SAND2012-1225P

Bandstructure influences on InGaN light-emitting diode efficiency

Weng Chow, Sandia National Labs.

Semiconductor lights, III-N material system

LED model

Efficiency droop: intrinsic or extrinic?

Thanks to:

Sandia's Energy Frontier Research Center (EFRC)

DOE, Basic Energy Sciences

Sonderforschungsbereich (SFB) 787

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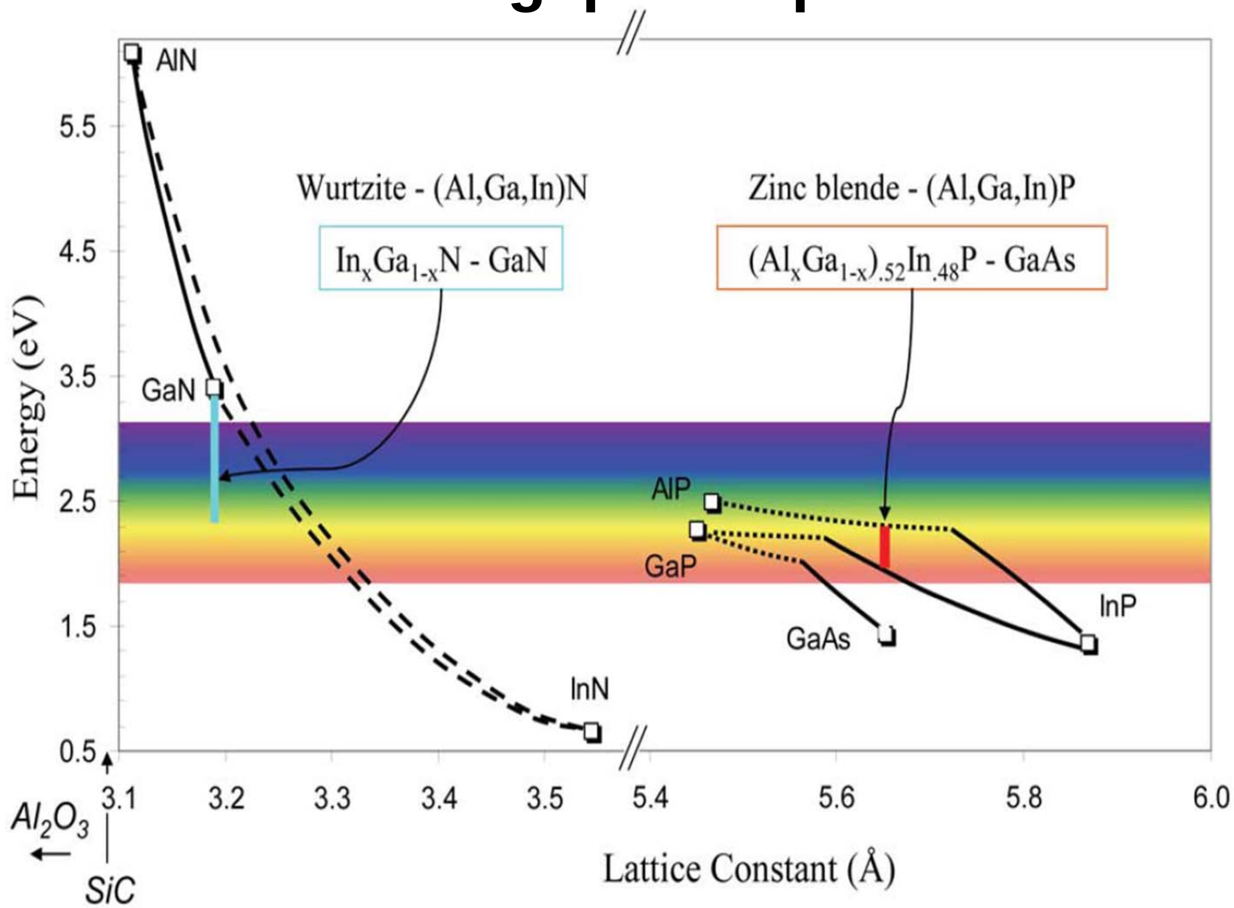
Wide bandgap Group-III Nitrides



Krames et al, J. Display Technology **3,** 1551 (2007)

