MOCVD growth system
General MOCVD growth features

• **Advantages**
  – Faster growth than MBE, can be a few microns per hour; multi-wafer capability easily achievable
  – Higher temperature growth; growth process is thermodynamically favorable
  – Quality of layers usually better than MBE

• **Disadvantages**
  – Difficult to monitor growth rate exactly (no Rheed possible due to higher pressure)
  – Not as abrupt a process as MBE due to gas flow issues and memory effects
  – Toxic gases are to be handled
MOCVD growth of III-nitrides

- Precursors for III: TMGa, TMA1, TMIn; for V: NH$_3$, Hydrogen carrier gas; 25-760 Torr pressure
- Growth of GaN is carried out at 1000 – 1100 °C, which is much higher than the MBE growth temperature
- Growth on both SiC and sapphire substrates have been optimized and used regularly
- If SiC is used as substrate, it can be etched \textit{in-situ} to get very smooth surface showing step flow
- Growth always results in Ga-face polarity irrespective of the nucleation layer used
- Problem of hydrogen passivation of p-type dopants, since hydrogen is used as the carrier gas
**Basics of MOCVD growth of Nitrides**

- **Important growth parameters:** growth temperature $T$ and $V/III$ ratio
  - $T$ too high: desorption, nitrogen vacancies. $T$ too low: impurities incorporation, low surface mobility, structure defects; Usually temperature $\sim 1050 \, ^\circ\text{C}$
  - $V/III$ ratio too high: III-atoms low surface mobility, structure defects. Too low: decompose, nitrogen vacancies, auto background doping

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**Diagram:**

- Best growth zone
  - **Diffusion controlled**
  - **Thermodynamics-limited**
  - **Kinetics-limited**

- **Growth rate**
  - Temperature
  - $\frac{1}{T} \times 10^4 \, (K^{-1})$
  - $NH_3$ Pressure (Torr)
  - $GaN (s) + \frac{3}{2} H_2 (g)$
  - GaN (s) + 3/2 H2 (g) fwd
  - gas-source MBE
  - ECR-assisted CVD
  - conventional CVD

- **Processes:**
  - Kinetics-limited
  - Thermodynamics-limited
  - Diffusion controlled
  - Best growth zone

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**Graphical Representation:**

- **X-axis:** Temperature
- **Y-axis:** Growth rate
- **Diagram:**
  - $NH_3$ Pressure (Torr)
  - $GaN (s) + \frac{3}{2} H_2 (g)$
  - Gas-source MBE
  - ECR-assisted CVD
  - Conventional CVD

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MOCVD growth of Nitrides on sapphire

- A two-step growth method is followed with the growth of a low temperature AlN layer.
- Before any growth, the sapphire surface is nitridated to reduce defect density by causing changes in surface energy.
- The low temperature layer can be either GaN, AlN or even AlGaN.
- In MOCVD growth (unlike growth by MBE), the polarity of the GaN film is always Ga-face.
Hetero-epitaxial growth: MBE vs. MOCVD

Mean free path $\lambda = \frac{kT}{1.414P\sigma} \approx \frac{5 \times 10^{-4}}{P}$ (m), at 1000 °C

where $\sigma$ is the collision cross-section

Ultra-high vacuum: $10^{-5}$-$10^{-11}$ Torr

Long mean-free path (> chamber length)

III: Solid source, V: NH$_3$ or N plasma

MBE: reactions occur only at the substrate, MOCVD: parasitic reactions can occur before the reactant species reach the substrate. MBE growth, unlike MOCVD growth, is not thermodynamically favorable and is governed by Kinetics
Growth of ternaries and quaternaries

• InGaN should be grown at lower temperature than GaN and at higher V/III ratio due to lower dissociation temperature and higher nitrogen partial pressure.

• AlGaN should be grown at higher temperature than GaN and at lower V/III ratio due to higher dissociation temperature and lower nitrogen partial pressure.

• Growth of quaternaries (InGaAlN) are difficult due to the conflicting growth conditions of AlN and GaN. Usually max. In incorporation is possible only up to ~5%.

<table>
<thead>
<tr>
<th></th>
<th>InGaN</th>
<th>GaN</th>
<th>AlGaN</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>Low 740 °C</td>
<td>High 1050 °C</td>
<td>Higher 1100 °C</td>
</tr>
<tr>
<td>P</td>
<td>200-400 torr</td>
<td>40-100 torr</td>
<td>30-50 torr</td>
</tr>
<tr>
<td>V/III</td>
<td>&gt;5000</td>
<td>1000-2000</td>
<td>&lt;=1000</td>
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Various problems associated with mismatches

<table>
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<tr>
<th>Substrate Property</th>
<th>Consequence</th>
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<tbody>
<tr>
<td>1. Lateral lattice constant (a-lattice constant) mismatch</td>
<td>1. All problems typically associated with high dislocation density</td>
</tr>
<tr>
<td>2. Vertical lattice constant (c-lattice constant) mismatch</td>
<td>2. Anti-phase boundaries, inversion domain boundaries</td>
</tr>
<tr>
<td>3. Coefficient of thermal expansion mismatch</td>
<td>3. Thermally induced stress, cracks in epitaxial films</td>
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<tr>
<td>4. Low thermal conductivity</td>
<td>4. Poor heat conduction; unsuitability for high power devices</td>
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<tr>
<td>5. Different chemical composition of the epitaxial film</td>
<td>5. Contamination, interface states, poor wetting of surface during growth</td>
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Strain and critical thickness

