

# CVDSim for Modeling of Epitaxy

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2010

## MOVPE process for horizontal reactors with reduced parasitic deposition

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The use of the inverted precursor supply allows 40 runs of 1.5 mm thick GaN without removing parasitic deposits instead of 10 growth runs for the conventional growth process

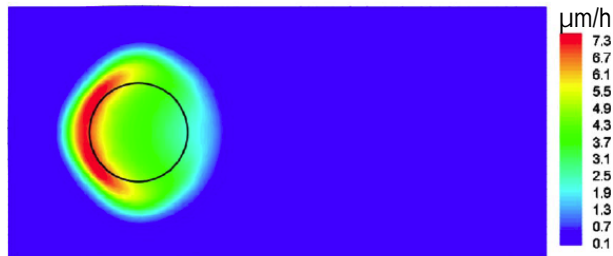
### Abstract

In this paper we report on a new MOVPE process for horizontal reactors in which care was taken to avoid the contact of group III source with the heated reactor walls. This effectively reduces parasitic deposition and leads to higher reproducibility and higher uptimes of the reactor without maintenance. A comparison between the standard and the new process for GaN growth is made. Results of modeling and experiments are presented.

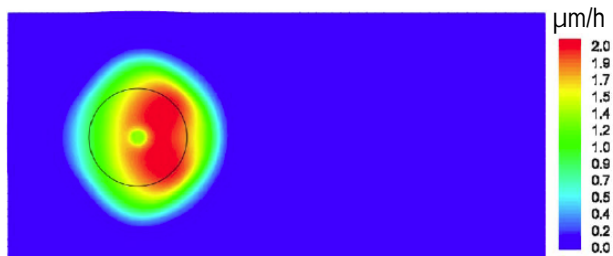
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### Deposition rate over the ceiling (modeling results)

conventional inlet

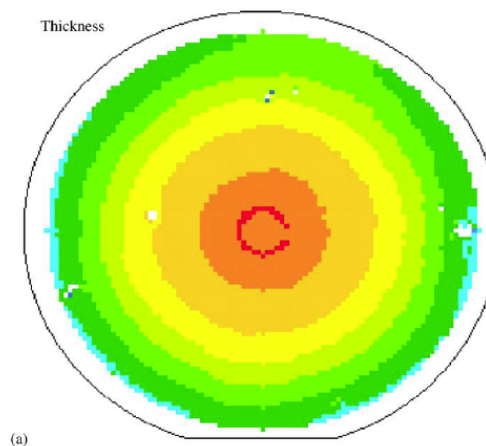


inverted inlet



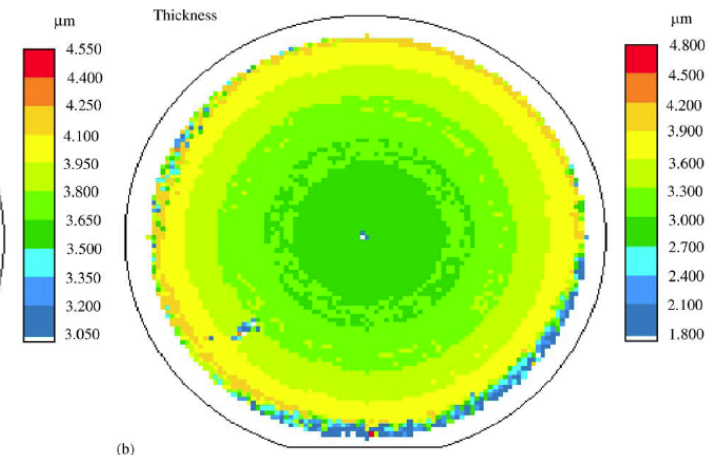
### Thickness mapping: from convex to concave profile

conventional inlet



(a)

inverted inlet



(b)

