Landscape localization theory of disorder in nitride semiconductors alloys and application to LED simulations

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Outline

• Introduction
• Implementation details of using Localized landscape theory into Poisson and drift-diffusion method.
• Simulation results on LEDs
• Remained challenges
Introduction: LED modeling

Basic LED concept might be easy, which is composed of p-i-n junctions. But the real problem is complicated. We need to consider these effects simultaneously.

1. Carrier transport issues.
2. Design of QWs. (compositions, numbers, balance of carrier distribution.
3. Suppression of defects and dislocations.
4. Electron blocking layer or hole blocking layers (for AGIP red LED).
5. Current spreading issues...
6. Light extraction issues.
7. Thermal managements.
8. ...  

For a better LED design, we need to improve all of them at the same time since some factors are coupled together.

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Issues in solving LEDs with simple normal QW assumption

- The traditional Poisson and Drift-diffusion solver with normal QW gave us very large turn-on voltage due to the strong polarization, which is not observed in experiments.

Many simulation works suggest to use a smaller polarization <50% to make I-V fit, but emission spectrum and QCSE might be missed as well. Therefore, it is hard to further predict the device performance.
Random alloy distribution in InGaN QW

Atom Probe Tomography (APT) Analysis: Indium composition fluctuation in QW.

Atom probe tomography of an InGaN/GaN LED

Y-R. Wu et al., APL 101, 083505 (2012)

Question:

How does this indium fluctuation affect the carrier transport behavior?

Multi-dimensional Scaling issues in device modeling

• How to compromise between Macroscopic model and microscopic scale factors?
  - parameters, simulation domains, ...

• Speed issues... For engineers, they don’t have time (days, months) to wait for just a simulation result.

• Accuracy....is the most important and a hard factor to consider...
Issues and Challenges

• Quantum models (atomistic or empirical) are usually used to calculate emission or absorption material properties.

  (1) Impractical for the full structure LED & injection & I-V curve with self-consistent solution. (2) difficulties in coupling with drift-diffusion

Multi-dimensional (E & X,Y,Z) & recombination, phonon scattering, impurity mechanism -> time consuming and convergence issues

• Quantum transport models such as NEGF are good to describe quantum effects such as tunneling which are absent from DD models.
Bohm’s quantum potential as an internal energy (PRB 85, p166, 1952) was proposed to be used as effective quantum potential seen by carrier.

\[
\psi = \psi(r, t) \text{ in physical space, } \mathbb{R}^3 \text{, is governed, in non-relativistic quantum mechanics, by the Schrödinger equation}
\]

\[
\frac{ih}{\partial t} \psi(r, t) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r, t) + V(r, t) \psi(r, t).
\]

Writing the wave function in polar form \( \psi(r, t) = R(r, t)e^{iS(r, t)/\hbar} \), and defining the quantum potential

\[
Q(r, t) = -\frac{\hbar^2}{2m} \frac{\nabla^2 R(r, t)}{R(r, t)}
\]

this equation is mathematically equivalent to the system of real equations


1. Get all eigen energies and wave functions \( R_i \)

2. \[ n = \sum f_i R_i^2 \]

2. The effective quantum potential can be described by

\[
Q_{\text{eff}} = -\frac{\hbar^2}{2} \left[ \frac{\nabla (M^{-1} \nabla n)}{2n} - \frac{\eta \nabla n \cdot M^{-1} \cdot \nabla n}{4n^2} \right] = -\frac{\hbar^2}{2} \gamma \frac{\nabla [M^{-1} \nabla (n^\alpha)]}{n^\alpha}. \tag{2}
\]

where we have defined the two parameters

\[
\gamma \equiv \frac{\sum_i \nabla [M^{-1} \nabla (f_i R_i^2)]}{\nabla [M^{-1} \nabla (\sum_i f_i R_i^2)]}, \quad \text{and}
\]

\[
\alpha \equiv 1 - \frac{1}{2} \sum_i f_i R_i^2 \left[ \sum_i f_i \nabla [M^{-1} (R_i^2)] \right] \sum_i \frac{f_i \nabla (R_i^2) M^{-1} \nabla (R_i^2)}{R_i^2}. \tag{3}
\]

\( Q_{\text{eff}} \) (effective quantum Potential)

New effective Q makes DD works, but it is **time consuming**, you need to solve eigen values and eigen functions!