Important applications: visible and ultraviolet lasers and LEDs

Interesting physics: Strong quantum-confined Stark effect

Strong many-body interaction

Significant excitation dependences in transition energies and matrix elements

Problem

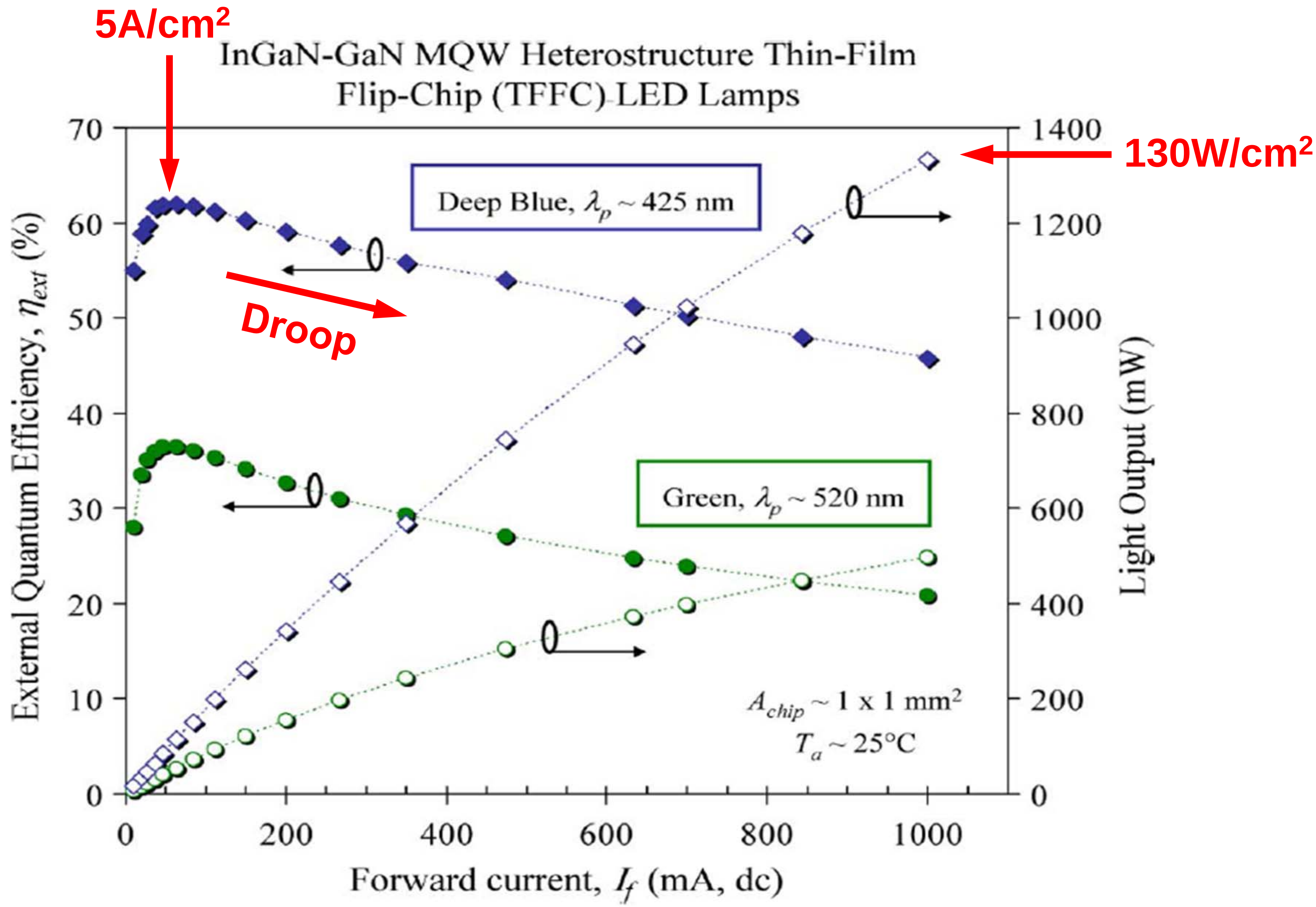


Fig. 8. External quantum efficiency and light output versus dc forward current for both blue and green InGaN-GaN QW-based TFFC LED lamps. Chip sizes are 1×1 mm^2.

Krames et al, J. Display Technology 3, 1551 (2007)

LED efficiency

Internal Quantum Efficiency

$$\frac{\#\ \text{photons created}}{\#\ \text{electrons injected}}$$

$$\textbf{Wall plug efficiency} = \frac{\hbar\omega}{eV}\ \underbrace{\text{IQE}\ \eta_{outcoupling}}_{\text{External quantum efficiency (EQE)}}$$

$$\frac{\mu_{eh}}{e} + IR$$

Chemical potential separation

Series resistance (=0 for ‘Manley-Rowe’ limit)

ABC model for LED efficiency

Carrier density rate equation

Injection efficiency
(carrier overshoot and escape)

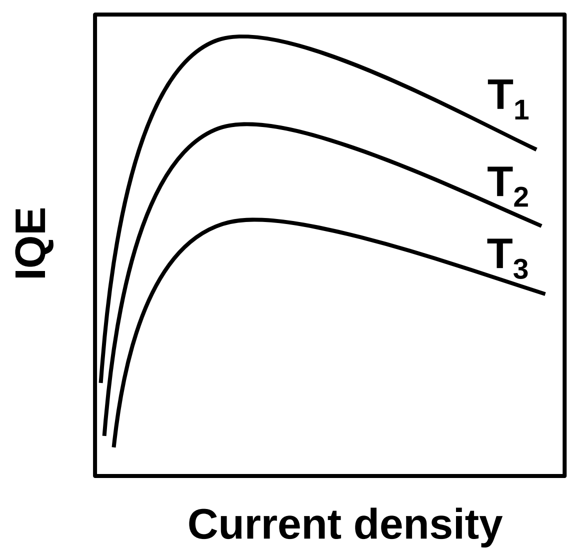
$$\frac{dN}{dt} = \frac{\eta_{inj} J}{ed} - AN - BN^2 - CN^3$$

Steady-state

$$\frac{dN}{dt} = 0 \Rightarrow \frac{\eta_{inj} J}{ed} = AN + BN^2 + CN^3$$

Internal quantum efficiency

$$\text{IQE} = \frac{BN^2}{\frac{J}{ed}} = \frac{\eta_{inj} BN^2}{AN + BN^2 + CN^3}$$