## Numerical and Experimental Study on Metal Organic Vapor-Phase Epitaxy of InGaN/GaN Multi-Quantum-Wells

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 Jongpa Hong  
 Jihye Shim  
 Bum Joon Kim  
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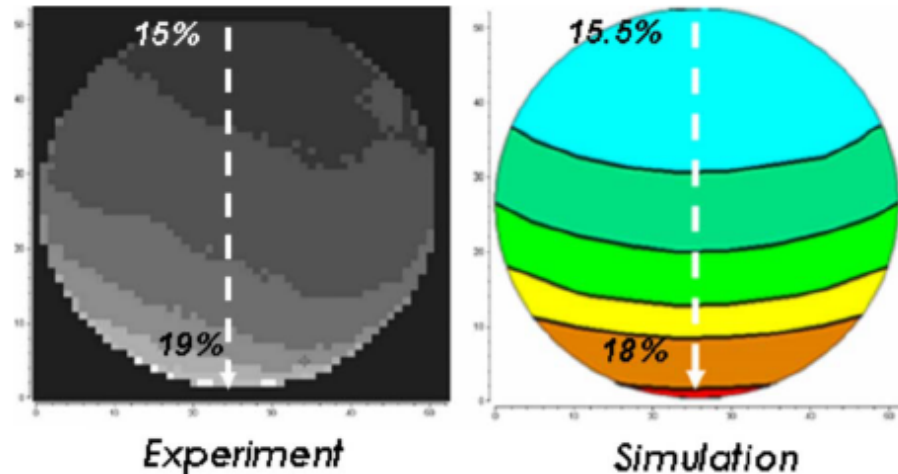
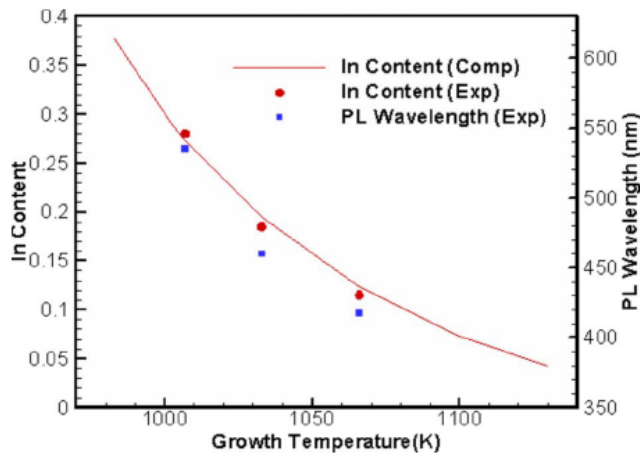
*A numerical and experimental study has been performed to characterize the metal organic vapor-phase epitaxy (MOVPE) growth of InGaN/GaN multi-quantum-wells. One of the major objectives of the present study is to predict the optimal operating conditions that would be suitable for the fabrication of GaN-based light-emitting diodes using three different reactors, vertical, horizontal, and planetary. Computational fluid dynamics (CFD) simulations considering gas-phase chemical reactions and surface chemistry were carried out and compared with experimental measurements. Through a lot of CFD simulations, the database for the multiparametric dependency of indium incorporation and growth rate in InGaN/GaN layers has been established in a wide range of growth conditions. Also, a heating system using radio frequency power was verified to obtain the uniform temperature distribution by simulating the electromagnetic field as well as gas flow fields. The present multidisciplinary approach has been applied to the development of a novel-concept MOVPE system as well as performance enhancement of existing commercial reactors. [DOI: 10.1115/1.2956513]*

*Keywords: metal organic vapor-phase epitaxy, InGaN, multi-quantum-well, light-emitting diode, surface chemistry, radio frequency power, electromagnetic field*

Combination of simulation and experimental analysis has been applied to improve the performance of the existing reactors and to develop a novel reactor concept

Corporate R&D Institute CAE Group,  
 SAMSUNG Electro-Mechanics Co. Ltd.,  
 Suwon, Gyeonggi-Do 443-743, Korea

Contour lines of indium composition



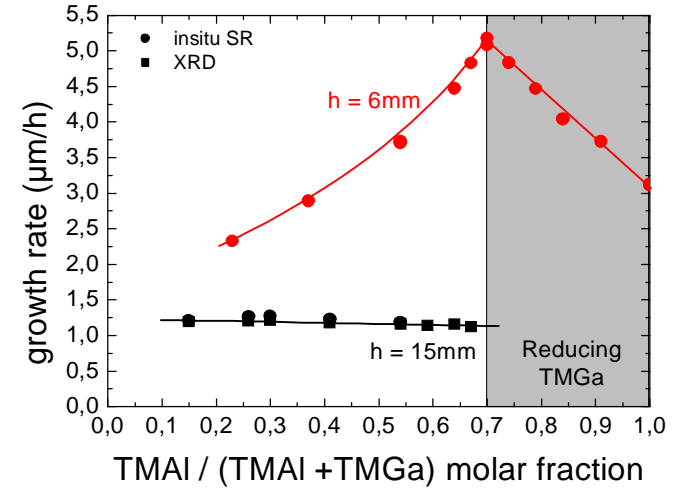
## Effect of the growth conditions and reactor height on the AlGa<sub>N</sub> growth rate and composition