Localized landscape model provides a quick path toward a full device modeling

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A new approach: a mathematical theory of localization applied to LEDs

Universal mechanism for Anderson and weak localization


Schrödinger equation

\[ (-\Delta + V)\psi = E\psi \text{ in } \Omega, \quad \psi|_{\partial\Omega} = 0 \]

Landscape equation

\[ (-\Delta + V)u = 1 \text{ with } u|_{\partial\Omega} = 0 \]

Much simpler
Much faster to calculate

InGaN QWs

Eigenmodes

Landscape \( u \)

Valleys network

\( \text{n-GaN} \) electrons

\( \text{p-GaN} \) holes

Photons
Comparison between traditional Poisson and Poisson-Schrodinger solver.

Comparison between 1/u- Poisson-DD solver and Poisson-Schrodinger solver.

1D comparison of carrier density from Schrodinger and landscape model. **Very good approximation!**
Further application of localized landscape theory

We further apply the landscape theory in the design of type II super lattice Infrared detector

With landscape theory to get the effective potential, we can couple it into 2D Poisson and drift-diffusion solver and obtain the responsivity curve directly. (Without landscape theory, it looks like multi-barriers)
We found that with a proper assumption, the application potential will not be only limited in studying the randomized system but some quantum structure studies, with a more efficient tool to assist engineers in device designs.
Target

Disorder effects: Localization & delocalization (quantum effects)

A fast solver ($Hu=1$, localization landscape) to include quantum effects

Transport issues: carrier injection and screening

- Overall studies from the fundamental material properties to the biasing device performance in a self-consistent framework.

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Methods

Generation of composition map

Mapping of Composition map into FEM solver

- Solve strain-stress equation
  \[ \mathbf{P}^{pz} = \varepsilon \cdot [\varepsilon] \]
  \[ \nabla \cdot \mathbf{P}_{\text{total}}(\mathbf{r}) = \rho_{\text{pol}}(\mathbf{r}) \]

- Solve Poisson equation
  \[ \nabla \cdot (\varepsilon \nabla \varphi) = q(n - p + N_A^- - N_D^+ \pm \rho_{\text{pol}}) \]

- Solve landscape equation
  \[ (-\frac{\hbar^2}{2m_{\text{e,h}}} \Delta + E_{e,h}) u_{e,h} = 1 \]

- Solve drift-diffusion equation
  \[ J_n = n \mu_n \nabla E_{F_n} \]
  \[ J_p = p \mu_p \nabla E_{F_p} \]

Get \( \psi_e, \psi_h \), eigen values with Schrodinger solver?
  Get I-V, IQE,

Converged?
  Yes, output converged profiles

No
Method for generating random alloy compositions

- Decide that each atom mesh grid is an In or Ga atom by using random number generator (rnd())
- Use Gaussian weighting to determine the In composition of each atom mesh grid.

\[
I(r_i) = \frac{\sum_j \text{atom}(j) \times e^{-\frac{(r_j-r_i)^2}{2\sigma^2}}}{\sum_j e^{-\frac{(r_j-r_i)^2}{2\sigma^2}}}
\]

This part has been discussed for many times that how the \( \sigma \) was decided. Since the empirical Schrodinger equations was used, we cannot choose single atom as a digital composition map. This may rely on TBM method for a correction. (See Schulz’s talk). Right now \( \sigma = 2a \) gives a better fit in emission and absorption (PRB paper II)
• Use 3D interpolation to fit into the FEM (Finite element method) mesh grid.

