



Modeling of MOCVD of GaN-based electronic devices

Outline :

1. Introduction
2. AlGaN buffer: parasitic reactions and uniformity
3. Carbon incorporation in GaN and AlGaN
4. AlGaN barrier layer: thickness and composition uniformity
5. Summary

Scope of modeling:

- Gas flow in the reactors
- Heat transfer and temperature distribution over the wafer
- Gas-phase and surface chemical reactions
- Prediction of the growth rate and layer composition, dopant concentration; distribution over the wafers
- Parasitic deposition and particle formation

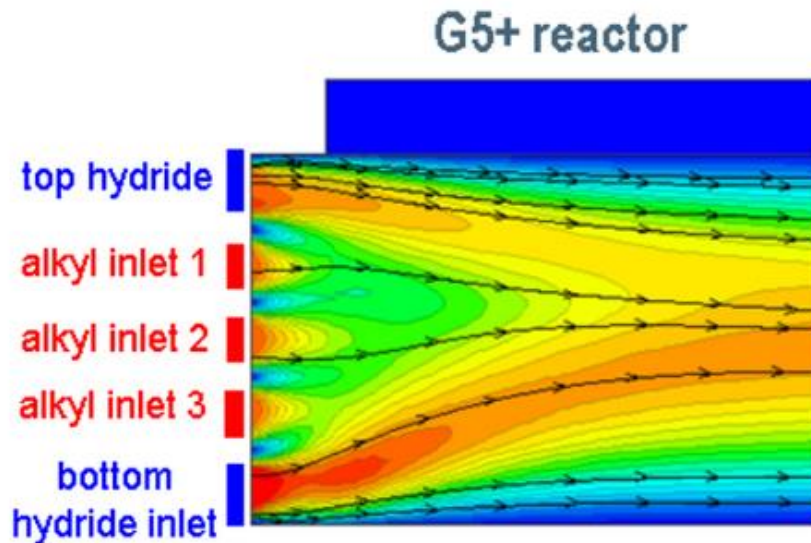


Typical GaN-on-Si device structure

What is needed:

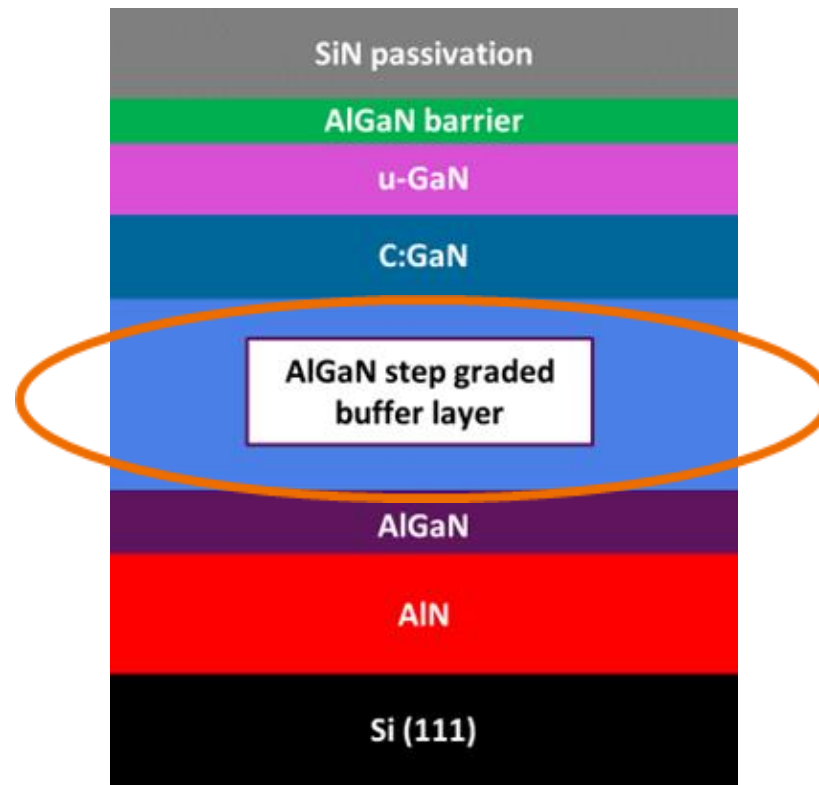
- Reasonable growth time
- Good uniformity
- Targeted electrical properties
- Strain control and crack suppression

Model of G5+C reactor:

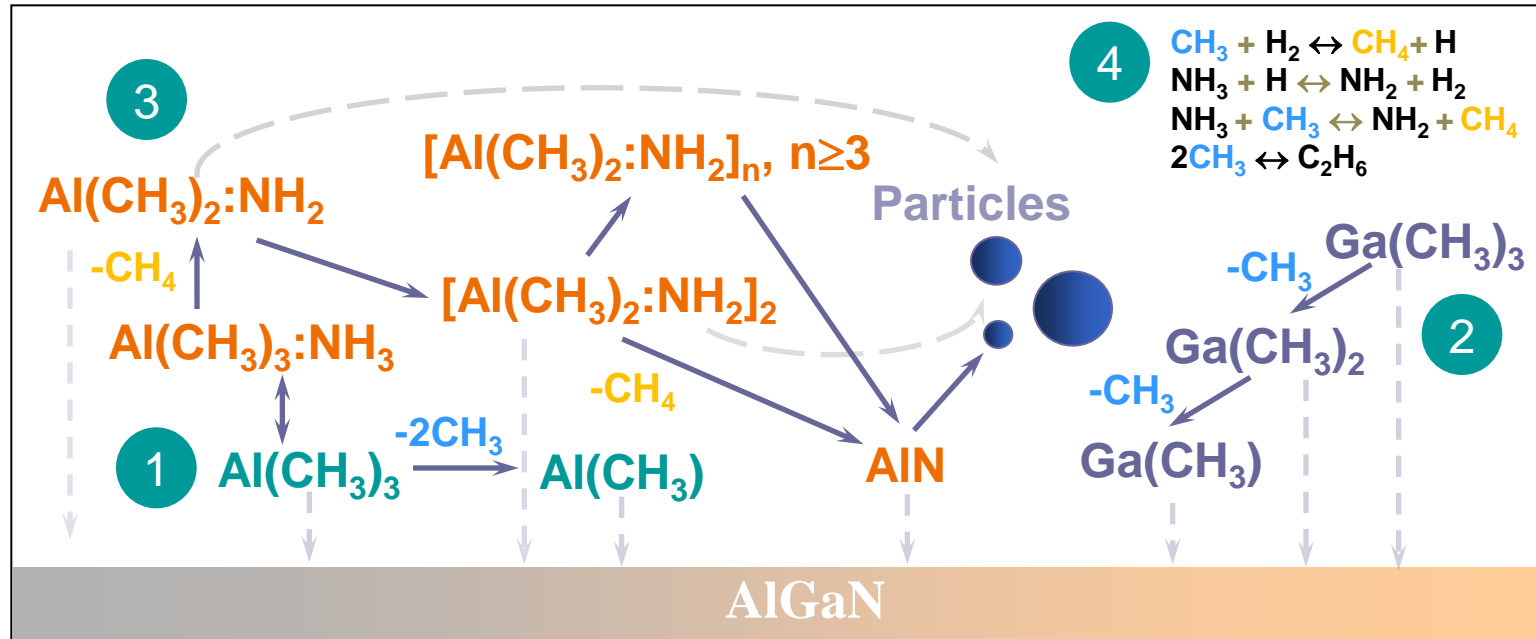


Detailed model of G5+C reactor is used to demonstrated simulation capabilities

Optimization of growth and uniformity of the buffer layers

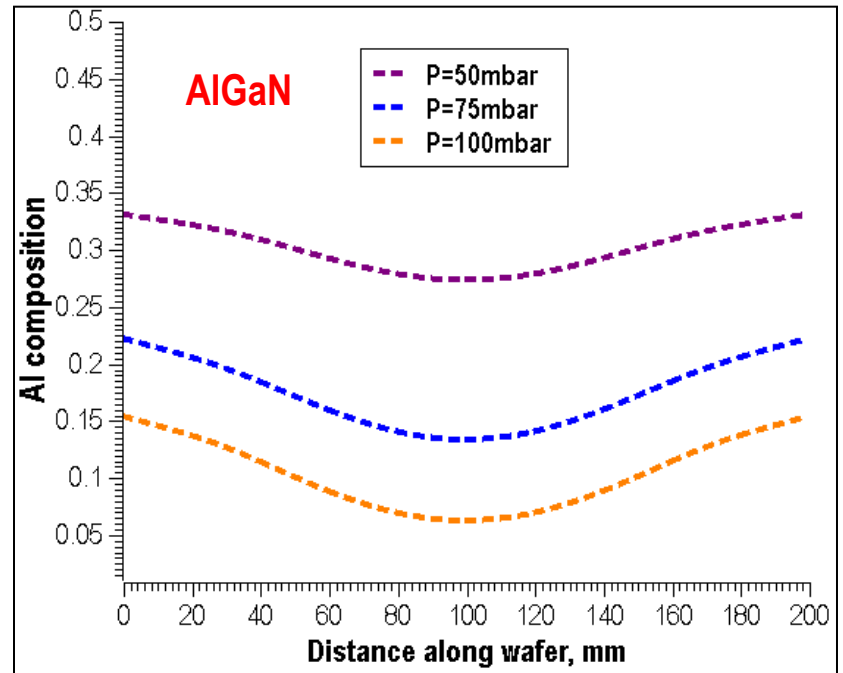
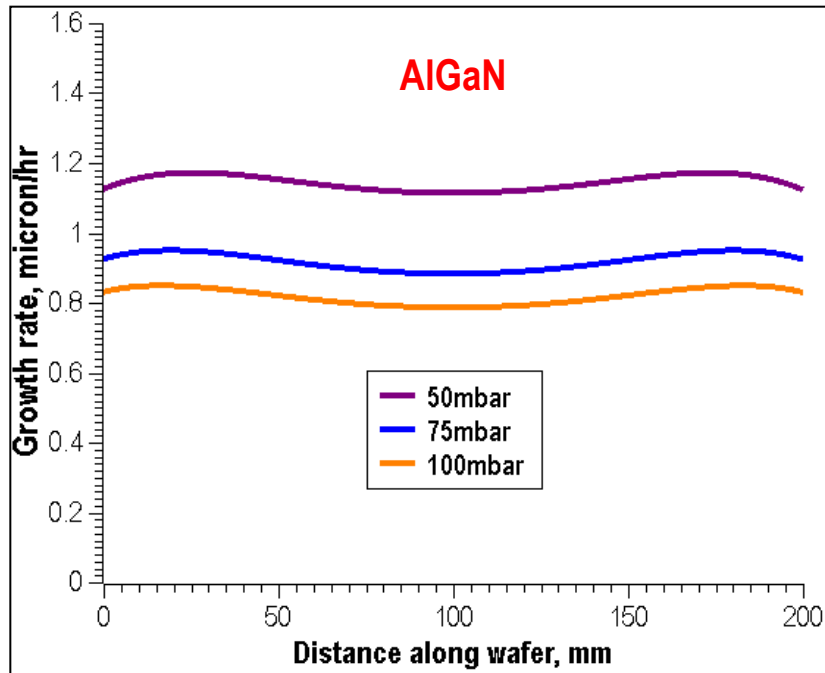