E.V. Yakovlev, A.V. Lobanova

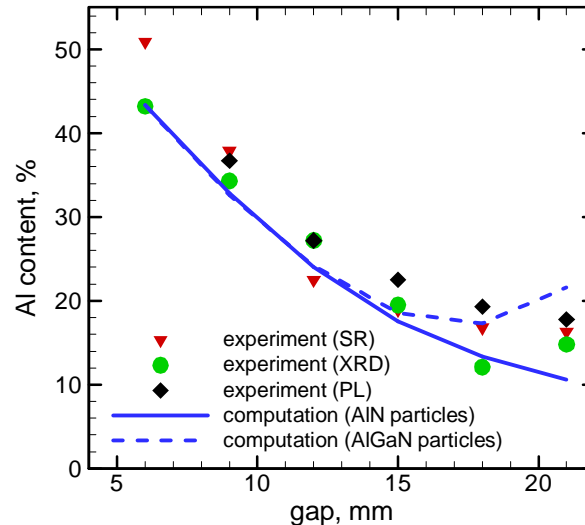
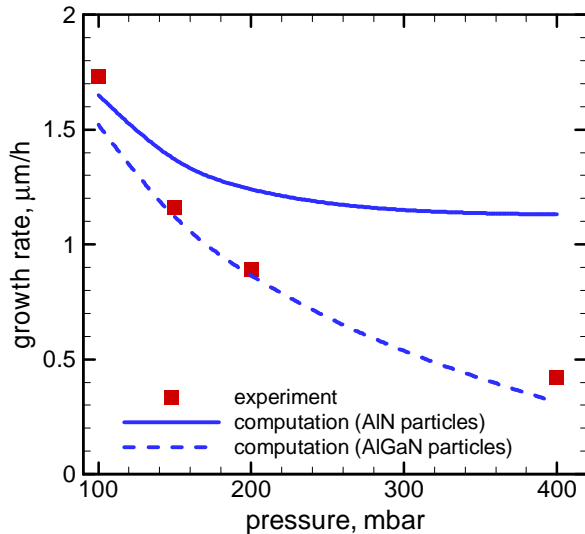
STR Group – Soft-Impact, Ltd., St.Petersburg, Russia

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Reproducible growth of AlGa<sub>N</sub> in the entire compositional range has been achieved with the growth rate above 3  $\mu\text{m/h}$



CVDSim has been applied to analyze the effect of operating conditions and reactor height during AlGa<sub>N</sub> MOVPE

## Modeling and process design of III-nitride MOVPE at near-atmospheric pressure in close coupled showerhead and planetary reactors

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### Abstract

The metalorganic vapor-phase epitaxy (MOVPE) growth of GaN from TMGa and NH<sub>3</sub> at higher process pressures up to near-atmospheric pressure in commercial production scale multi-wafer reactors is investigated. The Planetary Reactor<sup>®</sup> and close coupled showerhead reactor are compared and their suitability for near-atmospheric pressure growth is demonstrated. Advanced model development and its validation by growth experiments are carried out with particular emphasis on gas phase reaction kinetics and nucleation dynamics. Both are recognized to be crucial for nitride MOVPE at elevated pressures. Process and reactor design improvements to enhance growth efficiency of GaN at elevated pressures are discussed and the physical origin of the pressure dependence of growth efficiency is analyzed. Model predictions and growth experiments are in good agreement.