The atom composition map’s grid size is different from the FEM’s grid site, the linear interpolation is used to map the grid.
Method for strain calculation

\[ \sigma_{ij} \text{ is the shear stress} \]

\[
\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} + f_x = 0 \\
\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + f_y = 0 \\
\frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} + f_z = 0 
\]
Method for strain calculation

$$\sigma = [\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{zx}, \sigma_{xy}]^T$$

$$\varepsilon = [\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{yz}, \varepsilon_{zx}, \varepsilon_{xy}]^T$$

$$\sigma = D\varepsilon$$

$$D = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{pmatrix}$$

$$\varepsilon = \left[ \frac{\partial u}{\partial x}, \frac{\partial v}{\partial y}, \frac{\partial w}{\partial z}, \frac{\partial v}{\partial z}, \frac{\partial w}{\partial y}, \frac{\partial u}{\partial x}, \frac{\partial v}{\partial y} + \frac{\partial w}{\partial x}, \frac{\partial u}{\partial y} + \frac{\partial w}{\partial x}, \frac{\partial v}{\partial x} \right]^T$$

Rayleigh-Ritz method is used to solve the strain problem. And the displacement vector is used as the variable to solve the problem.

The external force $f$ is zero. However, the periodic boundary on the sidewall and fixed boundary on the bottom referred to buffer layer lattice (GaN buffer) is used in InGaN LED simulations.
Strain assuming fully strain according to composition without solving strain solver

\[ \varepsilon_{xx} \text{ and } \varepsilon_{yy} \]

fully strain

\[ \varepsilon_{xx} \text{ and } \varepsilon_{yy} \]

3D FEM

\[ \varepsilon_{yy} \]

3D FEM

In addition, the shear strain is also not zero. The program will obtain the strain \( \varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{yz}, \varepsilon_{zx}, \varepsilon_{xy} \ldots etc \ldots \)
After the strain was obtained in the system, we can calculated the piezoelectric field by

\[
P^{pz} = \begin{pmatrix}
0 & 0 & 0 & 0 & e_{15} & 0 \\
0 & 0 & 0 & e_{15} & 0 & 0 \\
e_{31} & e_{31} & e_{33} & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
e_{xx} \\
e_{yy} \\
e_{zz} \\
e_{yz} \\
e_{xz} \\
e_{xy}
\end{pmatrix} =
\begin{pmatrix}
e_{15}e_{xz} \\
e_{15}e_{yz} \\
e_{31}(e_{xx} + e_{yy}) + e_{33}e_{zz}
\end{pmatrix}
\]

\(P\) is equal to the dipole moment, with Gauss’s Law, We know that

\[\nabla P = \rho_{pol}\]

\(\rho_{pol}\) is the polarization charges, which will appear if the polarization is varying in space.
Poisson Equations:

Solve strain-stress equation

\[ \mathbf{p}^{zz} = \mathbf{[e]} \cdot \mathbf{[e]} \]
\[ \nabla \cdot \mathbf{p}_{\text{total}}(\mathbf{r}) = \rho_{\text{pol}}(\mathbf{r}) \]

\( \Rightarrow \mathbf{p}_{\text{pol}} \)

Solve Poisson equation

\[ \nabla \cdot (\varepsilon \nabla \varphi) = q(n - p + N_{a}^{-} - N_{d}^{+} \pm \rho_{\text{pol}}) \]

Solve landscape equation

\[ \left( -\frac{\hbar^{2}}{2m_{e,h}} - \Delta + E_{c,h} \right) \psi_{e,h} = 1 \]

Solve drift-diffusion equation

\[ J_{n} = n \mu_{n} \nabla E_{F_{n}} \]
\[ J_{p} = p \mu_{p} \nabla E_{F_{p}} \]

Converged?

