Modeling nanoscale device physics in COMSOL Multiphysics

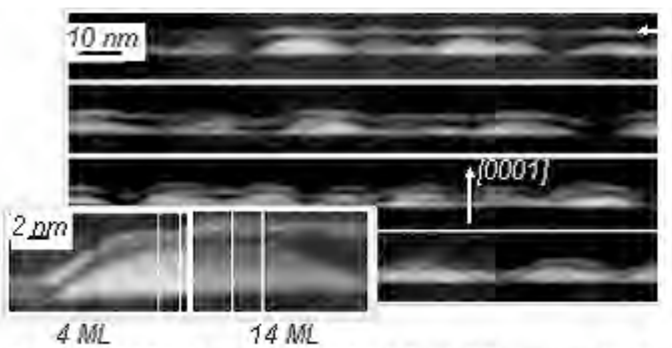
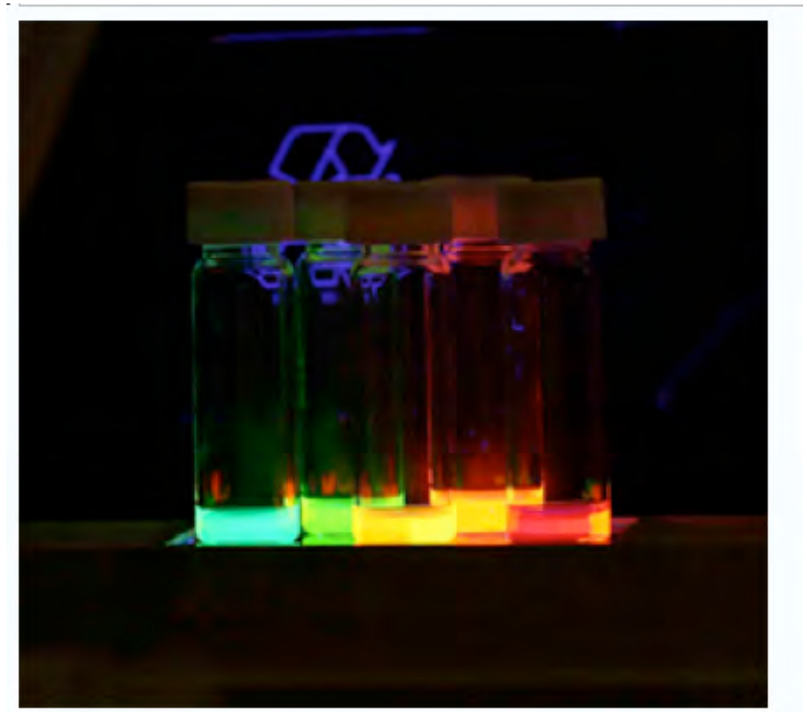


Figure 1 :HRTEM images of [0001] GaN QDs covered with various AlN spacers (in monolayers). Note the thin GaN layer above the spacers to visualize them. Inset : perfect dot wetting is shown for 4MLs AlN coverage. Smoothing of AlN layer is observed for 14MLs. coverage



