of Gases

Gases	AlN	$Al_{0.8}Ga_{0.2}N$	$Al_{0.5}Ga_{0.5}N$	$Al_{0.2}Ga_{0.8}N$
TMAl	100sccm	97 sccm	94 sccm	80 sccm
TMGa	-	3 sccm	6 sccm	20 sccm
NH_3	1 slm	1 slm	1 slm	1 slm
H_2	1 slm	1 slm	1 slm	1 slm

Table II: Extracted Output Parameters

Parameters		AlN	$Al_{0.8}Ga_{0.2}N$	$Al_{0.5}Ga_{0.5}N$	$Al_{0.2}Ga_{0.8}N$
Dislocation Density (/cm^2)		2.5X10^{11}	5.65x10^{11}	3.03x10^{12}	2.625x10^{12}
Lattice parameter (^{o}A)	a	3.8332	3.8277	3.8452	3.8861
	b	3.8419	3.8489	3.8866	3.8856
	c	7.6801	7.6948	7.7127	7.7208

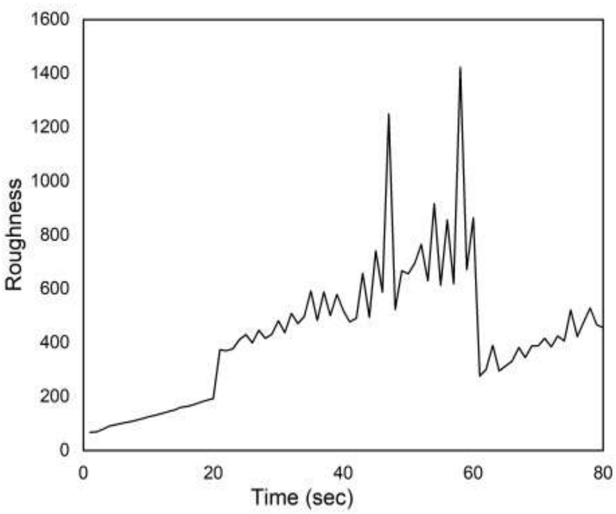

Fig.1a: Roughness plot with time

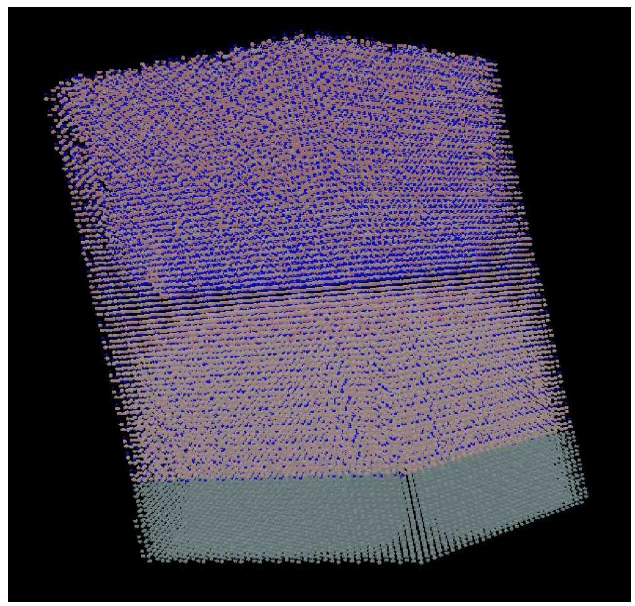

Fig.1c: Overall growth of all the layers on Silicon Substrate

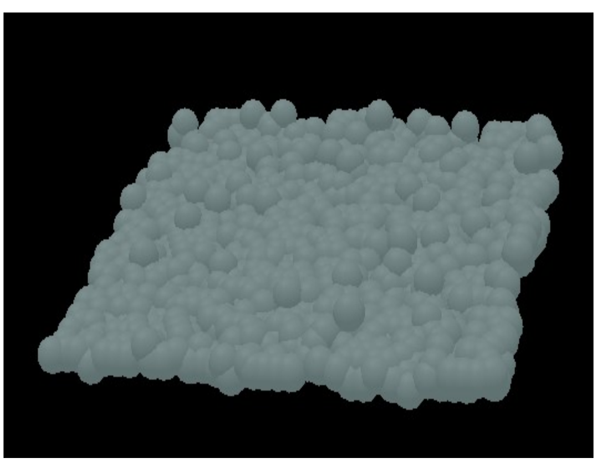

Fig.1b: Surface profile of $Al_{0.2}Ga_{0.8}N$ buffer layer