Yes, output converged profiles


Poisson Equations solve the potential if the charge distribution is well known

\[ \nabla \epsilon \nabla V = \nabla (\varepsilon \nabla (-E_{c}/q)) = q(n - p + N_{a}^{-} - N_{d}^{+} + \rho_{\text{pol}}) \]

However, in reality, \( n \) and \( p \) or even \( N_{a}^{-} \) and \( N_{d}^{+} \) are exponential function of \( E_{c} \) and \( E_{fn} \) and \( E_{fp} \). So it is actually a nonlinear equations

\[ n = \int_{E_{c}}^{\infty} \frac{N(E)}{1 + \exp \left( \frac{E - E_{fn}}{k_{B}T} \right)} dE = N_{c}F_{1} \left( E_{c}, E_{fn} \right) \]
\[ = N_{c}F'(E_{c}, E_{fn}) \exp \left( \frac{E_{fn} - E_{c}}{k_{B}T} \right) \]
\[ F' = 1 \text{ for Boltzmann approximation} \]

\[ p = \int_{-\infty}^{E_{v}} \frac{N(E)}{1 + \exp \left( \frac{E_{fp} - E}{k_{B}T} \right)} dE \sim N_{v}F'(E_{v}, E_{fp}) \exp \left( \frac{E_{v} - E_{fp}}{k_{B}T} \right) \]
Solve the Nonlinear Poisson Equation

\[ \nabla^2 E_c = -\frac{q^2}{\varepsilon} \left( N_c \exp\left( \frac{E_{fn}}{k_B T} \right) \exp\left( -\frac{E_c}{k_B T} \right) - N_v \exp\left( -\frac{E_{fp}}{k_B T} \right) \exp\left( \frac{E_v}{k_B T} \right) + N_B \right) \]

Note: \( E_v = E_c - E_g \)

\[ E_c = E_{c0} + \delta E_c \]

Assume that \( E_{fn} \) and \( E_{fp} \) are known, by one dimensional equation with an initial guess \( E_{c0} \)

\[ \exp\left( \frac{E_{c0} + \delta E_c}{k_B T} \right) = \exp\left( \frac{E_{c0}}{k_B T} \right) \exp\left( \frac{\delta E_c}{k_B T} \right) = \exp\left( \frac{E_{c0}}{k_B T} \right) \times (1 + \frac{\delta E_c}{k_B T}) \]

\[ \nabla^2 \delta E_c - \frac{q^2}{\varepsilon k_B T} N_c \exp\left( \frac{E_{fn}}{k_B T} \right) \exp\left( -\frac{E_{c0}}{k_B T} \right) \delta E_c \]

\[ = -\nabla^2 E_{c0} - \frac{q^2}{\varepsilon} \left( N_c \exp\left( \frac{E_{fn}}{k_B T} \right) \exp\left( -\frac{E_{c0}}{k_B T} \right) \right) \]

\( E_{c0} \) is an initial guess, known number, not a variable

Note: The nonlinear equation becomes a linear equation

Guess \( E_{c0} \) and then obtain \( \Delta E_c \), repeat the loop until \( \Delta E_c < \) tolerance value.

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According to the landscape equations, we need to solve

\[
\left( -\frac{\hbar^2}{2m^*_{e,h}} \nabla^2 + E_{c,v} \right) u_{e,h} = 1
\]

\(E_c\) and \(E_v\) can be obtained by Poisson solver. Then we can solve landscape equations to obtain the \(u_e\) and \(u_h\).

\[
n = \int_{1/u_c}^{\infty} LDOS_{3D}(E) \cdot \frac{1}{1 + \exp\left(\frac{E - E_{fn}}{K_B T}\right)} dE
\]

\[
p = \int_{-\infty}^{1/u_h} LDOS_{3D}(E) \cdot \frac{1}{1 + \exp\left(\frac{E_{fp} - E}{K_B T}\right)} dE
\]

\[
LDOS_{3D}(E) = \frac{\sqrt{2m^*_{e,h}}^{3/2}}{\pi^2 \hbar^3} \sqrt{E - 1/u_{e,h}}
\]
For the drift-diffusion solver

\[
J_n = -\mu_n n \nabla E_c - e D_n \nabla n = -\mu_n n \nabla E_{fn}
\]

\[
J_p = -\mu_p p \nabla E_v + e D_p \nabla p = -\mu_p p \nabla E_{fp}
\]