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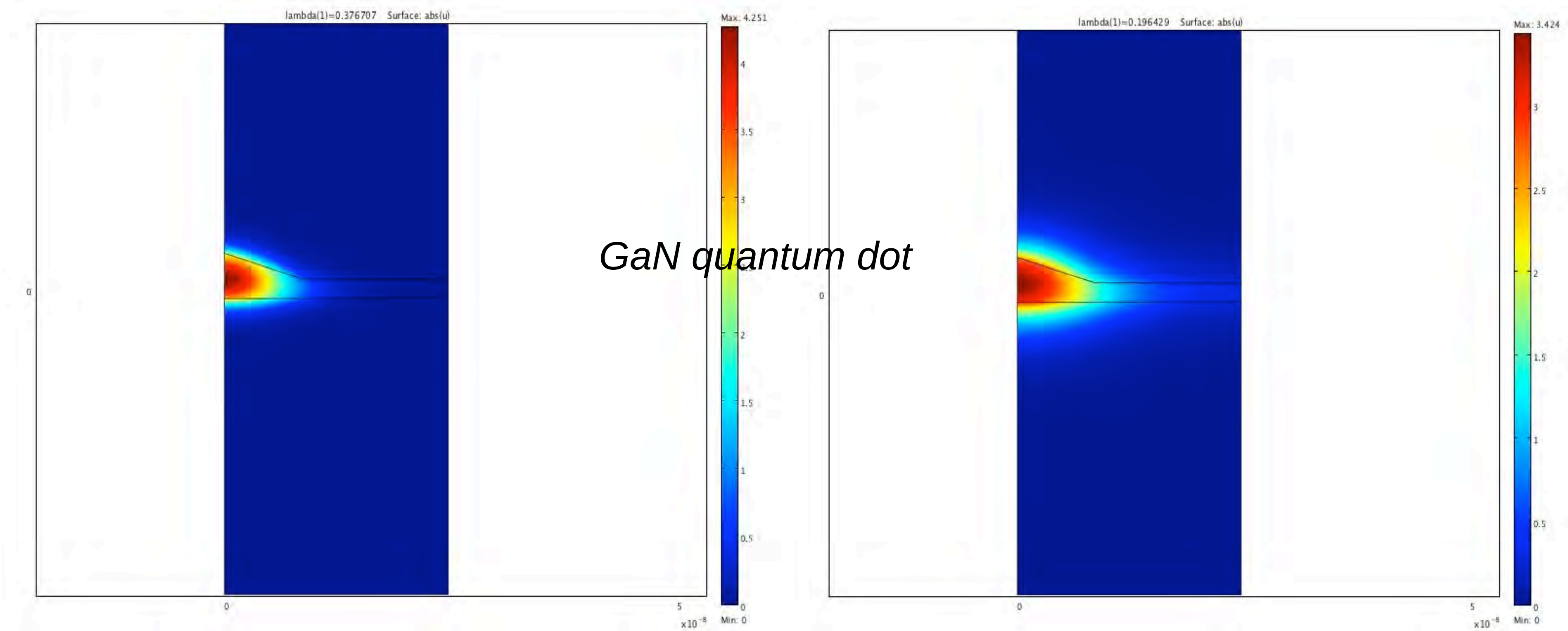
Many factors affects confinement



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

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

Structure	Degree of Confinement	
Bulk Material	0D	
Quantum Well	1D	1
Quantum Wire	2D	
Quantum Dot	3D	δ(E)

- 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

Structure of GaN quantum dot

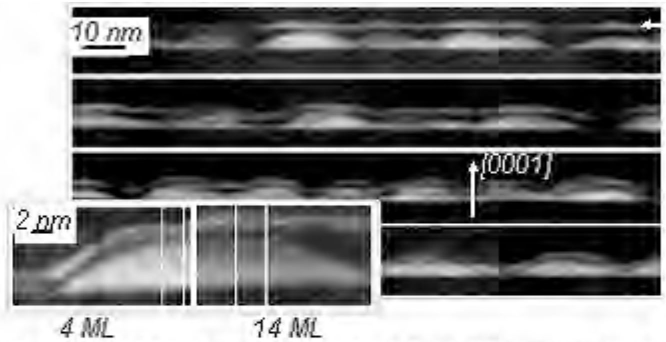
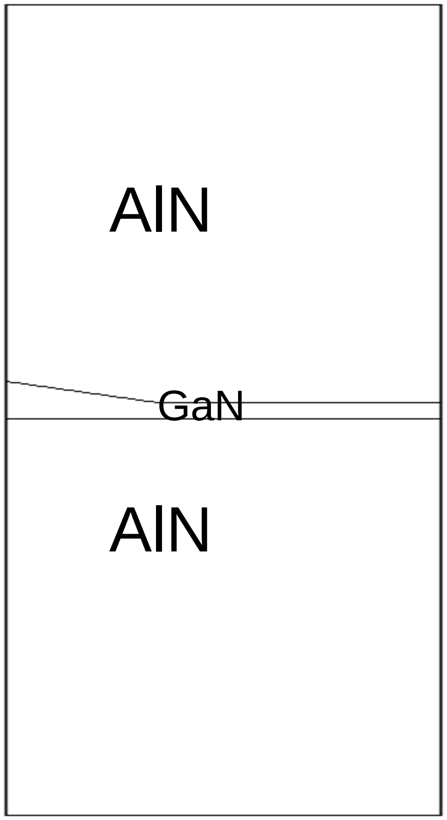


