Nanorod Visualizations

November 1, 2010

1 Volumetric Visualization of Electric Field Magnitude

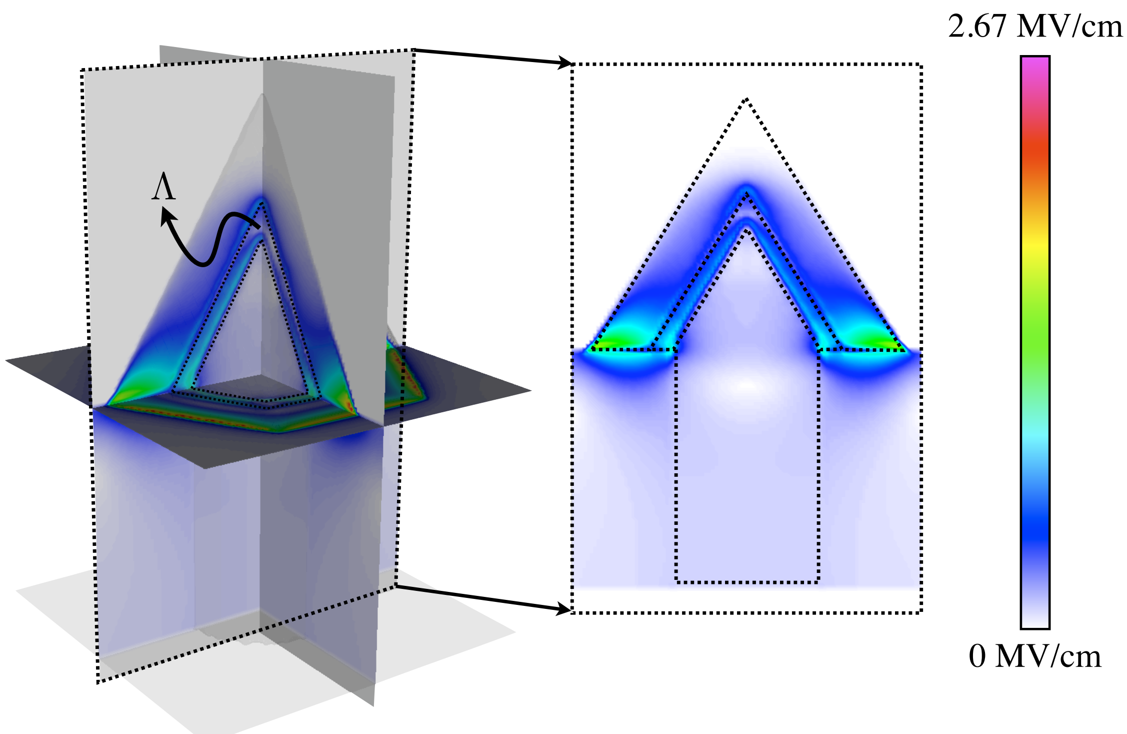

Figure 1: Electric field magnitude distribution in three dimensions. Region Λ is the low electric field region that is preferred for electron-hole recombination.

The electric field magnitude is obtained from "ElectricField.txt" according to:

$$|E| = \sqrt{E_x^2 + E_y^2 + E_z^2} \tag{1}$$

In all data files, the components of 0, 1 and 2 correspond to the coordinates of x, y and z.

1. Volumetric visualization of $|E|$ in the entire nanorod.

2. Zoom-in inset of the cross-section that emphasizes the Λ region.

3. Zoom-in inset of the cross-section that shows the high $|E|$ at the bottom of the pyramid.

2 IsoSurface of Electric Field Magnitude within the Quantum Well Region

Quantum well region is defined with $ID = 4$ ("microID.txt").

1. Show different layers of $|E|$ values within the quantum well region.

2. Show 3D Λ region.

3 Streamlines of Electric Field

Streamlines seedings are placed at $z = 5 \times 10^{-8}$, $z = 9 \times 10^{-8}$ and $z = 1.2 \times 10^{-7}$ ("microID.txt"). Both the streamlines of $+\vec{E}$ and $-\vec{E}$ are needed.