Gas-phase and surface chemistry



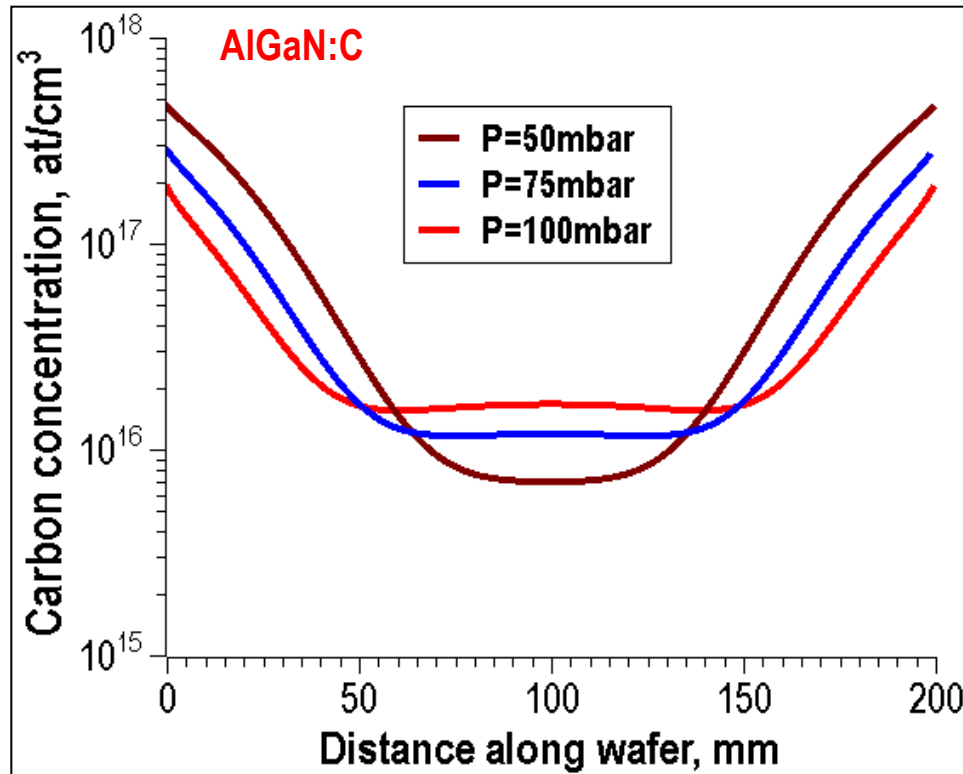
- 1 2 - TMAI and TMGa decomposition strongly temperature dependent
- 3 - Adduct formation and parasitic reactions: ammonia and pressure dependent
- 4 - Reactions with radicals

AlGaN buffer layer: growth rate and Al content



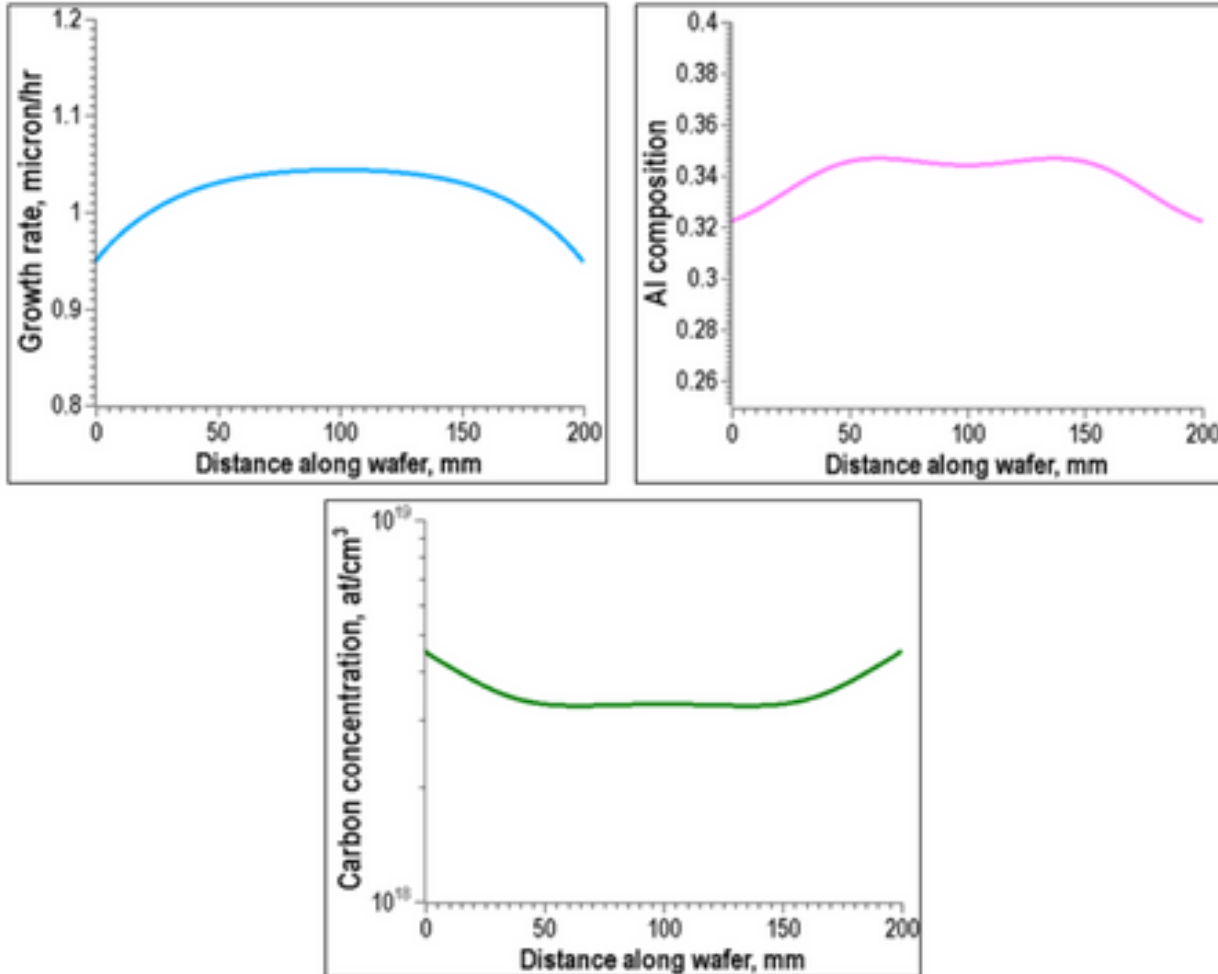
Growth rate and Al composition decrease due to parasitic reactions, uniformity gets worse