Figure 1 :HRTEM images of [0001] GaN QDs covered with various AlN spacers (in monolayers). Note the thin GaN layer above the spacers to visualize them. Inset : perfect dot wetting is shown for 4MLs AlN coverage. Smoothing of AlN layer is observed for 14MLs. coverage

- 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

COMSOL details-1



- Conical dot
- Height of cone 2nm
- Symmetry in the structure

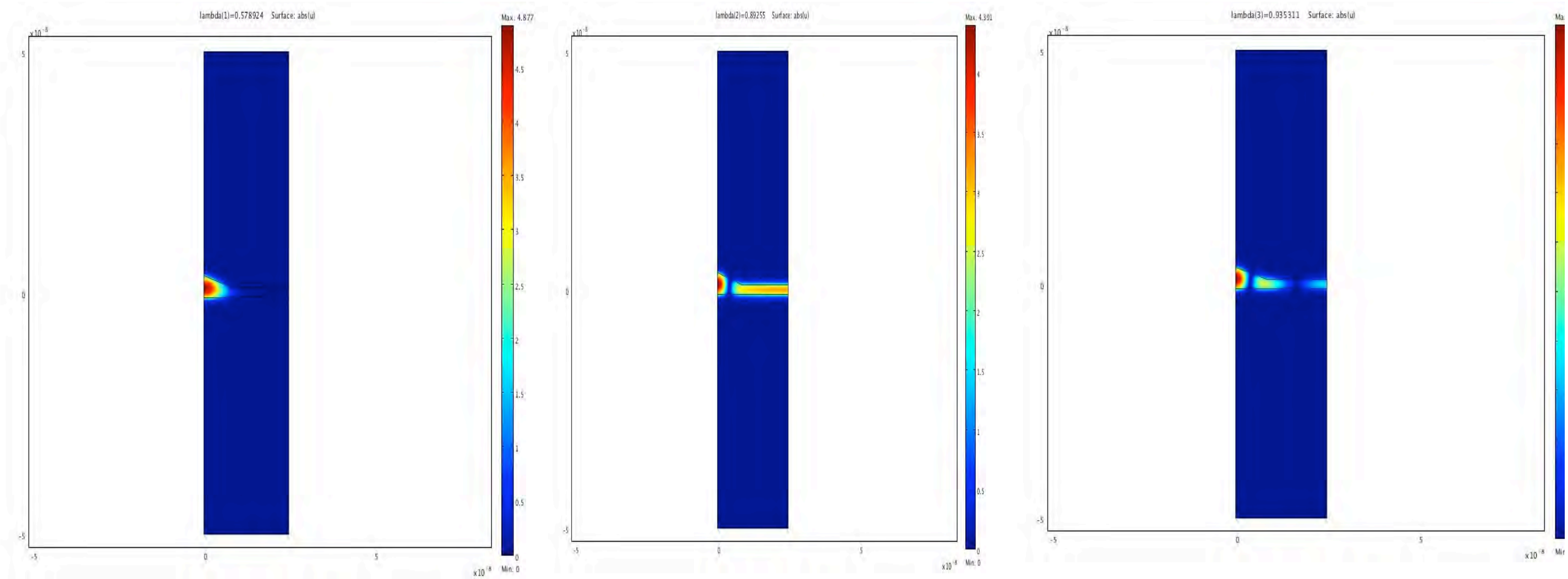
COMSOL details-2

$$-\frac{h^2}{8\pi^2}\frac{\partial}{\partial z}\left(\frac{1}{m_e}\frac{\partial\chi_l}{\partial z}\right)-\frac{h^2}{8\pi^2}\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e}\frac{\partial\chi_l}{\partial r}\right)+\frac{h^2}{8m_e\pi^2}\frac{l^2}{r^2}\chi_l+V_e\chi_l = E_l\chi_l$$

$$\nabla\cdot((-c\nabla u-\alpha u+\gamma)+a u+\beta\cdot\nabla u) = d_a\lambda u$$