4 Stress Tensor

Stress tensor has the following form:

$$\overleftrightarrow{\sigma} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{xy} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{xz} & \sigma_{yz} & \sigma_{zz} \end{bmatrix} \tag{2}$$

The stress components can be found in "Stress.txt". The hydrostatic stress is calculated as:

$$\sigma_h = \frac{1}{3} \left(\sigma_{xx} + \sigma_{yy} + \sigma_{zz} \right) \tag{3}$$

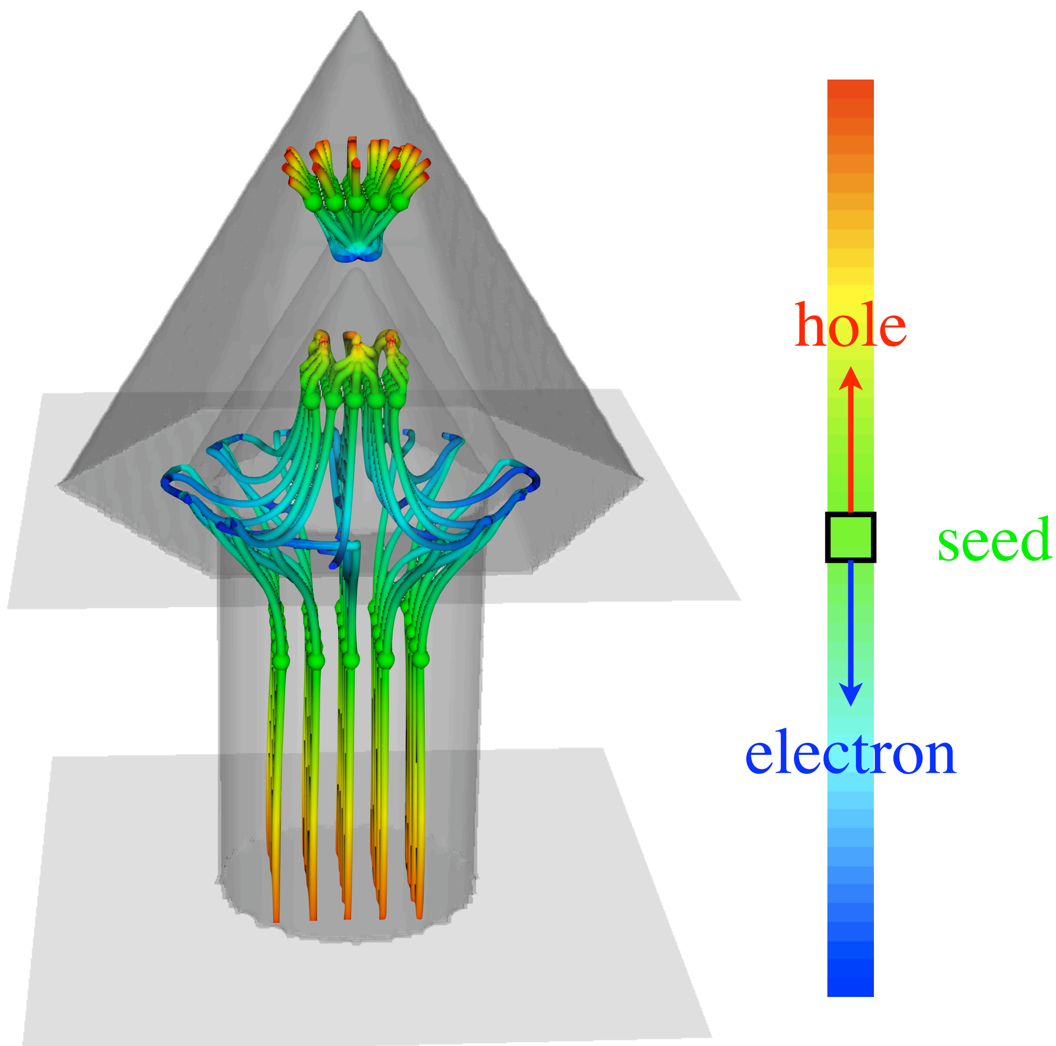

Figure 2: Electric field streamlines seeded (a) within the GaN pyramidal base and (b) within the GaN cap. The streamlines for $+\vec{E}$ correspond to the path along which holes are driven by the internal electric field, while the streamlines for $-\vec{E}$ correspond to electrons path. In order to maximize recombination in region Λ (see Figure 1), the results suggest p-type base and n-type cap.