Lattice mismatch \( f_m(x) = \frac{a_{epi}(x) - a_{sub}}{a_{epi}(x)} \)

In-plane strain \( \varepsilon(x) = -f_m(x) = \frac{a_{sub} - a_{epi}(x)}{a_{epi}(x)} \)

Strain relaxation \( r(x) = \frac{a_{epi}(x) - a_{sub}}{a_{epi,0}(x) - a_{sub}} \)

\( a_{epi,0}(x) = \) measured lattice constant, \( a_{epi,0}(x) = \) relaxed lattice constant, \( a_{sub}(x) = \) substrate lattice constant

Calculation of the critical thickness is very difficult experimentally, as it depends on many different factors such as in-plane strain, burgers vector of dislocations, growth methodologies etc.
Formation of dislocations

- Dislocations are formed in the epitaxial layers due to
  - Transfer of defects/dislocations already present in the substrate: Happens when substrate has high density of defects (example: dislocation in GaN epilayers when SiC is used as a substrate)
  - Misfit dislocation: When dislocations are caused by a difference in the lattice constant of the epitaxial layer and the substrate (Ex: dislocations in AlGaN layer ($d_{AlGaN} > d_{critical}$) grown on GaN)
  - Imperfections resulting from island coalescence (example: dislocations in GaN buffer layers grown on AlN nucleation layer)
- Main types of defects in GaN
  - Point defects (vacancies, self-interstitials, and antisites)
  - Threading edge dislocation
  - Threading screw dislocation
  - Mixed screw-edge dislocations
Dislocations

Simple cubic lattice

Extra half plane of atoms

Bonds

Displaced plane faces

Edge dislocation

Screw dislocation

Dislocations line structure in GaN film

\[
\left( \frac{1}{R_2} - \frac{1}{R_1} \right) = \frac{r_0}{r^2}, \quad r_0 = \frac{\mu b^2}{8\pi^2\gamma}
\]

For a given \( R_2 \), \( R_1 \) should be larger (i.e. the dislocation pit flatter) if \( r_0 \) is larger.

- \( b \) = magnitude of Burgers vector, \( \mu \) = shear modulus, \( \gamma \) = specific surface free energy, \( R_1 \) and \( R_2 \) inner and outer radii of curvature

- Whenever dislocation reach the surface it ends in a pit (this makes possible for AFM to record dislocations) due to equilibrium between the surface tension and line tension

- Screw dislocations have larger radii of surface pit than edge dislocations due to larger burger’s vector
Dislocation induced surface pits

- Dislocation with screw component reaching the surface will terminate steps. Usually 2 steps are terminated as the Burger’s vector has 2 times the magnitude of the step height (c/2)
- MBE grown GaN shows growth hillocks with 2 interlocking ramps around mixed screw dislocations

MOCVD grown GaN

MBE grown GaN on MOCVD templates
Dislocation characterization by AFM

Morphologies of AlGaN/GaN heterostructure on (a) SiC and (b) sapphire
Points to note about dislocations

- Step heights in nitride epitaxial films are ~2.6 Å (about half the unit cell height of 5.185 Å)
- Dislocations chains are formed around coalescing islands formed during the initial part of the growth
- Density of dislocations in epitaxial films grown on either sapphire or SiC is \(10^9 - 10^{10}\) cm\(^{-2}\)
- Screw and mixed edge-screw dislocations will terminate two steps as they both have a vertical component of the burgers vector equal to magnitude of the unit cell height \(c\)
- Screw and mixed-screw dislocations usually terminate in larger pits than edge dislocations due to larger burgers vector (pit-radius is proportional to the square of the burgers vector magnitude)
An estimate of density of acceptor states with dislocations

- Dislocation dangling bond density
  \[ = \left( \frac{2}{5.2 \times 10^{-8}} \right) \text{ cm}^{-1} = 3.85 \times 10^7 \text{ cm}^{-1} \]

- The density (per unit area) of dislocation induced states for 2 micron thick epitaxial layer
  \[ = 3.85 \times 10^7 \text{ cm}^{-1} \times 10^{10} \text{ cm}^{-2} \times (2 \times 10^{-4} \text{ cm}) = 7.7 \times 10^{13} \text{ cm}^{-2} \]

- Assuming just 10% of the states capture electrons there are \( 7.7 \times 10^{12} \text{ cm}^{-2} \) electrons lost

- Since the dislocations states are so close in real space they will form energy band in the reciprocal space along the c-axis
Detrimental effects of dislocations I

Leakage through dislocation states in a schottky contact

- Conduction through the dislocations states by hopping transport
- Tunneling assisted by the dislocation states.
- Dislocation induced leakage forms a major component of gate leakage current in HFETs

Recombination of electrons and holes via dislocation states

Dislocation states form a band in reciprocal space

Recombination process via defect states usually does not emit light. Even if it does, it will not be at the band-edge energy