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## Modelling of group-III nitride MOVPE in the closed coupled showerhead reactor and Planetary Reactor<sup>®</sup>

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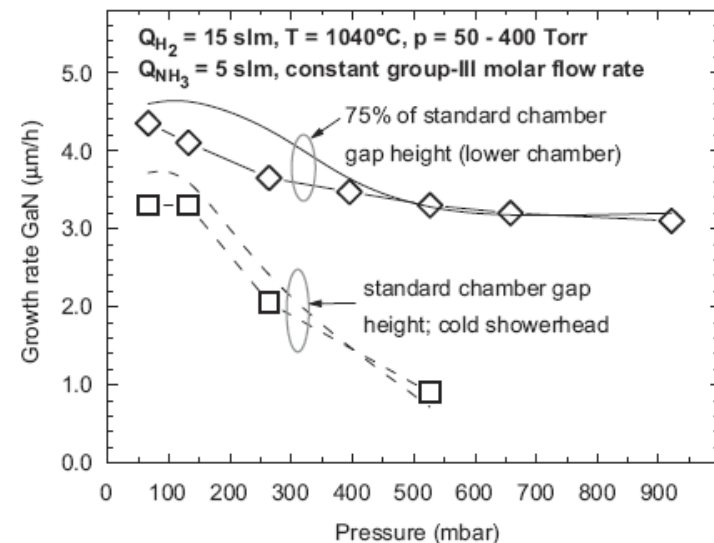
### Abstract

The modelling and subsequent experimental validation of nitride growth processes in commercial, production scale multi-wafer reactors is investigated with focus on group-III nitride compounds GaN and InGaN. The paper also deals with the development of group-III nitride growth processes at elevated process pressures, highlighting the effects of gas-phase nucleation phenomena on the growth efficiency of GaN. In addition, the latest hardware and process improvements to the Planetary Reactor<sup>®</sup> technology are presented, with focus on the development using a modelling approach, of a new gas injector design for III-nitride growth. Subsequent experimental validation of the new injector design, and its flexibility to changing process regimes for GaN and InGaN will be demonstrated for the 42 × 2" Planetary Reactor<sup>®</sup>.

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Modeling is actively used for the process optimization and design of commercial production-scale multi-wafer reactors

GaN growth rate vs pressure in 6x2" CCS reactor



## Influence of the reactor inlet configuration on the AlGaN growth efficiency

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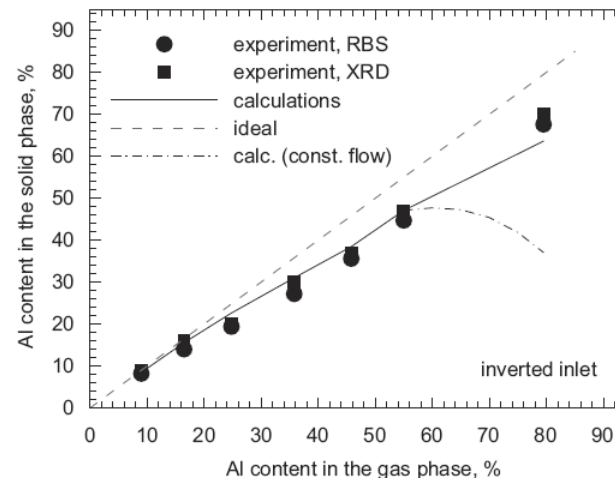
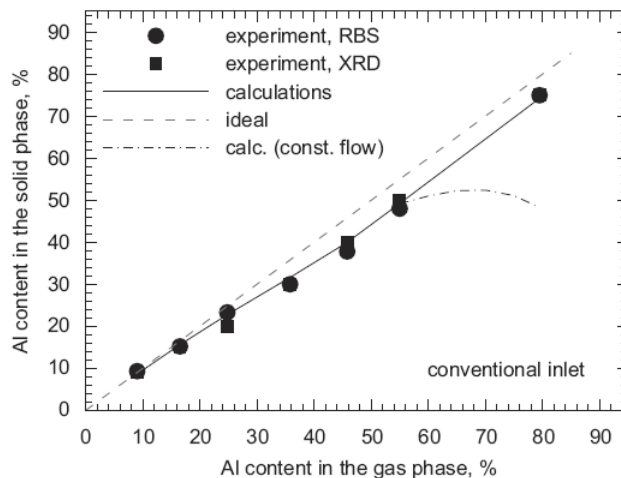
### Abstract

This paper discusses the results of a combined modeling and experimental analysis of AlGaN deposition in the horizontal two-flow AIX 200/4 RF-S reactor. The purpose of this study is to examine conventional and inverted supply of the precursors into the reactor with respect to the growth reproducibility and efficiency of the aluminum (Al) incorporation. It has been found that the use of the inverted inlet improves the reproducibility of the growth process and provides a good control of AlGaN deposition. At the same time, the Al content appears to be somewhat lower for the inverted inlet configuration. A good agreement between the experimental data and model predictions allows us to use the modeling results for interpretation of the experimental findings.