ABC model for LED efficiency

Carrier density rate equation

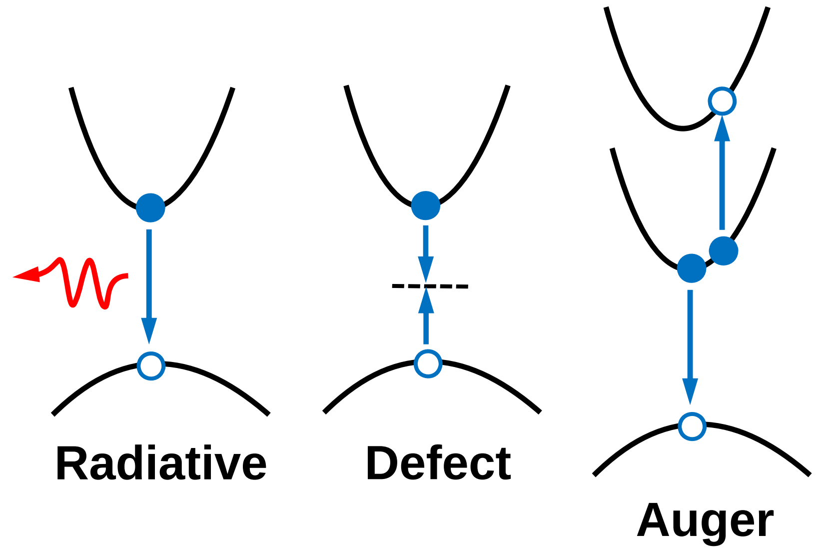
Injection efficiency
(carrier overshoot and escape)

$$\frac{dN}{dt} = \frac{\eta_{inj} J}{ed} - AN - BN^2 - CN^3$$

Defects *Auger*

Spontaneous emission

Carrier losses



Steady-state

$$\frac{dN}{dt} = 0 \quad \Rightarrow \quad \frac{\eta_{inj} J}{ed} = AN + BN^2 + CN^3$$

Internal quantum efficiency

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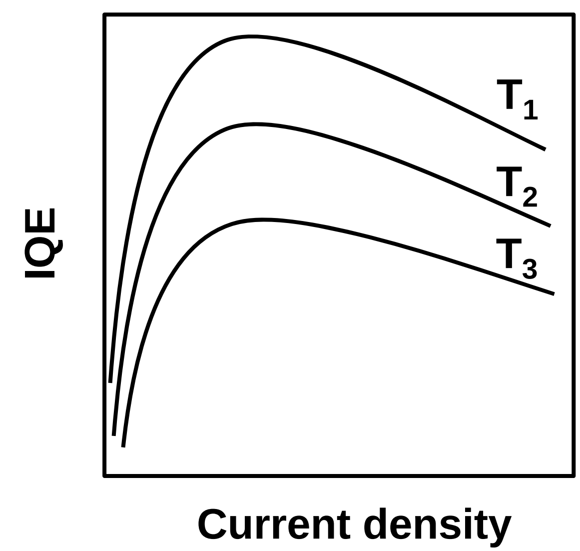
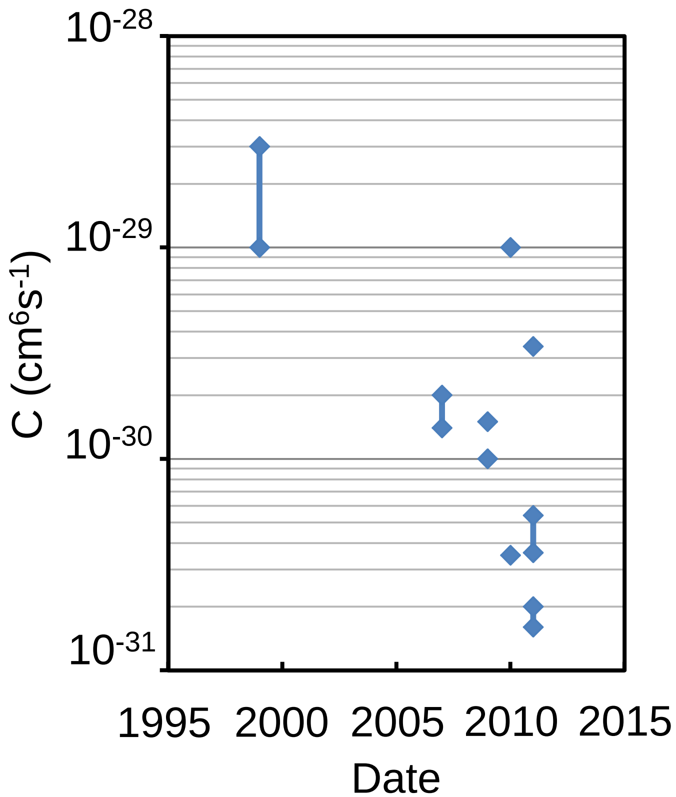


