Modeling and process design of III-Nitride MOVPE at near-atmospheric pressure in Close Coupled Showerhead and Planetary Reactors®

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Introduction and motivation

- Fundamental study of MOVPE gas phase processes and their impact on growth efficiency of high temperature grown GaN at pressures up to 1 atm
- Computational modeling of crucial gas phase kinetics and nucleation dynamics
- Two types of production scale reactors compared: Close Coupled Showerhead & Planetary Reactor®
- Discussion of process & reactor design to reduce gas phase depletion (via formation of clusters)
- Advantages of GaN MOVPE at near 1 atm include:
  - Lower threading dislocation density
  - Lower background impurity density
  - Improved magnesium activation in p-GaN

Modeling approach and features

- Major modeling features:
  - Chemically reacting gas flow and heat transfer
  - Reaction kinetics, gas phase nucleation, film growth

Gas phase kinetics in the TMGa – NH_3 system

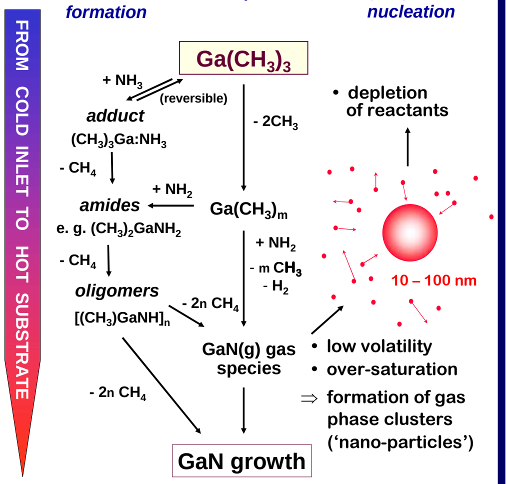

Fig. 1: Schematic of gas phase processes during MOVPE of GaN.

Close Coupled Showerhead Reactor

CCS Reactor principle:

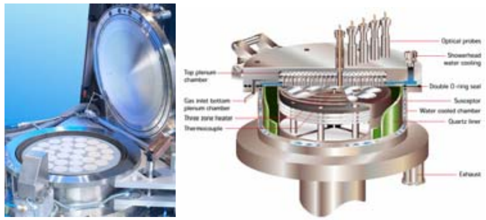

Fig 2: Opened CCS Reactor 30x2" (left), interior of CCS 19x2" (right)

- Reactor features:
  - Water cooled multi-plenum showerhead gas inlet
  - Separate supply of group-III precursors and NH_3
  - Shallow process chamber, uniform boundary layer

Pressure dependence of growth efficiency

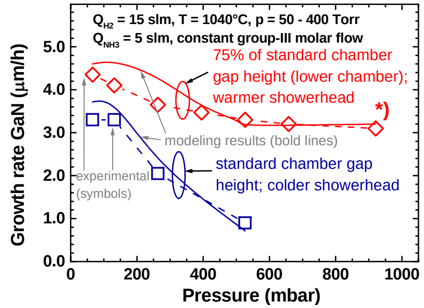

Fig. 3: Effect of pressure, chamber height and thermal environment on growth efficiency of GaN; CCS 6x2", T = 1040°C, Q_{tot} = 20 slm.

*) Chamber gap height reduction was partially obtained arranging an additional plate at the showerhead process face.
⇒ top wall of process volume turned out hotter by ~150°C!

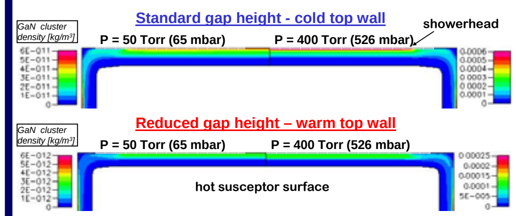

Fig. 4: CCS 6x2": distribution of GaN nano-cluster density (kg·m⁻³) in the process chamber; T = 1040°C, Q_{tot} = 20 slm, p = 50 / 400 Torr, standard gap height (top) and lower gap \ hotter top wall (bottom).

Planetary Reactor®

Planetary Reactor® principle:

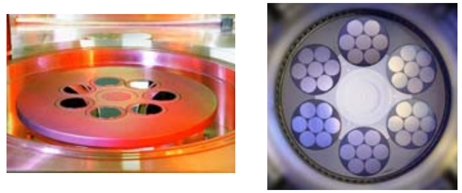

Fig. 5: Planetary Reactor® configurations: 6x2" (left), 42x2" (right).

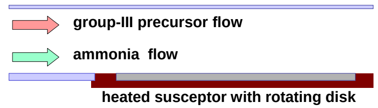

Fig. 6: Schematic of Planetary Reactor® principle: radial flow depletion.

Pressure dependence of growth efficiency

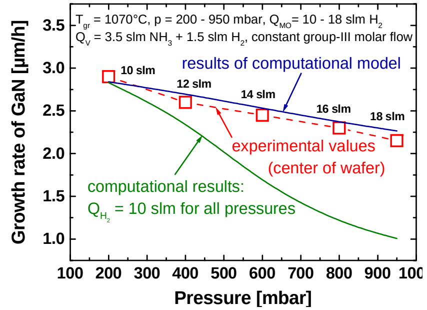

Fig. 7: Planetary Reactor® 6x2" configuration: effect of pressure and flow rate on the growth efficiency of GaN; T = 1070°C.

Effect of carrier gas flow rate

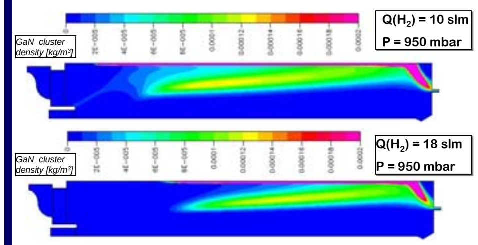

Fig. 8: Planetary Reactor® 6x2" configuration: effect of carrier gas flow rate on GaN nano-cluster density (kg·m⁻³); T = 1070°C, p = 950 mbar.

Discussion of phenomena

- Growth efficiency of GaN using TMGa and NH_3 at higher pressure is governed by formation of nano-sized clusters in the gas phase
  - Nano-clusters swept out of process volume by flow
  - Gas phase partially depleted by group-III reactants
- Rate of cluster formation highly sensitive on
  - Intermolecular collision frequency (i. e. pressure, residence time, dilution of reactants by carrier gas)
  - Reduction of nano-cluster growth rate by H_2-etching effects, that is affected by local gas temperature, and carrier gas (H_2 or N_2)
- Influence of thermophoresis
  - Thermophoretic forces acting on suspended nano-clusters tend to drive them away from the hot substrate surface towards the colder zones of the process volume (e. g. ceiling or showerhead).

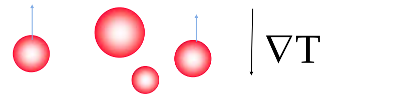

Fig. 9: Illustration of thermophoretic forces acting on nano-clusters

  - Enhanced depletion effect, reduced H_2 etching rate
  - Control of top wall temperature increases GaN growth efficiency significantly.

Conclusion

- Capability to grow GaN at pressures up to 1 atm in commercial production scale MOVPE reactors has been demonstrated.
- Gas phase nucleation and cluster formation has been identified as the most important governing factor forGaN growth efficiency at high pressure.
- Various reactor and process design strategies discussed to improve efficiency at high pressure.

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