AlGaIn buffer layer: carbon concentration vs P



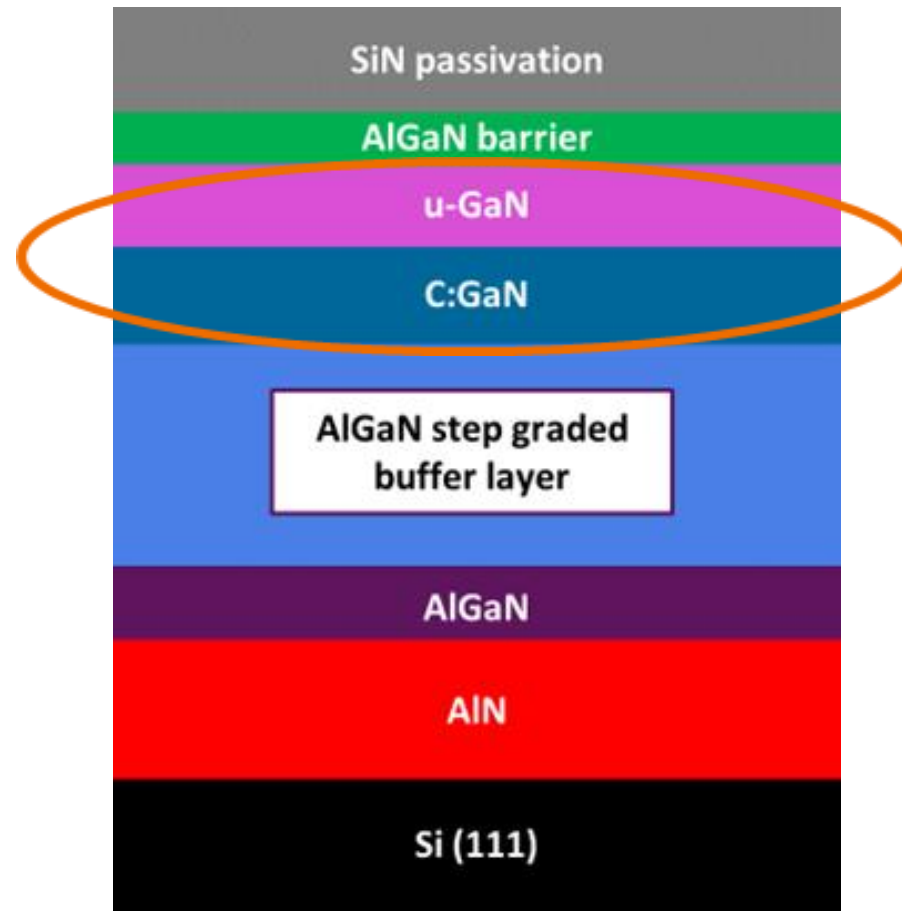
However carbon concentration uniformity gets better because of the difference in growth and doping mechanism

AlGaN buffer layer: optimized conditions



Optimized conditions allow to improve the uniformity and keep reasonable growth rate

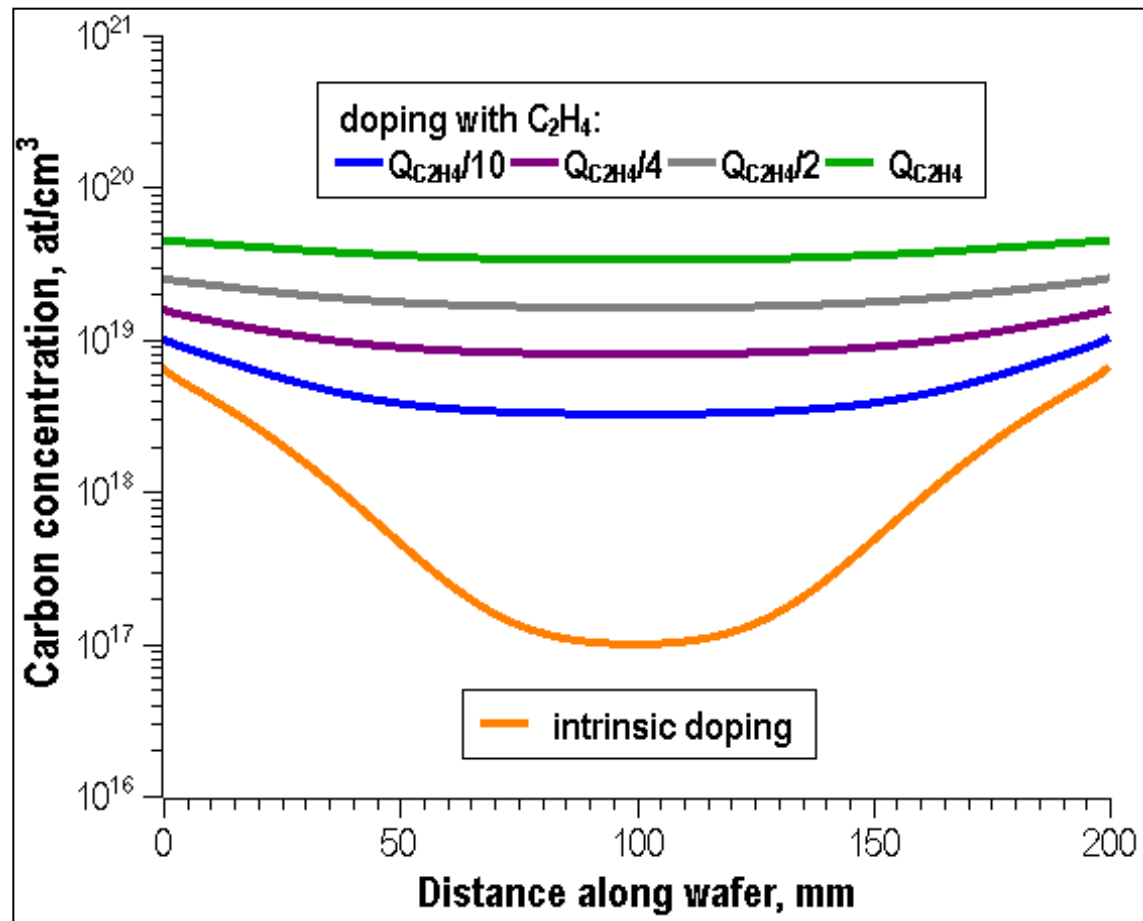
GaN: doping and uniformity



Carbon incorporation to GaN is sensitive to:

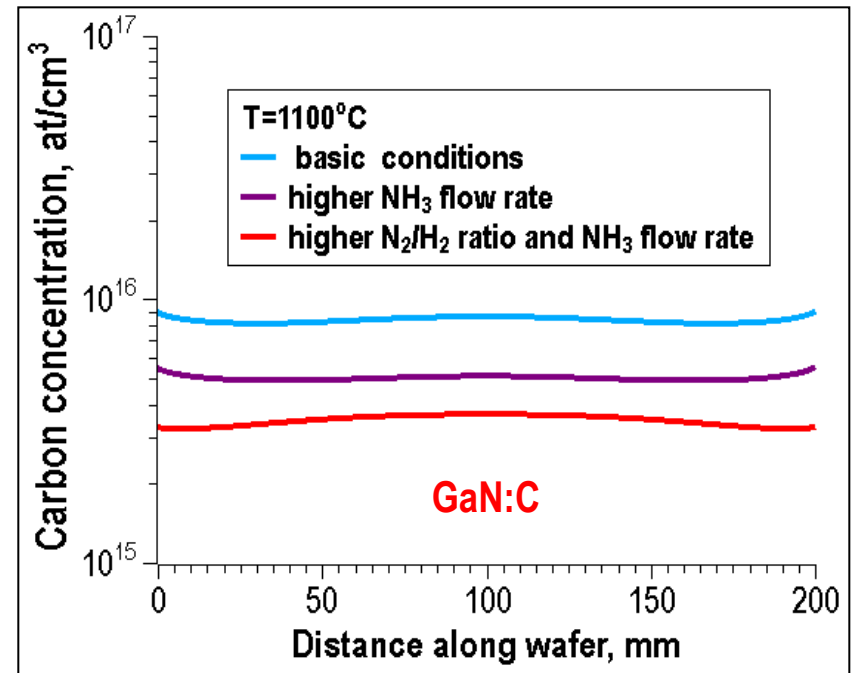
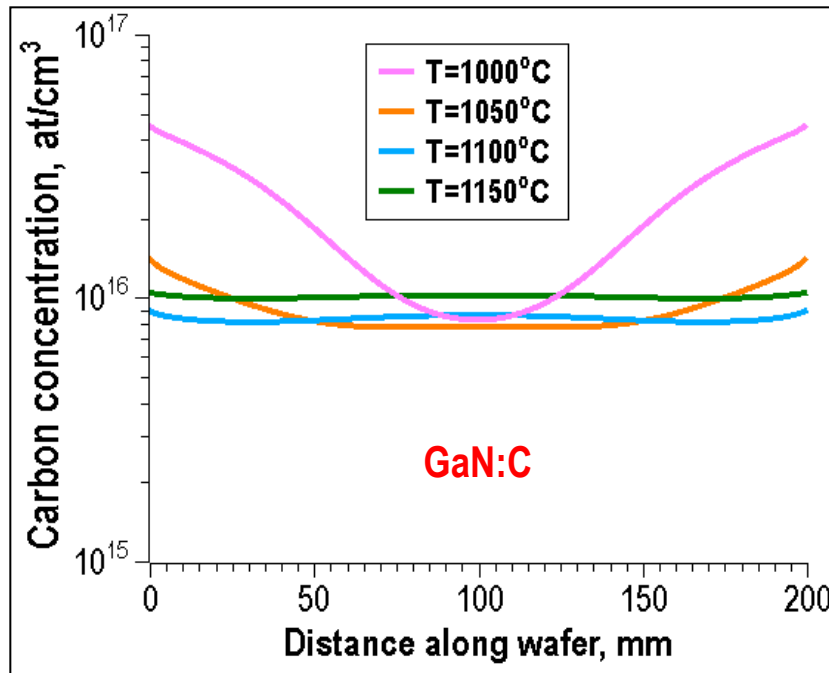
- **Temperature**
- **Carrier gas**
- **Precursor flow rates**
- **Pressure**
- **Reactor type**

GaN:C layer: carbon incorporation



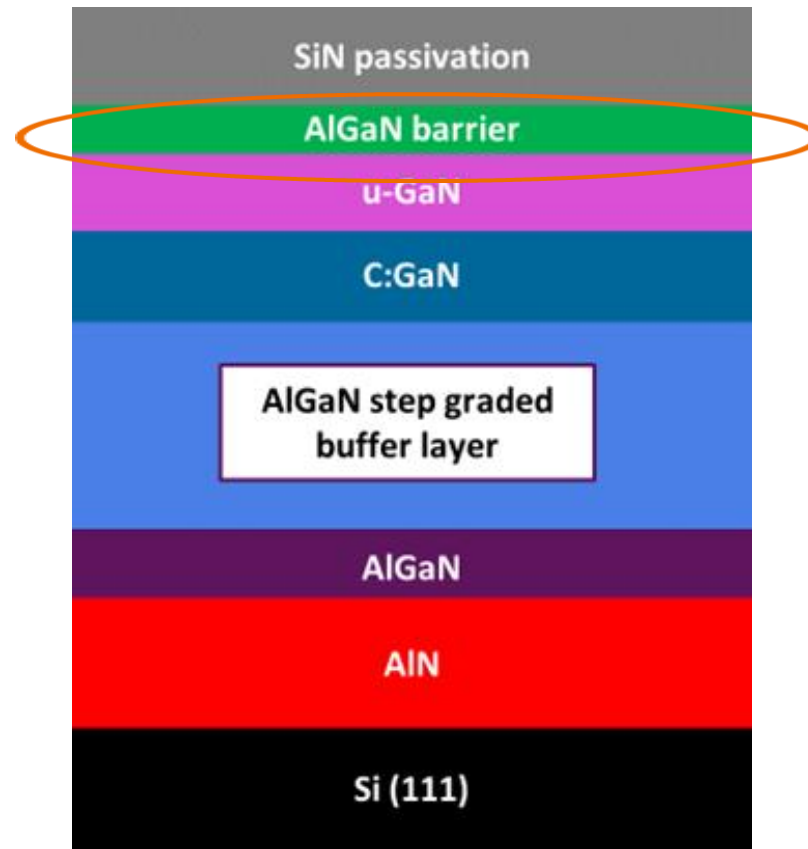
Desired carbon concentration and uniformity can be reached by using external doping source