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Modeling allows the interpretation of the experimental findings related to aluminum incorporation. A way to enhance the growth efficiency is suggested

### AlGaN solid-vapor relationship for different inlet configurations



## Hydrogen effects in III-nitride MOVPE

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A3. Metalorganic vapor phase epitaxy

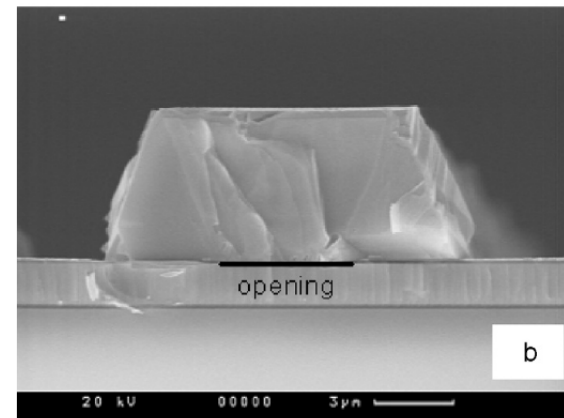
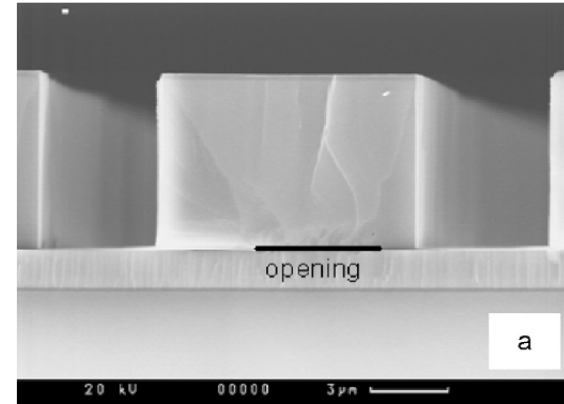
A3. Selective epitaxy

B1. Nitrides

### ABSTRACT

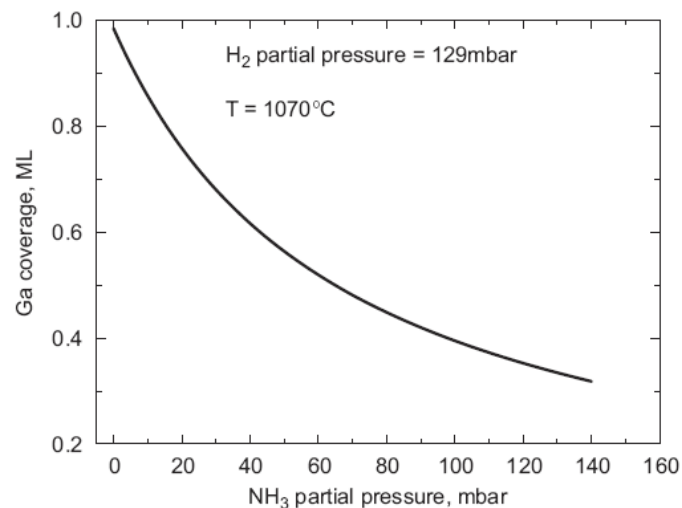
Influence of hydrogen on the growth of III-nitride materials by MOVPE is discussed using modeling and experimental study. The main conclusion, coming from the modeling and supported by numerous experimental observations, is that hydrogen affects the growth of III-nitrides in two different ways: via layer etching at elevated temperatures and via surface coverage with metal adatoms. The adatoms are found to accumulate on the surface due to interaction with hydrogen in a wide temperature range, including reduced temperatures. With regard to these effects, one can control such important characteristics as layer composition, growth anisotropies, surface quality, and even material properties (like p-doping level) by adjusting the carrier gas composition and other growth parameters.

