Modeling nanoscale device physics in COMSOL Multiphysics

Figure 1: HREM images of [0001] GaN QDs covered with various AlN spacers (in monolayers). Note the thin GaN layer above the spacers to visualize them. Inset: perfect dot wetting is shown for 4MLs AlN coverage. Smoothening of AlN layer is observed for 14MLs coverage.

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Many factors affects confinement

- Possible causes
  - Defects
  - Temperature
  - Stress effects
- Nanoscale devices are very sensitive to other effects.
- Need to quickly incorporate other physics in simulations

GaN quantum dot
Plan of the talk

• Motivation
• Using GaN Quantum dots for sensing:
  – How can we tune them?
• GaN Quantum dot system
  – Basic physics of Quantum dot
  – Simulation results
  – Effect of defects and temperature
  – COMSOL handles these problems in a natural fashion
• Conclusions and future work
  – Nano devices need other physics
  – Present day device simulators are hard to customize
Motivation

- GaN LEDs have caused a great deal of interest in GaN optical properties.
- Nanoscale device simulation needs to incorporate many physical models.
- Simulation tools are lagging behind
  - No easy way incorporate different physics: temperature, stress.
  - Quantum devices need new transport models
  - Self-consistent solutions for very large systems
  - Multiphysics approach needed.
Basics of quantum dots

- 3D confinement (like a finite 3D well)
- Small bandgap dot surrounded by a larger one (GaN dot in AlN matrix)
- Excitons generated inside the quantum dot
- Discrete energies

<table>
<thead>
<tr>
<th>Structure</th>
<th>Degree of Confinement</th>
<th>( \delta(E) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk Material</td>
<td>0D</td>
<td></td>
</tr>
<tr>
<td>Quantum Well</td>
<td>1D</td>
<td>1</td>
</tr>
<tr>
<td>Quantum Wire</td>
<td>2D</td>
<td></td>
</tr>
<tr>
<td>Quantum Dot</td>
<td>3D</td>
<td></td>
</tr>
</tbody>
</table>
Structure of GaN quantum dot

- Conical dots have been shown to be grown by MBE
- GaN dots separated by AlN spacers
- Size is assumed to be 2 times Bohr radius
- Conical dot
- Height of cone 2nm
- Symmetry in the structure
• Use PDE mode, coefficient form
• Solve the single band Schrödinger equation
• Solve for lowest energy \( l=0 \)
• Get solutions for first 2 eigenvalues
Some solutions corresponding to $l=0$

- Confinement is almost 80% in unperturbed dot system
Band bending due to spontaneous e-field

- Polarization charge at the AlN/GaN interface bends the bands.
- This changes confinement
- Could enhance or degrade confinement
Band bending results

- Finite well could bend into triangular well due to surface charge
- Confinement reduces by 60% due to band bending
Temperature dependent bending

- Bandgaps reduce due to temperature.
- Couple with surface charge induced band bending
- Affects confinement adversely 65 % confinement
Conclusions

- Confinement gets adversely affected by external factors
- Coupling temperature, stress and charge effects is easy in COMSOL
- To improve efficiency of nanoscale devices (QDs) we need better understanding of the coupled physics
- Coupling temperature, stress and charge effects is easy in COMSOL
- Making better nanoscale devices needs incorporation of many physics.