Motivations for a more detailed model

Variation in Auger coefficient from IQE curve fitting with ABC model



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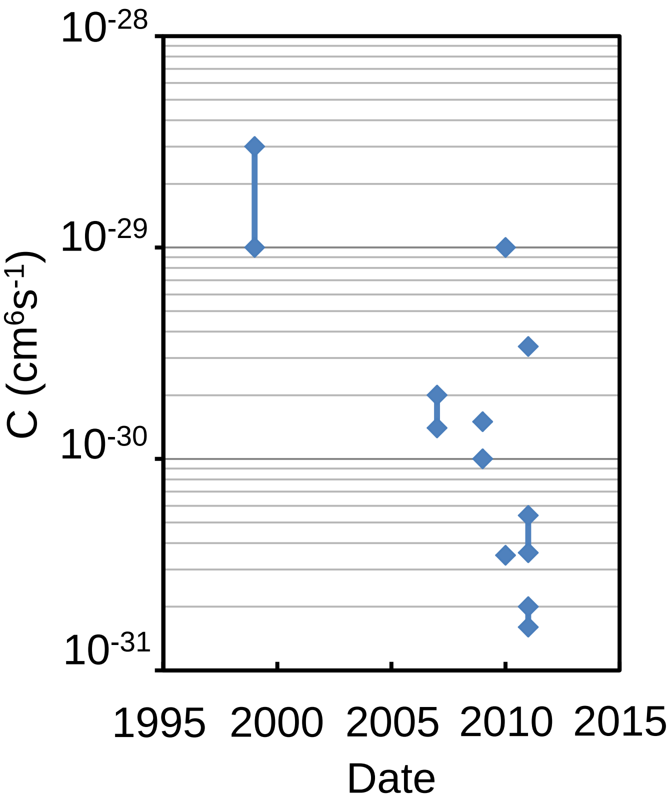
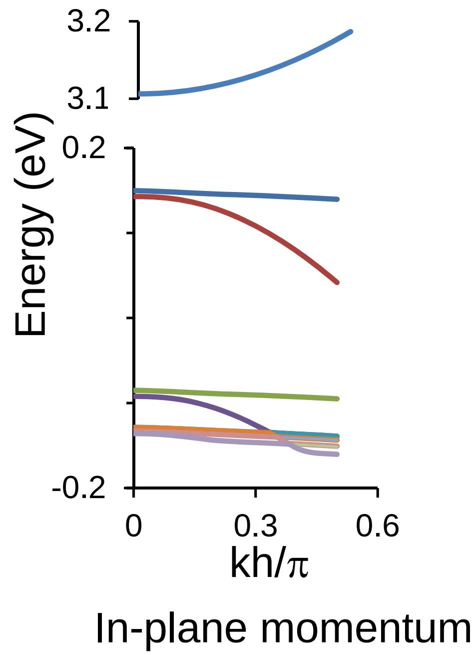
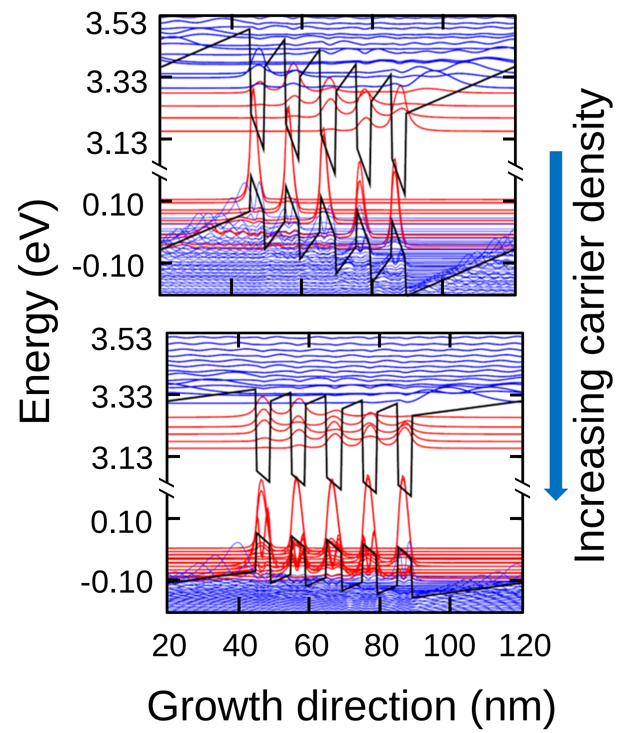