Undoped GaN channel: carbon incorporation

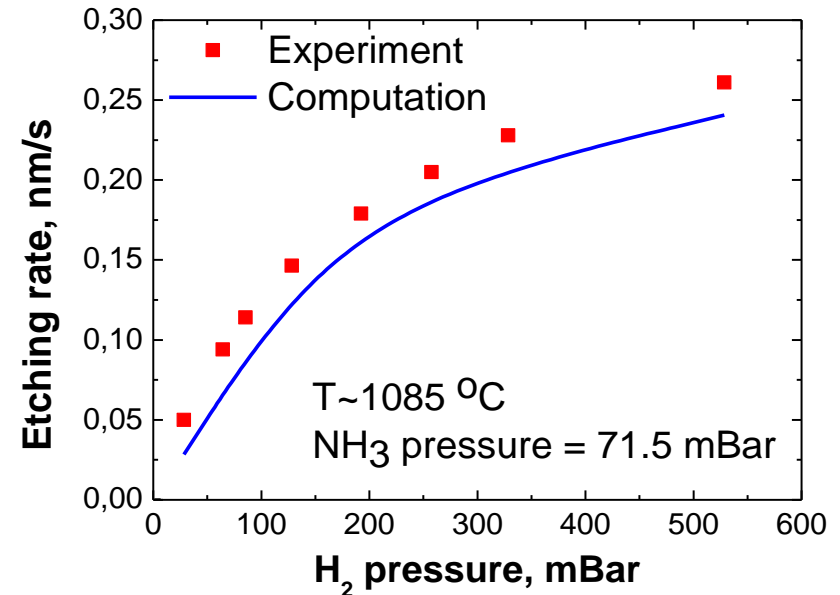
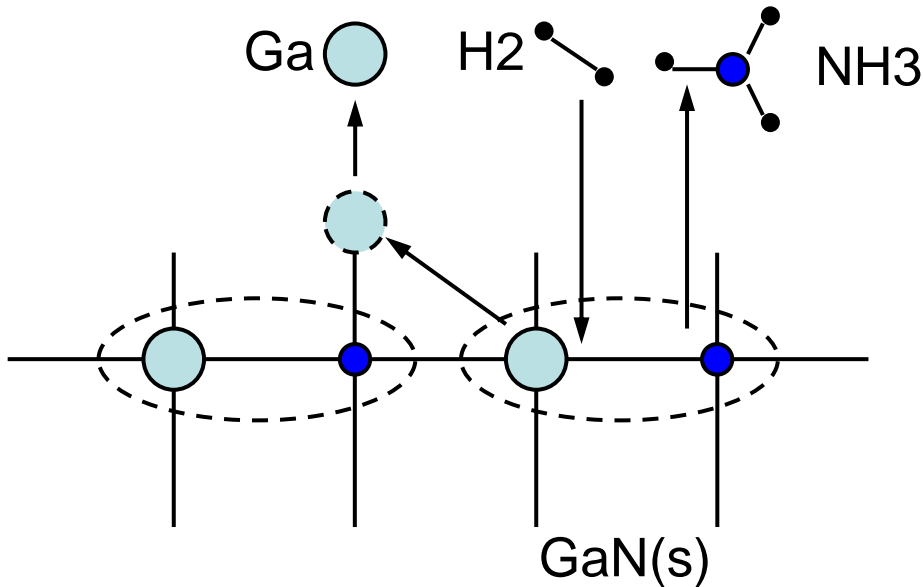


Highly pure and uniform layers can be grown by applying proper growth conditions

AlGaN barrier layer: thickness and composition uniformity



GaN surface chemistry: etching by H₂



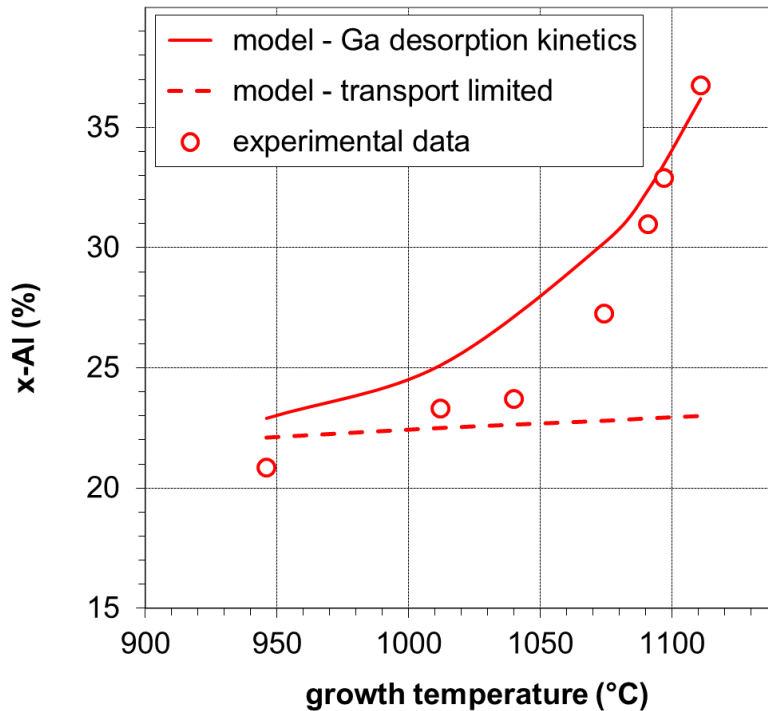
$\text{GaN(s)} + _V + (3/2)\text{H}_2 \rightleftharpoons \text{Ga_V} + \text{NH}_3$ – Ga is removed from bulk to surface