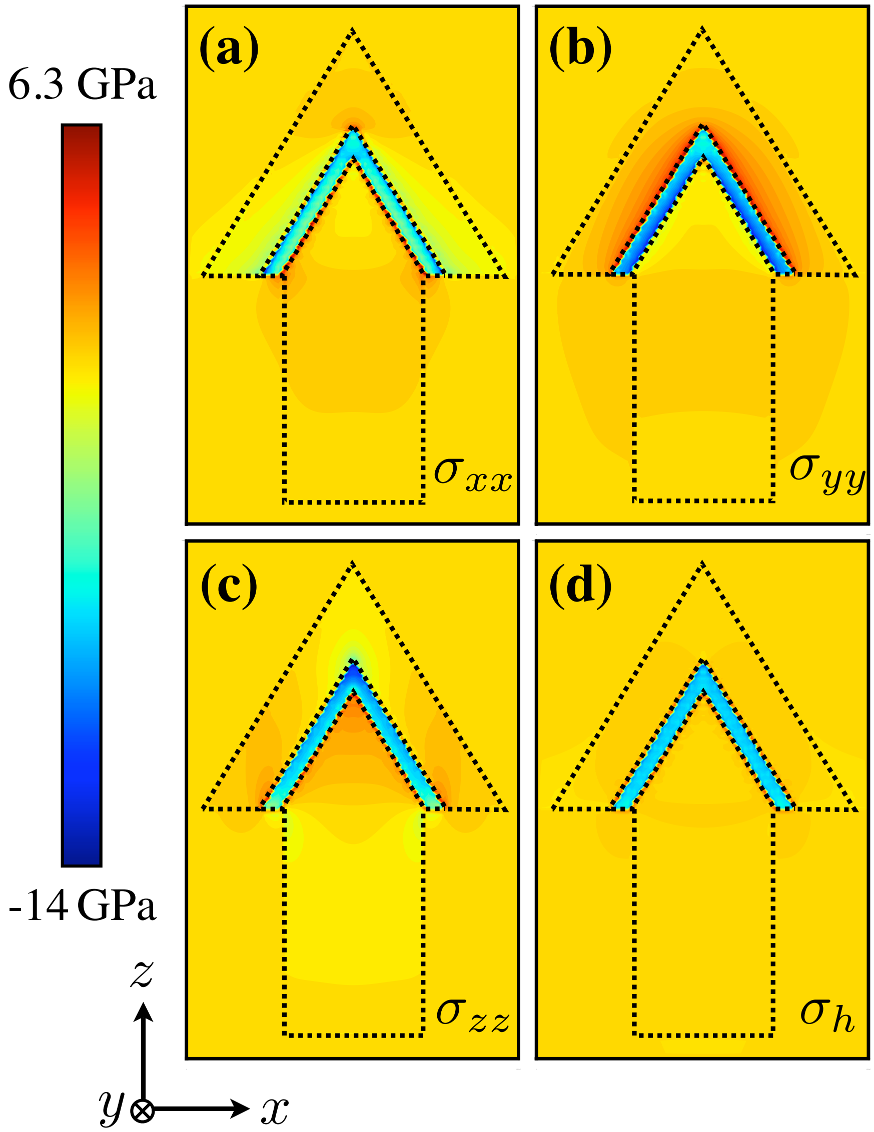

Figure 3: The cross-sectional distributions of stress components, (a) σ_{xx}, (b) σ_{yy}, (c) σ_{zz} and (d) hydrostatic stress, σ_h, for the nanorod structure.

1. Volumetric visualization of σ_{xx}, σ_{yy}, σ_{zz} and σ_h are needed.

2. Stress fields should emphasize the negative values within the quantum well region.

3. Visualization of σ_{zz} should clearly show the variation around the tip of the quantum well.

4. Negative, positive and zero stress levels are to be identified clearly.

5 Polarizations

The vector of total polarization have three contributions: dielectric, spontaneous, and piezoelectric polarizations:

$$P^{total} = P^{dielectric} + P^{spontaneous} + P^{piezoelectric} \tag{4}$$

in which P^{total} is found in “TotalPolarization.txt”, $P^{spontaneous}$ is found in “SpontaneousPolarization.txt”, $P^{piezoelectric}$ is found in “PiezoelectricPolarization.txt”. So, $P^{dielectric}$ can be obtained. The z components of these polarizations, *i.e.*, the third column, are of interest.