Energy dispersions



Carrier density dependent band structure changes



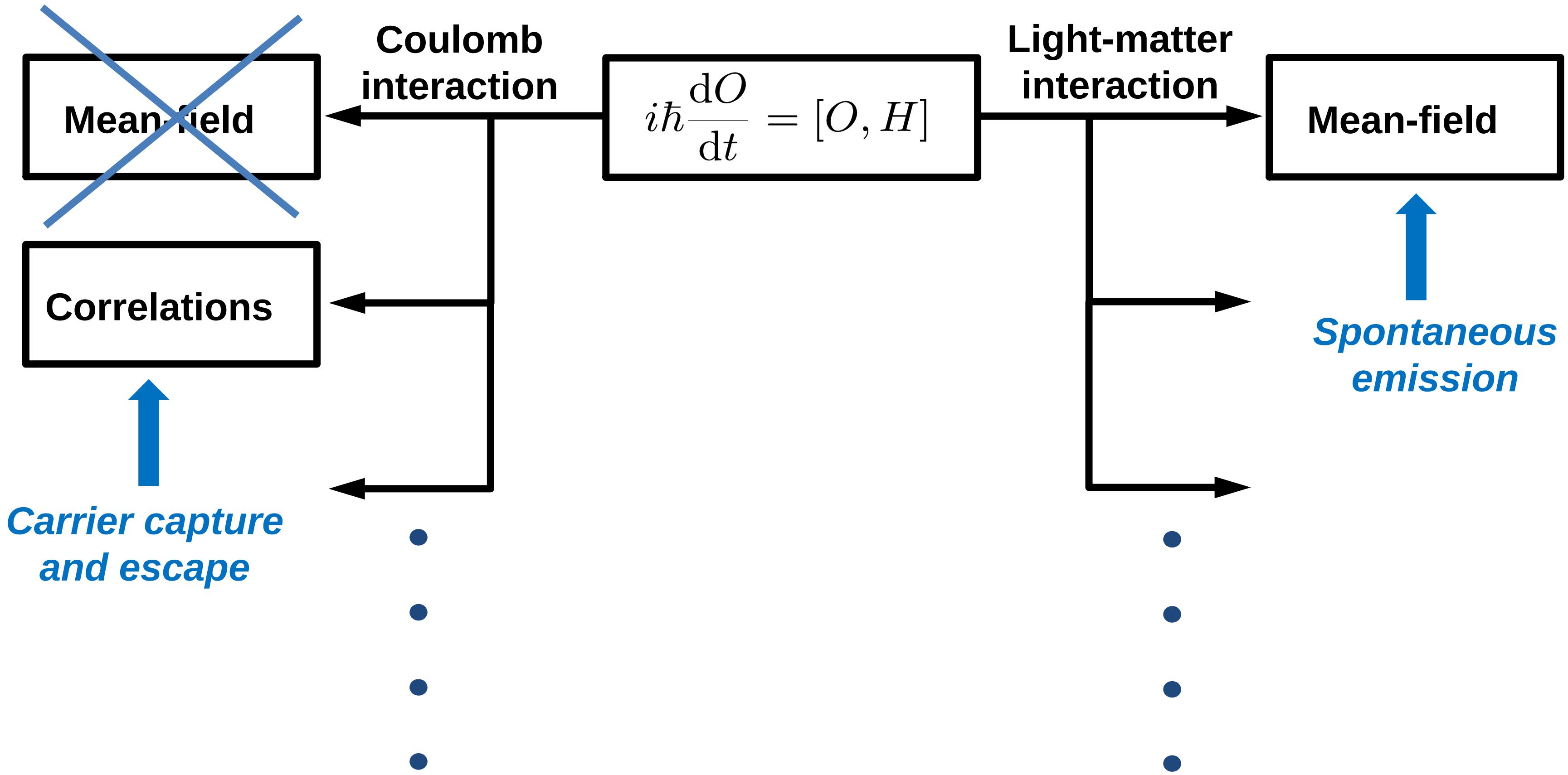
Approach

<u>Hamiltonian</u>

$$H=\overbrace{\sum_i \varepsilon_i^e a_i^\dagger a_i + \sum_j \varepsilon_j^h b_j^\dagger b_j + \sum_q \hbar\Omega_q c_q^\dagger c_q}^{\text{Single-particle energies}} - \overbrace{\sum_{i,j,q} \wp_{ij}\sqrt{\frac{\hbar\Omega_q}{V\epsilon_b}}\left(a_i b_j c_q^\dagger + c_q b_j^\dagger a_i^\dagger\right)}^{\text{Light-matter interaction}}$$

+ Coulomb interaction

Hiesenberg Picture



Model

e* or *h

$$
\begin{aligned}
\frac{\mathrm{d}n_{\sigma,\alpha_\sigma,k_\perp}}{\mathrm{d}t} = & -n_{\sigma,n_\sigma,k_\perp}\sum_{\alpha_{\sigma'}} b_{\alpha_\sigma,\alpha_{\sigma'},k_\perp} n_{\sigma',\alpha_{\sigma'},k_\perp} - A n_{\sigma,n_\sigma,k_\perp} \\
& -\gamma_{c-c}\left[n_{\sigma,n_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_\sigma,T\right)\right] \\
& -\gamma_{c-p}\left[n_{\sigma,n_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_\sigma^L,T_L\right)\right]
\end{aligned}
$$

$$
\begin{aligned}
\frac{\mathrm{d}n^b_{\sigma,k}}{\mathrm{d}t} = & -b_k n^b_{e,k} n^b_{h,k} + \frac{J}{eN^p_\sigma} f\left(\varepsilon^b_{\sigma,k},\mu^p_\sigma,T_p\right)\left(1-n^b_{\sigma,k}\right) + A_b n_{\sigma,k} \\
& -\gamma_{c-c}\left[n^b_{\sigma,k} - f\left(\varepsilon^b_{\sigma,k},\mu_\sigma,T\right)\right] \\
& -\gamma_{c-p}\left[n^b_{\sigma,k} - f\left(\varepsilon^b_{\sigma,k},\mu^L_\sigma,T_L\right)\right]
\end{aligned}
$$

Similar for holes

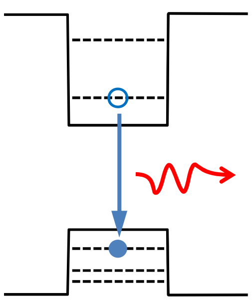
IEEE JQE **38** 402, 2002 (for QW); IEEE JQE **41** 495, 2005 (for QD); APL 97, 121105, 2010 (for InGaN LEDs)

Model

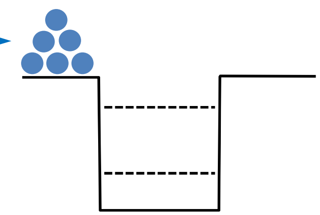
e or h

$$\frac{\mathrm{d}n_{\sigma,\alpha_\sigma,k_\perp}}{\mathrm{d}t} = \overbrace{-n_{\sigma,n_\sigma,k_\perp}\sum_{\alpha_{\sigma'}} b_{\alpha_\sigma,\alpha_{\sigma'},k_\perp} n_{\sigma',\alpha_{\sigma'},k_\perp}} - An_{\sigma,n_\sigma,k_\perp}$$
$$-\gamma_{c-c}\left[n_{\sigma,n_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_\sigma,T\right)\right]$$
$$-\gamma_{c-p}\left[n_{\sigma,n_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_\sigma^L,T_L\right)\right]$$