$\text{Ga_V} \rightleftharpoons \text{Ga} + _V$ – Ga desorption

E.E. Zavarin et al, ECS Proc, 2005-09 (2005) 299

AlGaN etching by H₂

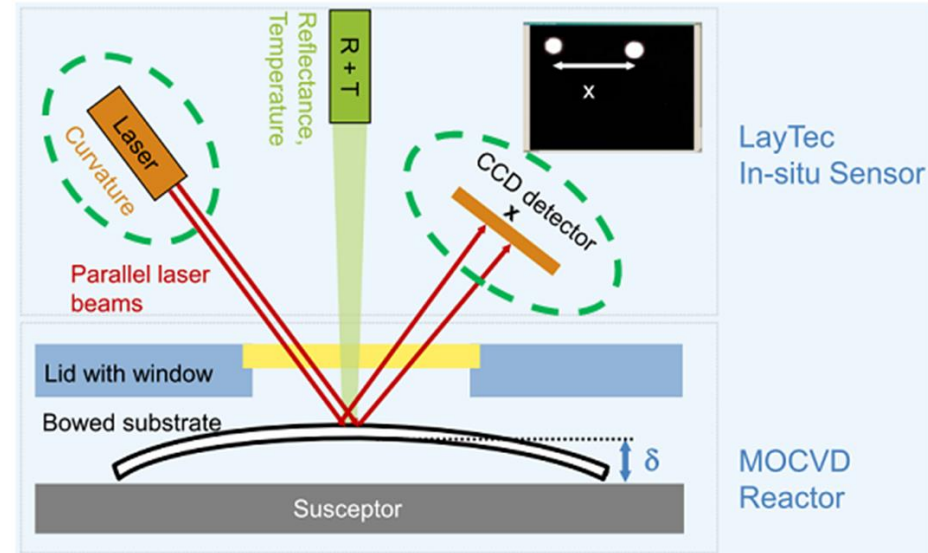
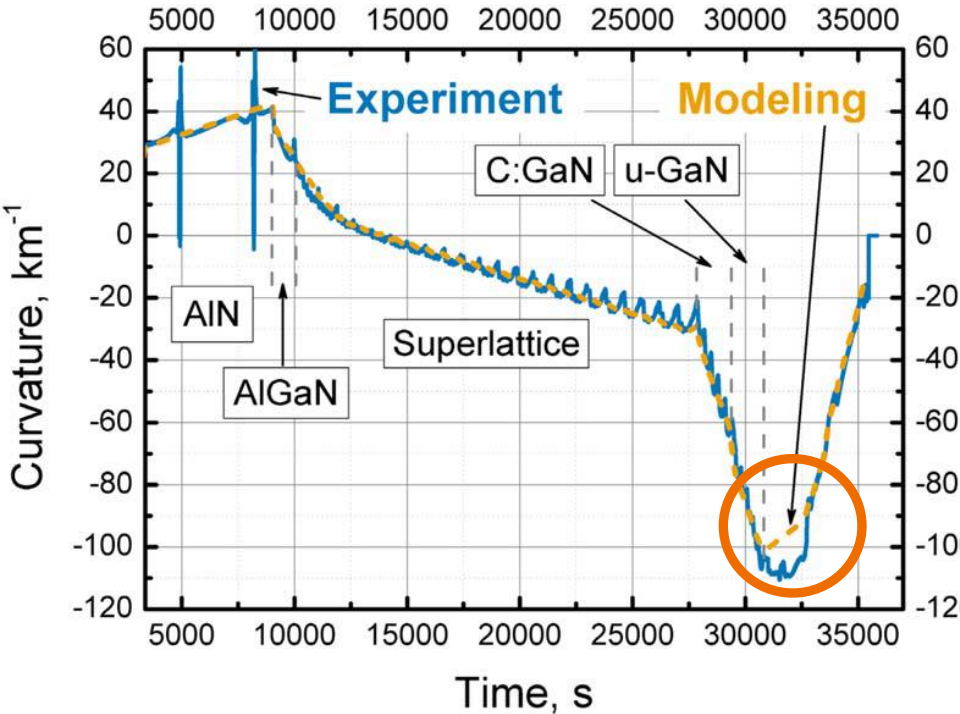
M. Daulesberg et al, JCG 393 103 (2014)



- **Dependence of AlGaN composition and thickness on temperatures is caused by hydrogen etching reaction**

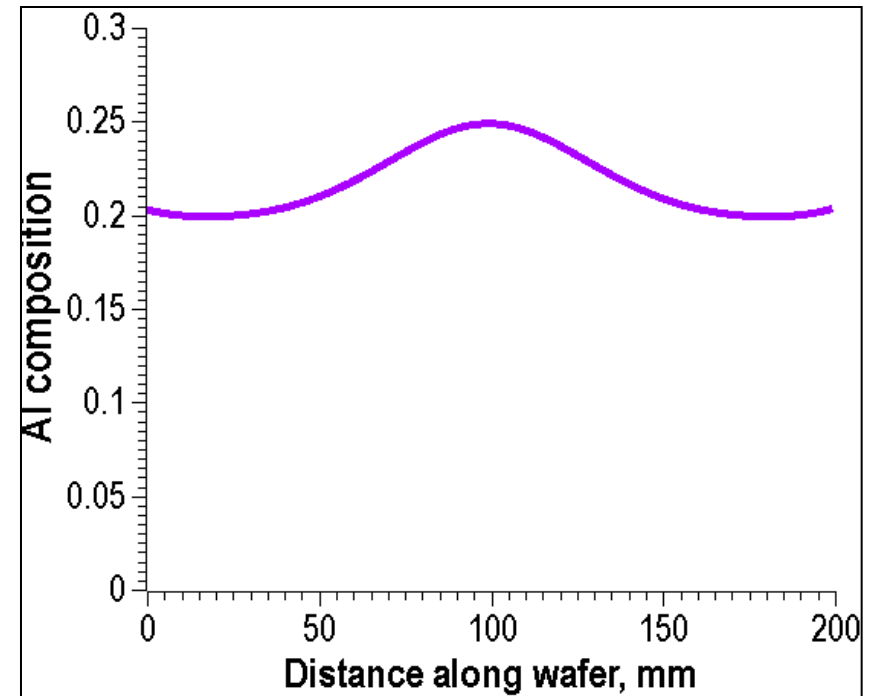
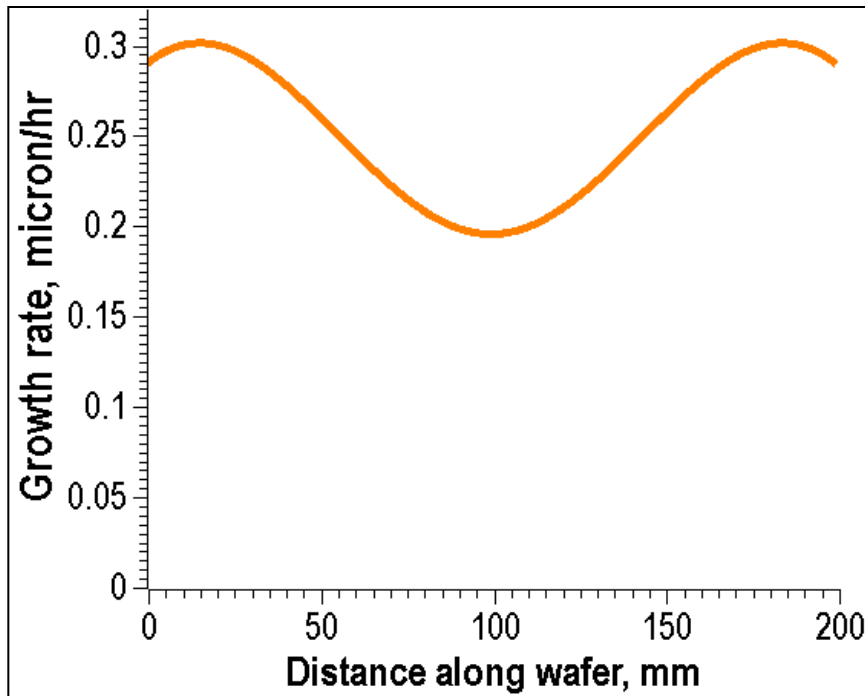
- **This effect is critical for barrier layer uniformity**