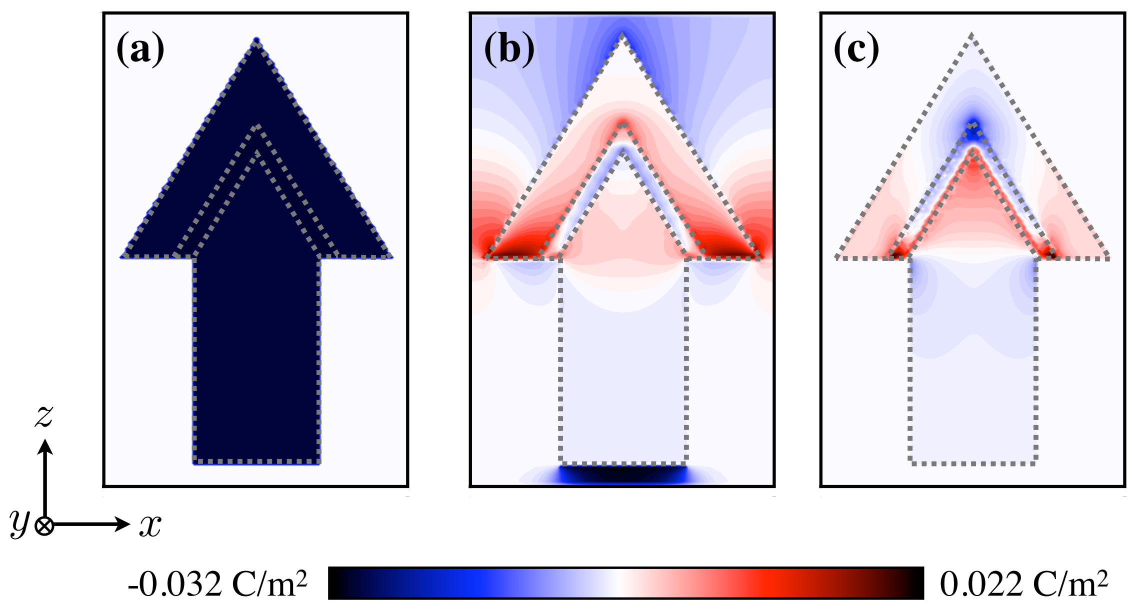

Figure 4: Distributions of polarizations (z component) contributed from (a) spontaneous polarization, (b) dielectric polarization, and (c) piezoelectric polarization.

1. Volumetric visualizations of $P_z^{dielectric}$, $P_z^{spontaneous}$ and $P_z^{piezoelectric}$ are needed.

2. Should emphasize the negative, positive and zero values of these polarization fields.

3. Show clearly that $P_z^{spontaneous}$ does not vary much, while $P_z^{dielectric}$ and $P_z^{piezoelectric}$ have large spatial variation and similar trends.

6 Truncated Pyramid

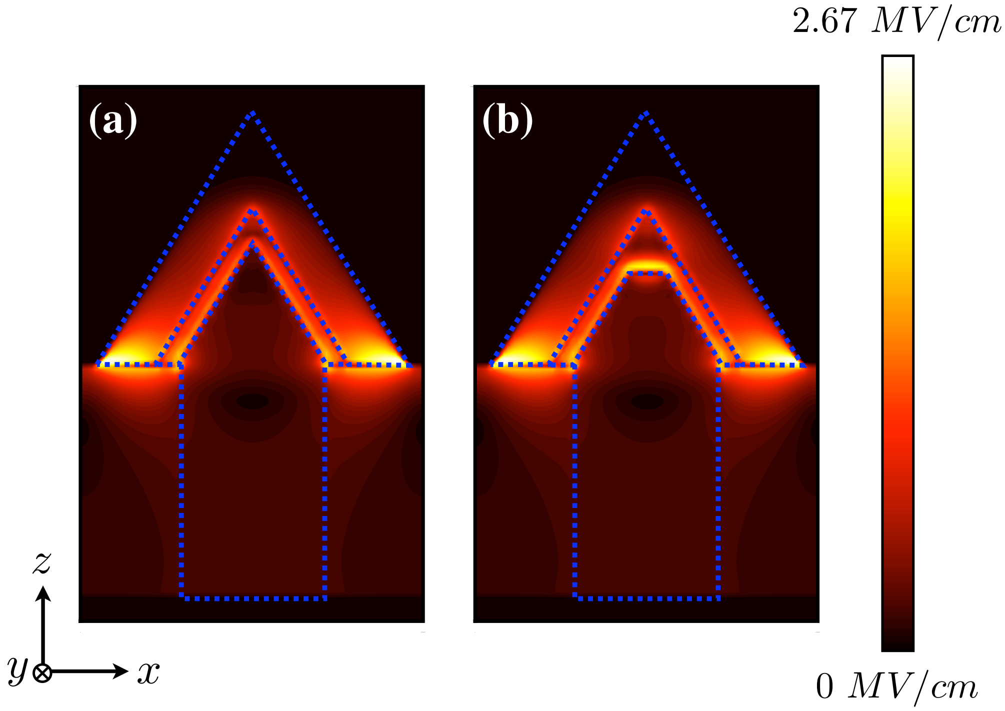

Figure 5: Cross-sections of electric field magnitude distribution for (a) sharp pyramidal nanorod and (b) truncated pyramidal nanorod.

Electric field magnitude of the truncated pyramid geometry shows a different low $|E|$ region that shaped like the letter of A. It would be interesting to compare against the sharp pyramid. Possibilities:

1. IsoSurface of the low $|E|$ regions for these two geometries.

2. Volumetric visualization.