Spontaneous emission (>ns)



Carrier injection



$$\frac{\mathrm{d}n^b_{\sigma,k}}{\mathrm{d}t} = \overbrace{-b_k n^b_{e,k} n^b_{h,k}} + \overbrace{\frac{J}{eN^p_\sigma} f\left(\varepsilon^b_{\sigma,k},\mu^p_\sigma,T_p\right)\left(1-n^b_{\sigma,k}\right)} + A_b n_{\sigma,k}$$
$$-\gamma_{c-c}\left[n^b_{\sigma,k} - f\left(\varepsilon^b_{\sigma,k},\mu_\sigma,T\right)\right]$$
$$-\gamma_{c-p}\left[n^b_{\sigma,k} - f\left(\varepsilon^b_{\sigma,k},\mu^L_\sigma,T_L\right)\right]$$

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Model

e or h

$$\frac{\mathrm{d}n_{\sigma,\alpha_\sigma,k_\perp}}{\mathrm{d}t} = -n_{\sigma,n_\sigma,k_\perp}\sum_{\alpha_{\sigma'}} b_{\alpha_\sigma,\alpha_{\sigma'},k_\perp} n_{\sigma',\alpha_{\sigma'},k_\perp} - An_{\sigma,n_\sigma,k_\perp}$$
$$-\gamma_{c-c}\left[n_{\sigma,n_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_\sigma,T\right)\right]$$
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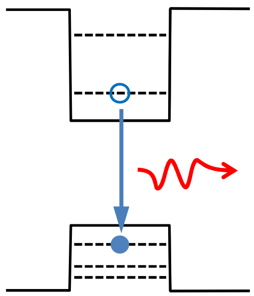
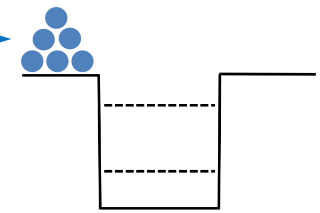
Spontaneous emission (>ns)



Carrier injection



$$\frac{\mathrm{d}n^b_{\sigma,k}}{\mathrm{d}t} = -b_k n^b_{e,k} n^b_{h,k} + \frac{J}{eN^p_\sigma} f\left(\varepsilon^b_{\sigma,k},\mu^p_\sigma,T_p\right)\left(1-n^b_{\sigma,k}\right) + A_b n_{\sigma,k}$$
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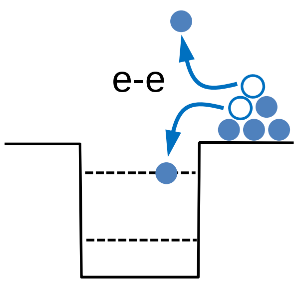
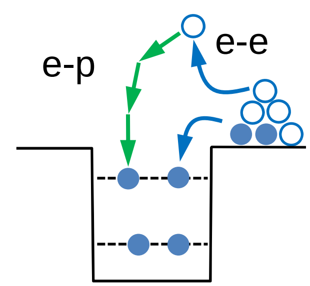
$$-\gamma_{c-p}\left[n^b_{\sigma,k} - f\left(\varepsilon^b_{\sigma,k},\mu^L_\sigma,T_L\right)\right]$$

Carrier-carrier (100fs)



Carrier-phonon (<1ps)