And again,

\[
\nabla J_{n,p} = \nabla (-\mu_n n \nabla E_{fn}) = q (R - G)
\]

\[E_c \text{ and } E_v \text{ are replaced by } 1/u_e \text{ and } 1/u_h\]

Please note that \(n\) and \(p\) are in the exponential form of \(E_c\), \(E_v\), \(E_{fn}\), and \(E_{fp}\). If we use \(n\) and \(p\) as variables, they change very fast in space even in a small \(\delta x\). It is very easy to get negative charge density if we directly use \(n\) as variable without proper treatment. Therefore, usually we need to treat it as nonlinear equation again, or use \textbf{Scharfetter-Gummel’s approximation} for carrier density treatment.
### Comparison table: computation time

<table>
<thead>
<tr>
<th>One Iteration</th>
<th>Node number (matrix size)</th>
<th>Computation time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D Poisson</td>
<td>428,655</td>
<td>25</td>
</tr>
<tr>
<td>3D Drift-diffusion (e &amp; h)</td>
<td>428,655</td>
<td>50</td>
</tr>
<tr>
<td>3D Localization landscape (e &amp; h)</td>
<td>428,655</td>
<td>50</td>
</tr>
<tr>
<td>Schrödinger (solving eigen values, over 100 states found)</td>
<td>428,655</td>
<td>63,650 (~18 hour)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>&quot;Self-consistent&quot; solver for 45 bias points</th>
<th>“Estimated” Total computation time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D Poisson-DD</td>
<td>54,000</td>
</tr>
<tr>
<td>3D Poisson-DD-Schrödinger</td>
<td>45,882,000 (~531 days!!)</td>
</tr>
<tr>
<td>3D Poisson-DD-1/u</td>
<td>90,000 (~1 day)</td>
</tr>
</tbody>
</table>

- **ARPACK** Eigen solver
- **PARDISO** sparse inverse solver
- **2 Intel Xeon E5-5650V2 8 cores 2.6 GHz** CPUs with 396 GB memory.
- The landscape model coupled to the Poisson-DD equations is much more computationally efficient with respect to state-of-the-art quantum solvers, while still incorporating quantum effects such as tunneling and quantum confinement. (1000X faster than Schrodinger eigen solver!!)
Outline

• Introduction
• Implementation details of using Localized landscape theory into Poisson and drift-diffusion method.
• Simulation results on LEDs
• Remained challenges
Effective Quantum potential

Smoothed & raised potential (quantum confinement in z direction)

- The landscape theory flattens the rapid fluctuations not “seen” by the quantum states of the disordered system.
- Quantum confinement manifests itself by the appearance of closed crest lines of the effective potential $1/u$, creating localization regions.
- Difference between the $E_v$ and $1/u_h$ maps is much smaller. (larger hole effective mass)

Holes are very localized due to random fluctuation

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• The current finds percolation paths through lower potential regions, enabling a decrease of the turn-on voltage.
• The existence of such percolation paths with high current densities is the basis of the reduced turn-on voltage caused by In fluctuations induced by disorder.

z-component current and the corresponding effective quantum potentials
Comparison of potential between different methods

The landscape model with random indium fluctuation accounts the quantization and tunneling effect, which will give a lower turn on voltage.
The classical Poisson-DD solver treats carriers as particles.

In the landscape model, quantum effects are included and the smoother effective potentials.

Better representative of the standing wave nature of the localized quantum states.
Modeling result on ideality factor (IF)

Ideal current density

\[ J \propto N_c N_v \exp \left( -\frac{E_g}{k_B T} \right) \exp \left( \frac{eV}{k_B T} \right) \]

\[ \approx n_i^2 \exp \left( \frac{eV}{k_B T} \right) \]

\[ IF = \frac{q}{k_B T} \frac{\partial V}{\partial \ln(J)} \]

- 1/u-Poisson-DD model including random alloy fluctuations provides an excellent overall description of the transport properties of LEDs.
Comparison of IF (n) to the published papers

\[ I = I_s \left[ \exp \left( \frac{V}{n k_B T} \frac{q}{n} \right) - 1 \right] \]

- The simulation of the trend of IF factor matches well with the experimental curve! (Note that experimental case has no EBL and only 5 QWs, which is not exactly the same as ours)


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Internal Quantum efficiency

- Peak IQE obtained from 1/u is slightly higher than the classical particle based Poisson-DD model on fluctuated QWs because of the more homogeneous in-plane radiative efficiency and carrier injection in each QW.

