Simulation of Bandgap in MOVPE Selective Area Growth of InGaAsP-based Photonic Integrated Circuits

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Background

Research on selective area MOVPE
- A method to realize low cost monolithic photonic integrated circuits
  (EA modulator integrated laser, laser array and all-optical switch, etc)
- A tool to analyze and model the growth process

Compared to other schemes of active-passive integration, it has
- Flexibility to design different bandgap with a single growth step
- Real application in the industry for BH lasers

Problems of TCAD design tools for SA-MOVPE
- Modeling parameters are dependent on used source material
  (organic/inorganic group V) and other conditions
- Simultaneous modeling of reactor and growth mechanism in required
- Gas phase diffusion based model proposed by Gibbon*
  • Binary growth rate profile only

Why Simulate Bandgap?

- Bandgap helps determine operating wavelength, bias current/voltage

Q 1: How much is the influence of neighboring masks?
Q 2: Can we predict the bandgap correctly?
Q 3: Can we design proper mask for desired performance?

Example PIC – An Array of SOA Integrated With Passive Waveguides

Bandgap helps determine operating wavelength, bias current/voltage
Outline

• Background
• Mechanism of Selective Area MOVPE
• Model of SA-MOVPE
• Simulation Parameters
• Simulation of Bulk and Quantum Wells
  – Arrayed mask
  – Step mask
  – Tapered mask
• Parameter Dependence and Accuracy
• Conclusion
Mechanism of Selective Area MOVPE

Causes → Effects
No growth on the SiO₂ masks → Concentration gradient of growth precursors
Concentration gradient → Lateral and surface diffusion
Near mask, an extra supply of ingredient → Increased growth rate
Indium reacts more easily than Galium → In-richness causes smaller bandgap (red-shift)
Quantum wells gets thicker → Lower quantum levels (red-shift)
Assumptions

• Only gas phase diffusion is considered, because surface diffusion is limited to only few µm from mask edge
• No selectivity for group V elements, only group III dominates
• Surface reaction rate independent of V/III ratio and As/P ratio
• Constant temperature across the region → Uniform rate of diffusion
• No crystal orientation dependence
• Mask silica is thin
• Boundary condition
  – At sufficient height from substrate, concentration is constant
  – On the masked area, flux is zero (no growth)
  – On the growth area, flux is proportional to concentration of species
Model of Growth Region

Satisfies Diffusion equation and Fick’s law

Parameter definitions:
- $C$ = group III precursor concentration
- $D$ = diffusion constant of precursor in $H_2$
- $k_s$ = surface reaction rate constant
- $C_0$ = normalized constant concentration

MOVPE Reactor: AIX 200/4, Pressure=$10^4$Pa, $T=883K$

<table>
<thead>
<tr>
<th>Precursor</th>
<th>Gas Phase Diffusion Constant $D$ [m$^2$s$^{-1}$]</th>
<th>Surface Reaction Rate Constant $k_s$ [ms$^{-1}$]</th>
<th>$D/k_s$ [µm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Indium (CH$_3$In)</td>
<td>$2.98 \times 10^{-03}$</td>
<td>41.97</td>
<td>71</td>
</tr>
<tr>
<td>Galium (CH$_3$Ga)</td>
<td>$2.67 \times 10^{-03}$</td>
<td>23.41</td>
<td>110</td>
</tr>
</tbody>
</table>


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Width of growth window: 20µm
Mask width: 20, 30, 40, 50µm
Mask-to-mask distance: 20 to 300µm
Concentration Distribution of Growth Species

- Finite Element Method analysis done by using commercial 3D finite element solver*
- Concentration is calculated separately for Ga and In precursors
- Symmetry and adaptive mesh used for fast calculation and accuracy

(*FEMLAB by Comsol Inc.)
GRE (Growth Rate Enhancement)
For modeling of $\text{In}_{1-x}\text{Ga}_x\text{As}_y\text{P}_{1-y}$ ...

- $y = y_{\text{planar}}$ (group V does not show much selectivity)
- For group III
  - Growth Rate Enhancement
    $\text{GRE} = (\text{GR of masked area})/(\text{GR of planar area})$
  - calculated from the concentration on the surface
  - Ga composition $x$ is taken as:
    \[
    x = \frac{E_{Ga}x_0}{E_{Ga}x_0 + E_{In}(1 - x_0)}
    \]
    - $E_{Ga}$, $E_{In}$ : GRE of Ga, In
    - $x_0$ : Ga composition sufficiently far from the mask
- Bandgap is calculated from the composition $(x, y)$:
  \[
  E_g = 1.35 + 0.668x - 1.068y + 0.758x^2 + 0.078y^2 - 0.069xy - 0.322x^2y + 0.03xy^2
  \]
Consideration of Strain and Quantum Level

• Compensation for biaxial strain

\[ \Delta E_g = -2A \frac{C_{11} - C_{12}}{C_{11}} \Delta a + B \frac{C_{11} + 2C_{12}}{C_{11}} |\Delta a| \]

• Calculate the quantum levels by solving the Schrödinger Eq. for C.B. and V.B.

\[
\begin{align*}
\left[ E_C^B - \frac{\hbar^2}{2m_B} \nabla^2 \right] \psi(r) &= E \psi(r) \\
\left[ E_C^W - \frac{\hbar^2}{2m_W} \nabla^2 \right] \psi(r) &= E \psi(r)
\end{align*}
\]

• Composition dependence of the parameters

• Photoluminescence peak wavelength was estimated from the bandgap and compared with measured values
When strain relaxation is assumed, better agreement is achieved with experimental data.
Simulation for Quantum Well

Scan direction

D/ks_Ga=110, D/ks_Ga=71
D/ks_Ga=110, D/ks_Ga=50
Measured

Position Along Growth Region [µm]
PL Peak Wavelength [nm]
Strain Relative to InP [ppm]

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Effect of Mask-to-Mask Distance

Stronger influence of neighboring mask as the distance decrease

→ Can be useful to increase the bandgap shift

→ Qualitative agreement, discrepancy due to $D/k_s$ parameter
Bandgap Energy Distribution in Other Mask Patterns

Designing for tailored device properties, such as bandwidth, uniformity of array and gradation of bandgap possible

Conclusions

- 3D and 2D modeling of selective area MOVPE by considering gas phase diffusion was done.
- Based on the concentration distribution, we estimated the composition, strain and bandgap of InGaAsP layers.
- For both quaternary bulk layer and QW, relatively fair agreement was achieved, even for complex masks.
- We can predict bandgap profile for arbitrary mask, as well as diffusion enhancement due to neighboring mask.
- Further improvements may be done with consideration of strain distribution.
The Parameter $D/k_s$

- $D$ : Diffusion constant [$m^2/s$]
  
  $$D = \frac{0.00266 T^{3/2}}{PM \sigma \Omega}$$
  
  (Chapman-Enskog Eq.)

- $k_s$ : surface reaction rate constant [$m/s$]

- $D/k_s$ is experimentally found from binary (GaAs and InP) growth

- $k_s$ can be estimated (a function of precursor type and temperature)

Arrhenius plot of $k_s$ for group III precursors (TMI and TMGa)