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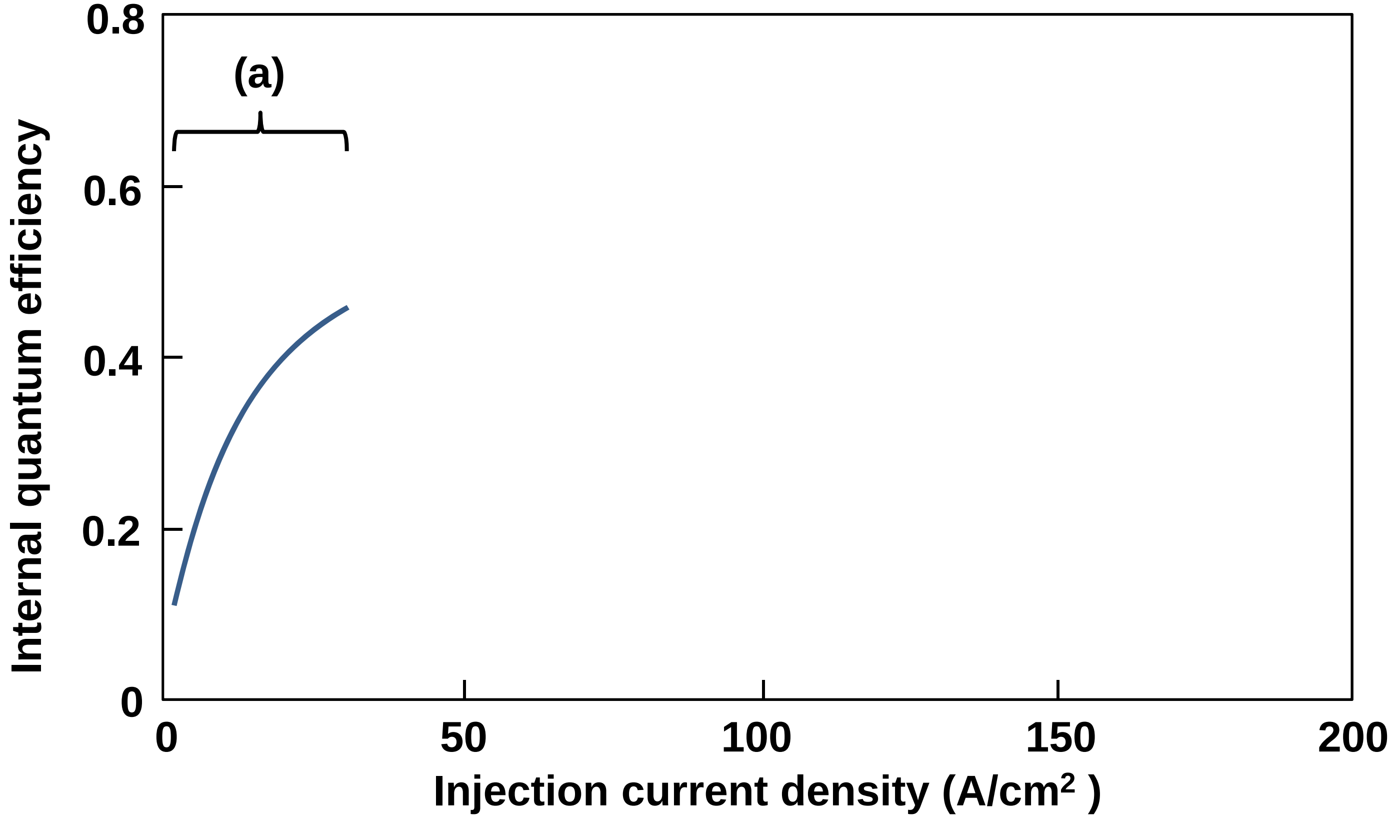
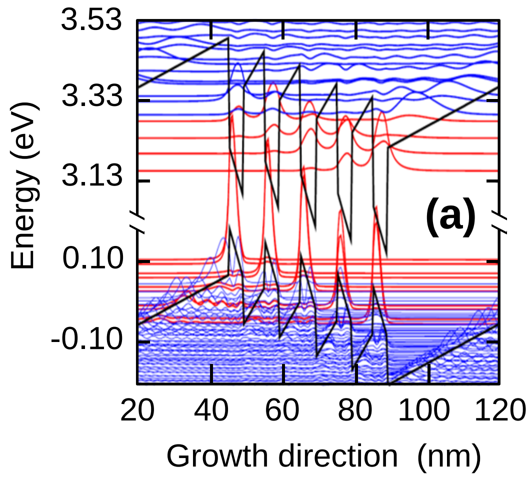
4nm $In_{0.2}Ga_{0.8}N$/6nmGaN, T_L = 300K, $\gamma_{c\text{-}c} = 5\times10^{13}s^{-1}$, $\gamma_{c\text{-}p} = 10^{13}s^{-1}$, $A = 10^{-7}s^{-1}$, C = 0