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Non-coalesced a-GaN ELOG structures grown under identical growth conditions, using hydrogen (a) and nitrogen (b) as a carrier gas

### Ga coverage vs NH<sub>3</sub> partial pressure



The ability to adjust the surface coverage is found to underlie various experimental findings related to both planar and selective growth of GaN layers

## Effect of metallic surface coverage on material quality in III-nitride MOVPE

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Pinholes and pits are well known types of defects characteristic for nitride growth by MOVPE. This paper reports on studies of the correlation between the defect appearance and MOVPE growth conditions and discusses the ways to improve the material quality. A decrease of the ammonia flow at a constant total flow during MOVPE of GaN in a hydrogen-ammonia atmosphere at moderate temperatures (750-900 °C) has revealed the overgrowth of pinholes up to their almost

complete disappearance. The same effect was observed by the addition of a certain amount of trimethylindium to the gas phase. In both cases the improvement in morphology was associated with an accumulation of metallic (Ga and In, respectively) atoms in the adsorption layer at the growing surface. This conclusion was supported by surface kinetics model computations. The model suggests possible strategies for the growth of pinhole-free layers in various device structures.

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We suggest strategies for the pinhole density decrease and improvement of the surface morphology during GaN MOVPE via accumulation of metallic atoms in the adsorption layer

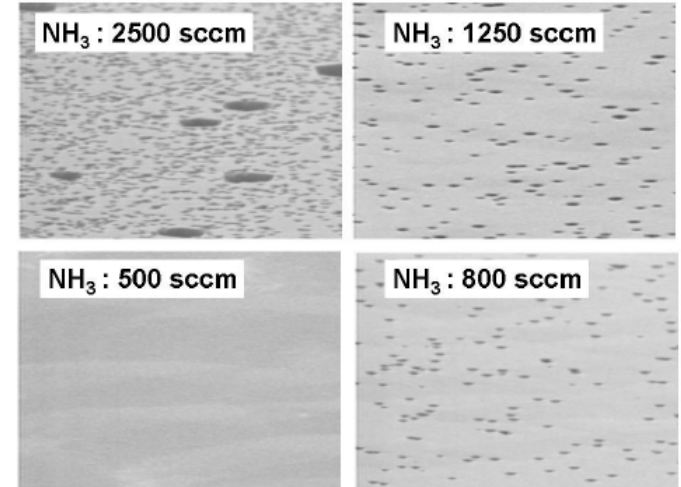


Figure 1 SEM images of GaN surface grown in Epiquip reactor under reduction of ammonia flow rates ( $T = 850\text{ °C}$ ,  $P = 200\text{ mbar}$ , Total flow ( $\text{H}_2 + \text{NH}_3$ ) = 7 slm).

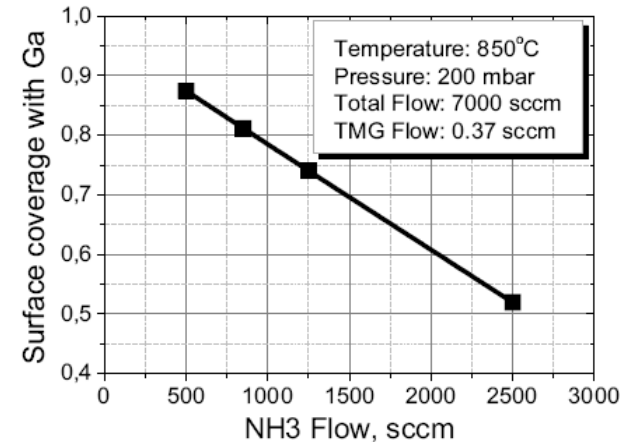


Figure 2 Model prediction for variation of atomic Ga coverage on GaN surface with ammonia flow in Epiquip reactor.



## Growth conditions and surface morphology of AlN MOVPE

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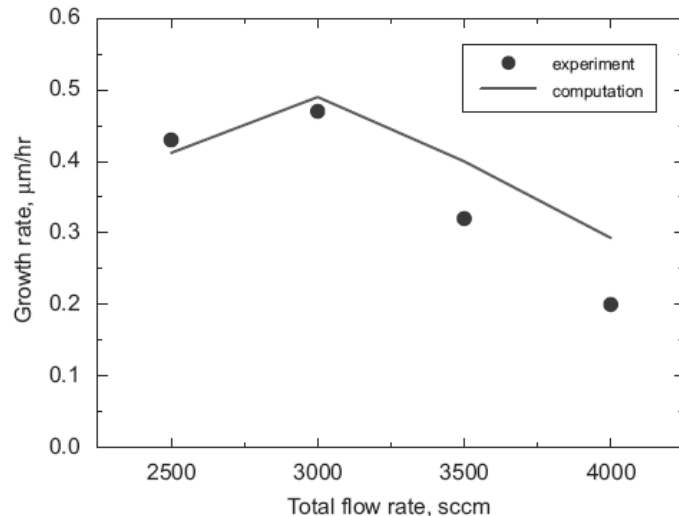
### ABSTRACT