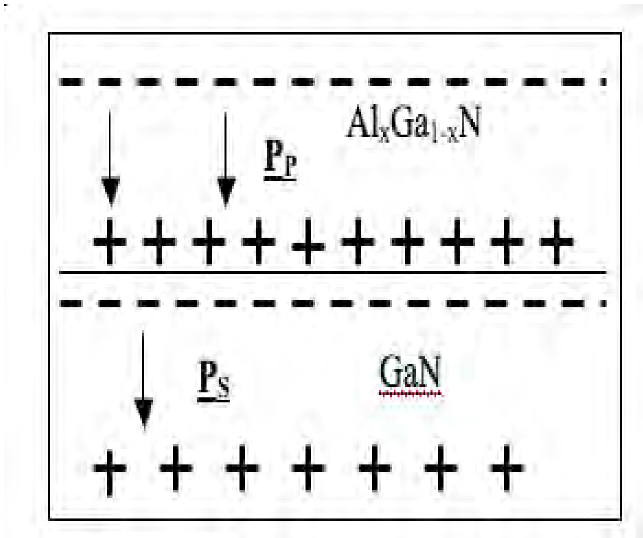
- Use PDE mode, coefficient form
- Solve the single band Schrödinger equation
- Solve for lowest energy l=0
- Get solutions for first 2 eigenvalues