**Spreads out in the 1/u-Poisson-DD model**

![Graph showing IQE vs. Current density](image)

- **Poisson and drift-diffusion (50% pol. uniform QW)**
- **Poisson and drift-diffusion (fluc. QW)**
- **Poisson and drift-diffusion with 1/u (fluc. QW)***

![Map showing radiative recombination rate](image)

- **Radiative recombination rate** (cm^{-3}s^{-1})
  - 1x10^{22} to 2x10^{28}

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Green LED: Calculated I-V curve of 5 QWs

• In Green LEDs, the $P_{ez}$ in barrier is too high even with atom scale alloy fluctuation. Other possible percolation path needs to be explored. The accurate I-V curve is even harder to be obtained.
• A larger scale QW thickness fluctuation will be further considered.


No sheet resistance in simulation
A pure consideration of random alloy cannot explain the behavior of IV in green LED

In green LED, larger scale fluctuation is also observed

The larger scale fluctuation may come from (1) dislocation (2) V-pits (3) strain relaxation region .....
Influences on bowing terms choices

The bandgap of alloy is decided by 

\[ E_{g In_x Ga_{1-x}N} = x E_{g InN} + (1 - x)E_{g GaN} + b(1 - x)x \]

1. The bowing term is “b”. In different references, the bowing term varies from -1.4eV \(^1\) to -2.3eV \(^2\).

2. For QW=3nm emitting at green wave length ranges, the APT results show that average indium composition is around 20% to 24%.

3. \(b=2.3\) eV might give a better fitting, we will use \(b=-2.3\) eV for later studies.

4. We need to better calibration of Indium composition versus \(E_g\) in bulk material to avoid QC effects.

\(^2\) Miguel A. Caro PRB 88, 214103 (2013)
Indium map and Emission peak of the thickness fluctuation model

This is the emission peak of the thickness fluctuation model

- QW thickness 3nm,
- $L_A$ width is 150 nm,
- $L_B$ width is 30 nm
- $h = 0.849$nm.

- In addition, the In average composition peak of $L_A$ and $L_B$ are 21.59% and 11.95%, respectively.
Indium composition map of different h thickness

Simulation results shows that h =0.849nm might have a better fit to green LED’s experimental I-V curves.
Influence of $L_B$ to the I-V curves

- $L_A = 150\text{nm}$
- $L_B = 10-50\text{nm}$
- $h = 0.849\text{nm}$.

For a fixed $L_A$ and $h$, the turn-on voltage is directly affected by the length of $L_B$. However, when $L_B > 30\text{nm}$, the influence to I-V is not significant. $L_B < 20\text{nm}$ and $L_B > 40\text{nm}$ all have a smaller IQE. One is due to hole injection problem. The later one is due to smaller active volume.
Influence of $L_A$ to the I-V curves

- $L_A = 50$-$350$ nm
- $L_B = 30$ nm
- $h = 0.849$nm.

When $L_B = 30$nm, the increase of $L_A$ only increases voltage slightly. The IQE actually becomes better when $L_A$ increases due to larger affective volume.

When dislocation density $= 10^9$ cm$^{-2}$, the average spacing of dislocation lines is 316nm, which is similar to the spacing of $L_A = 300$-$350$nm. The influences of dislocation line might be also within 30nm ($L_B$). Dislocation line might be one possible sources for the thickness fluctuation.

We think $L_A > 350nm$ might give similar effects as long as $L_B > 30$nm.