Experimental and modeling studies of AlN metal-organic vapor phase epitaxy (MOVPE) are aimed at the analysis of surface morphology variations with growth conditions. It was found that flattest surfaces can be obtained at high temperature, reduced growth rate, and optimal V/III ratio. Detailed simulation of AlN growth and comparison of the results with trends reported in the literature point out that the improvement of the surface morphology is due to the reduced parasitic gas-phase reactions and increased migration length of adsorbed species on the surface.

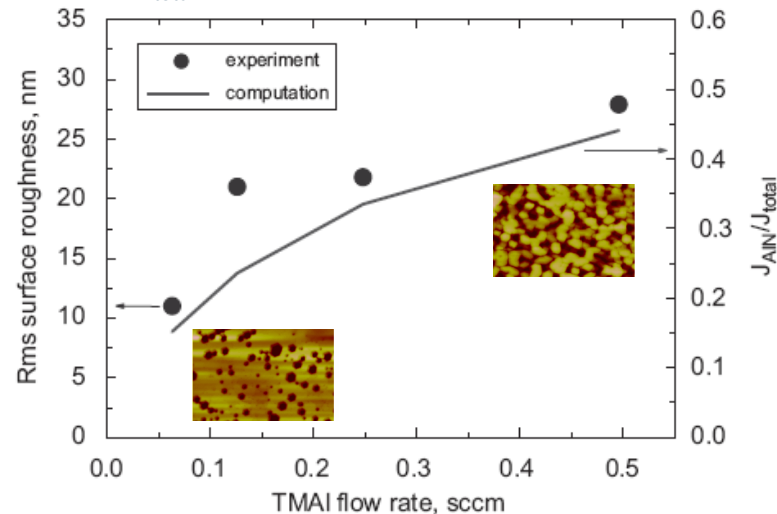
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Correlations between AlN surface roughness and growth conditions have been established using modeling and experimental study

Growth rate vs total flow



Surface roughness (experimental) and  $J_{AlN}/J_{total}$  ratio (computed) vs TMAI flow



## Surface chemistry and transport effects in GaN hydride vapor phase epitaxy

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## Reactor and growth process optimization for growth of thick GaN layers on sapphire substrates by HVPE

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P. Brückner<sup>b</sup>, F. Scholz<sup>b</sup>, Yu. Makarov<sup>c</sup>, A. Segal<sup>c</sup>, J. Kaeppler<sup>d</sup>

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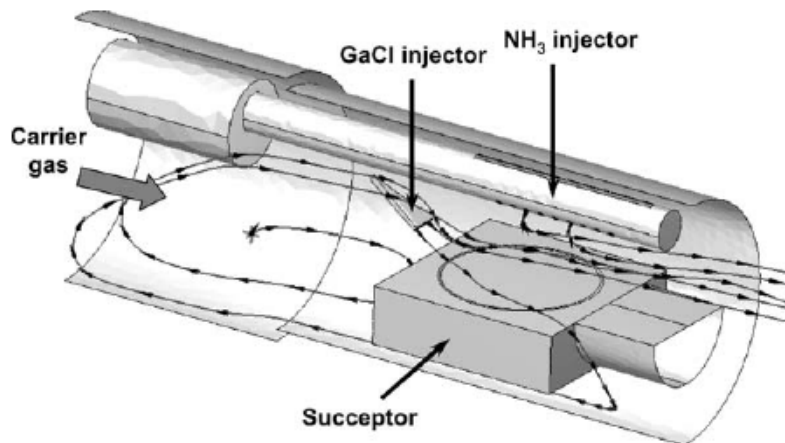
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Modifications of the operating parameters and reactor design have been suggested, using modeling, to enhance the process efficiency

### Case 1: bottom GaCl injector + nozzle



### Case 2: gas regulation chamber