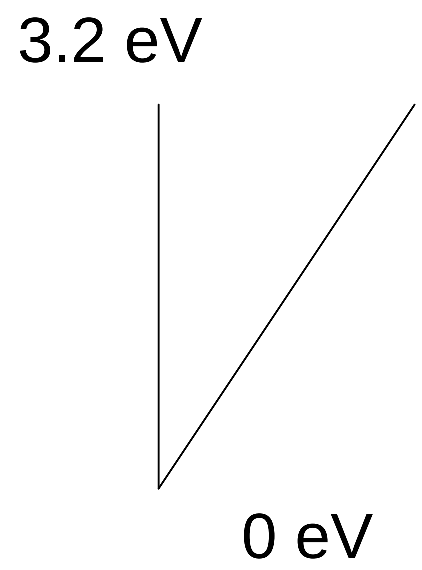
Some solutions corresponding to l=0



- Confinement is almost 80% in unperturbed dot system

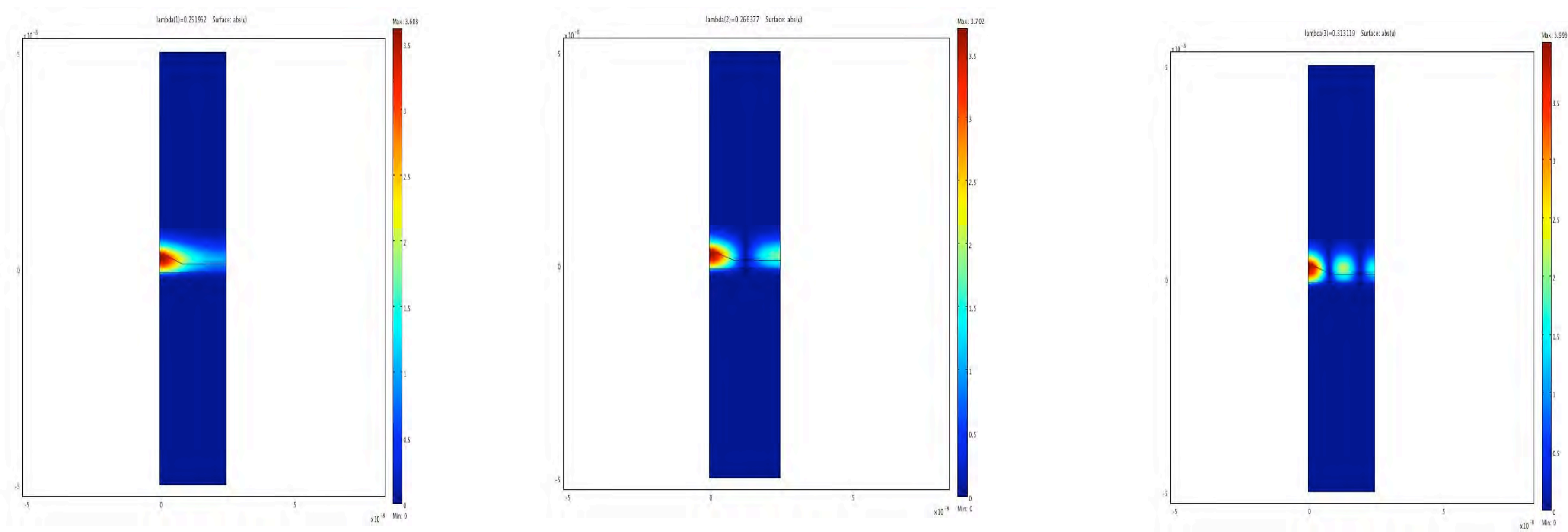
Band bending due to spontaneous e-field





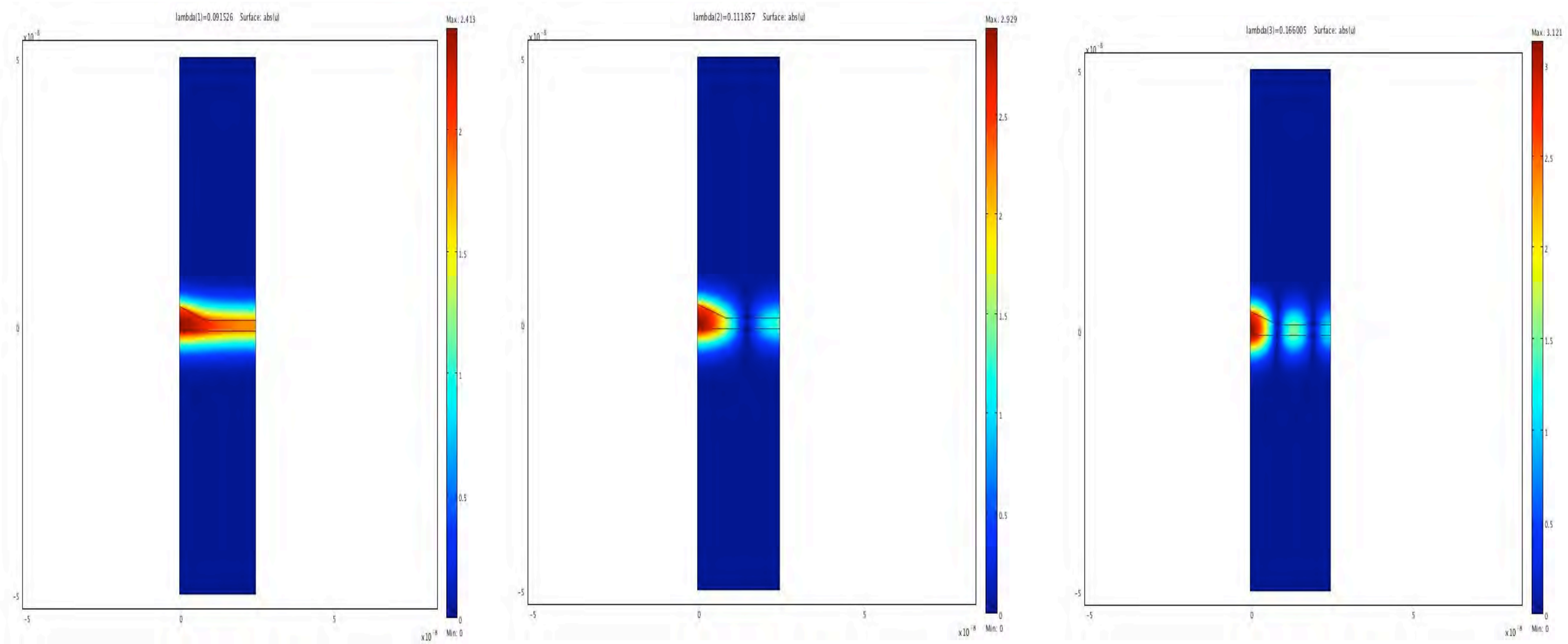
- Polarization charge at the AlN/GaN interface bends the bands.
- This changes confinement
- Could enhance or degrade confinement

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.