Temperature distribution on the wafer



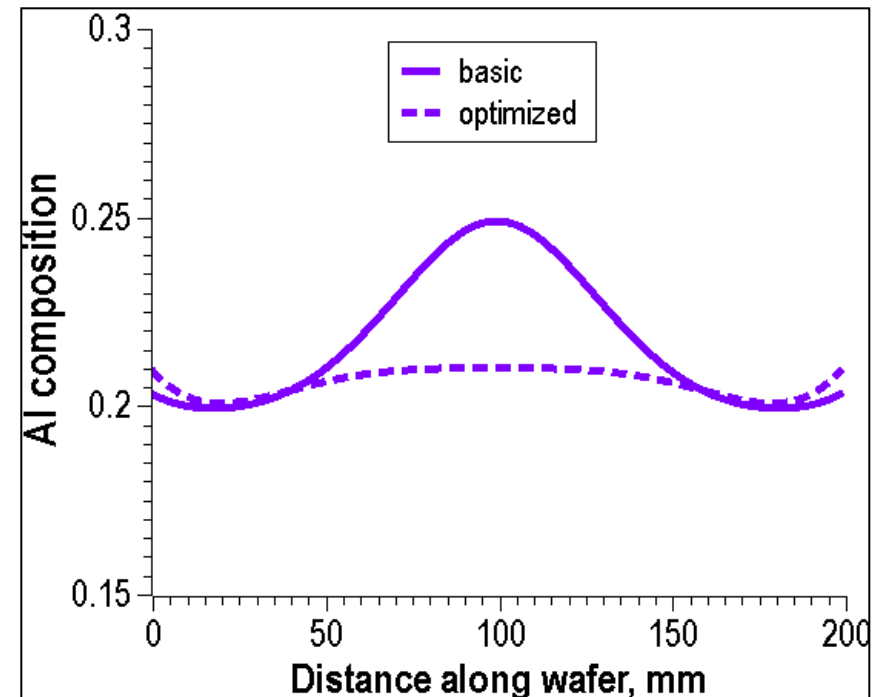
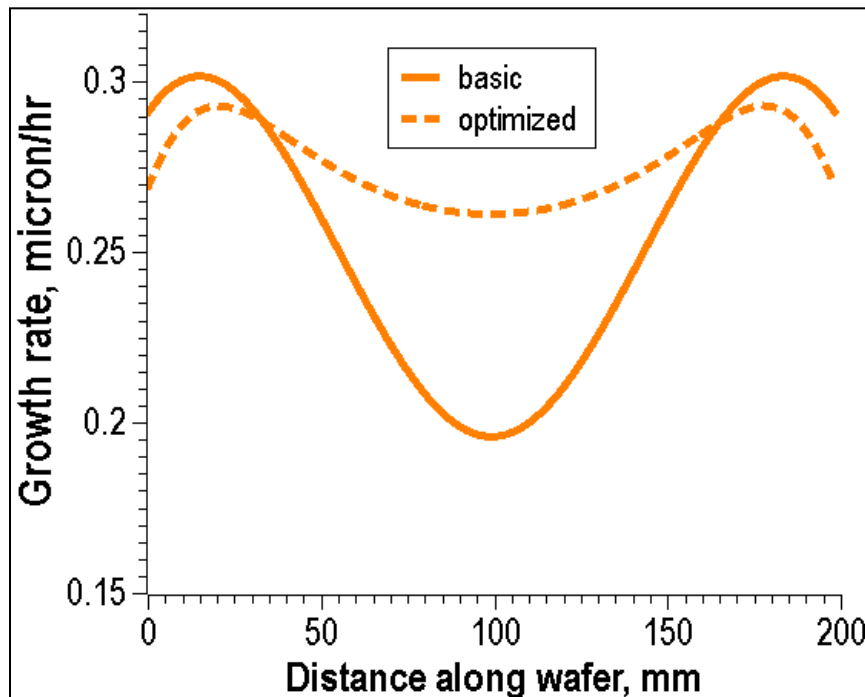
Strong convex bowing results in non-uniform wafer temperature

Barrier layer uniformity: basic conditions



Temperature non-uniformity in non-uniform thickness and composition distribution of the barrier

Barrier layer uniformity: optimized conditions



Optimized conditions allow improving barrier layer uniformity

Summary:

- **MOCVD process model can be used to analyze the productivity and uniformity at all stages of GaN-on-Si epiwafer growth**
- **AlGaN composition uniformity depends on gas-phase parasitic reactions and temperature distribution over the wafer and can be optimized by proper growth conditions**
- **Carbon concentration in GaN and AlGaN strongly depends on process parameters**
- **MOCVD modeling can be effectively used to improve the process characteristics and reduce the cost of production of GaN-based electronic devices**