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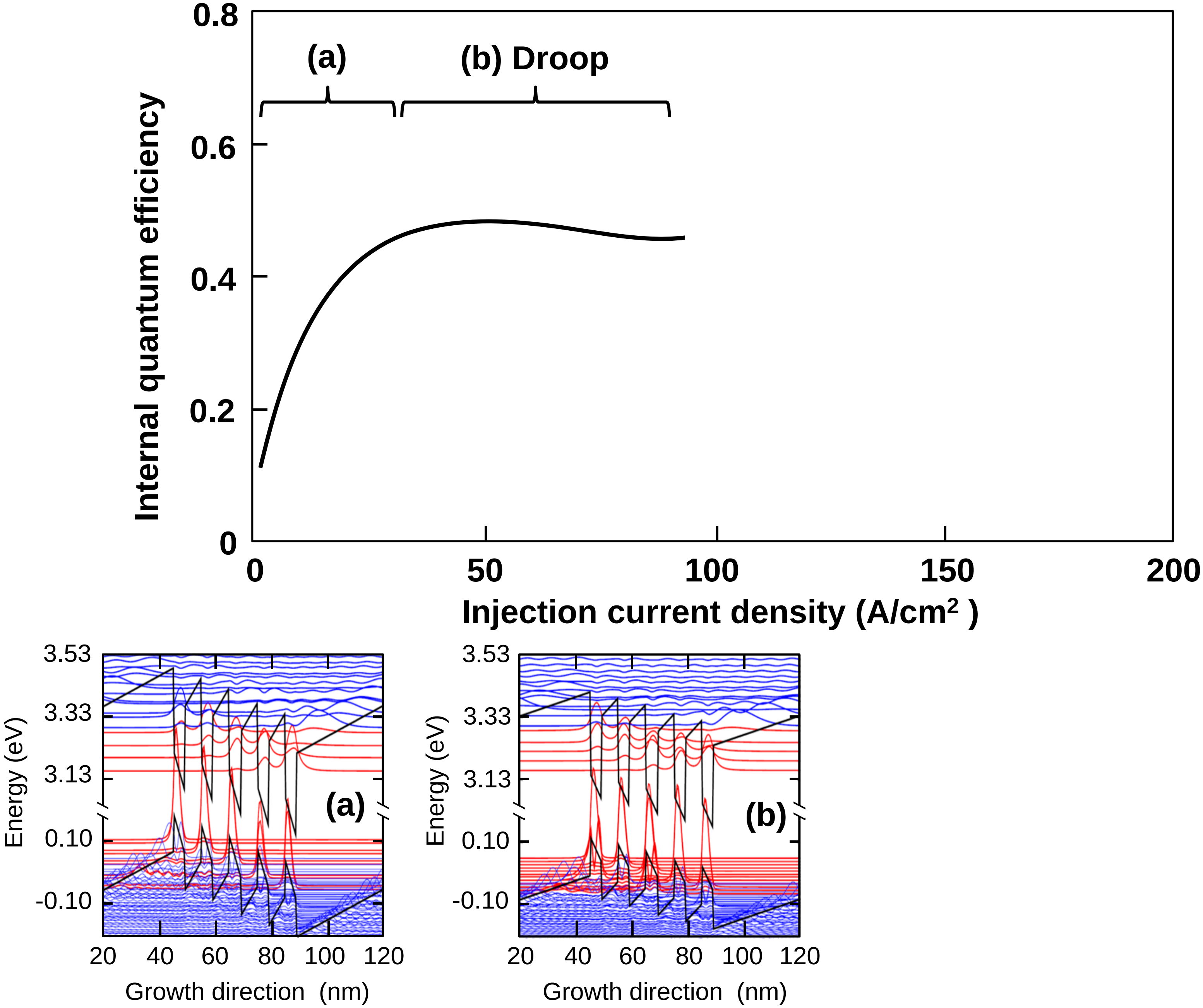
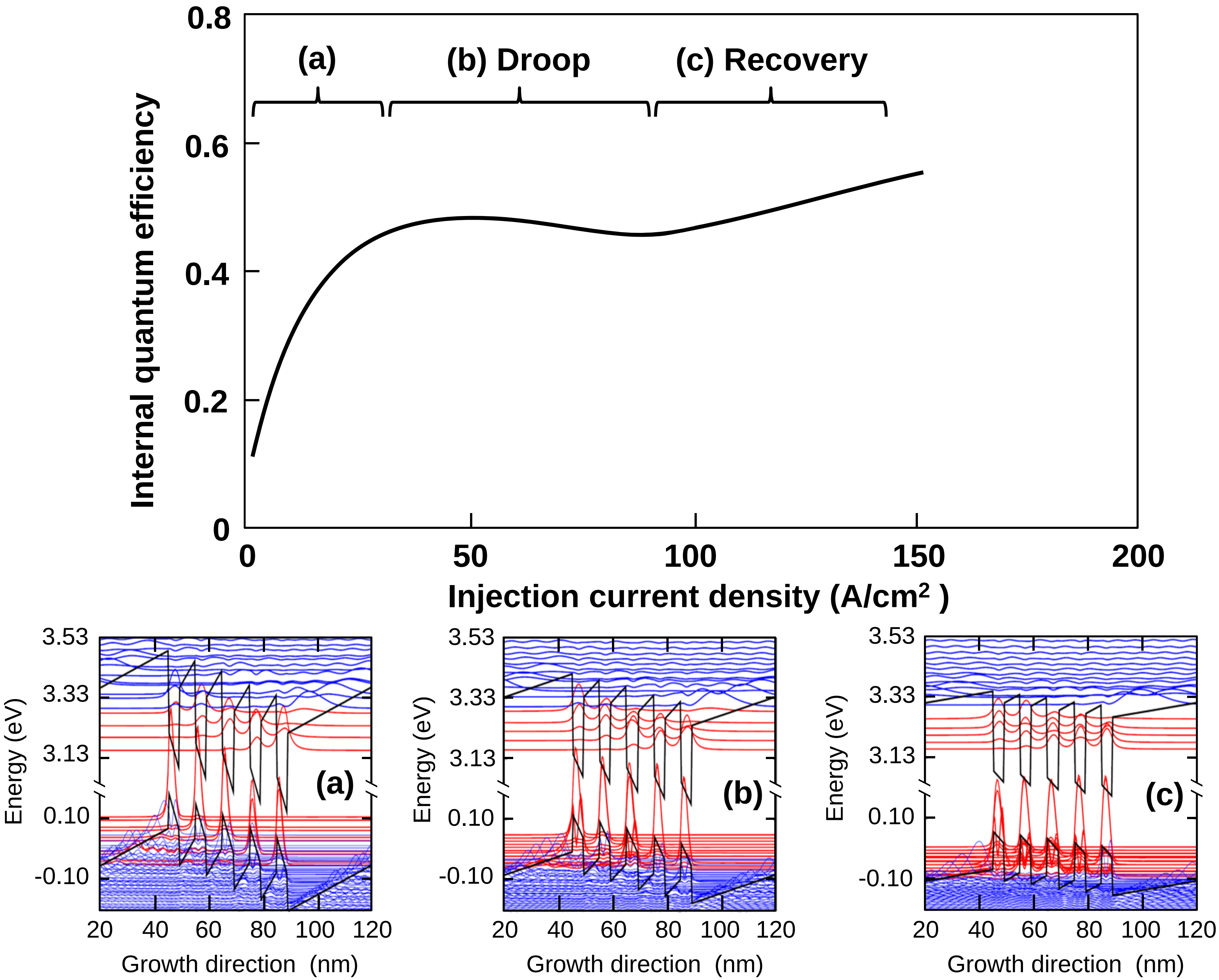


4nm $In_{0.2}Ga_{0.8}N$/6nmGaN, T_L = 300K, $\gamma_{c\text{-}c} = 5\text{x}10^{13}s^{-1}$, $\gamma_{c\text{-}p} = 10^{13}s^{-1}$, $A = 10^{-7}s^{-1}$, $C = 0$



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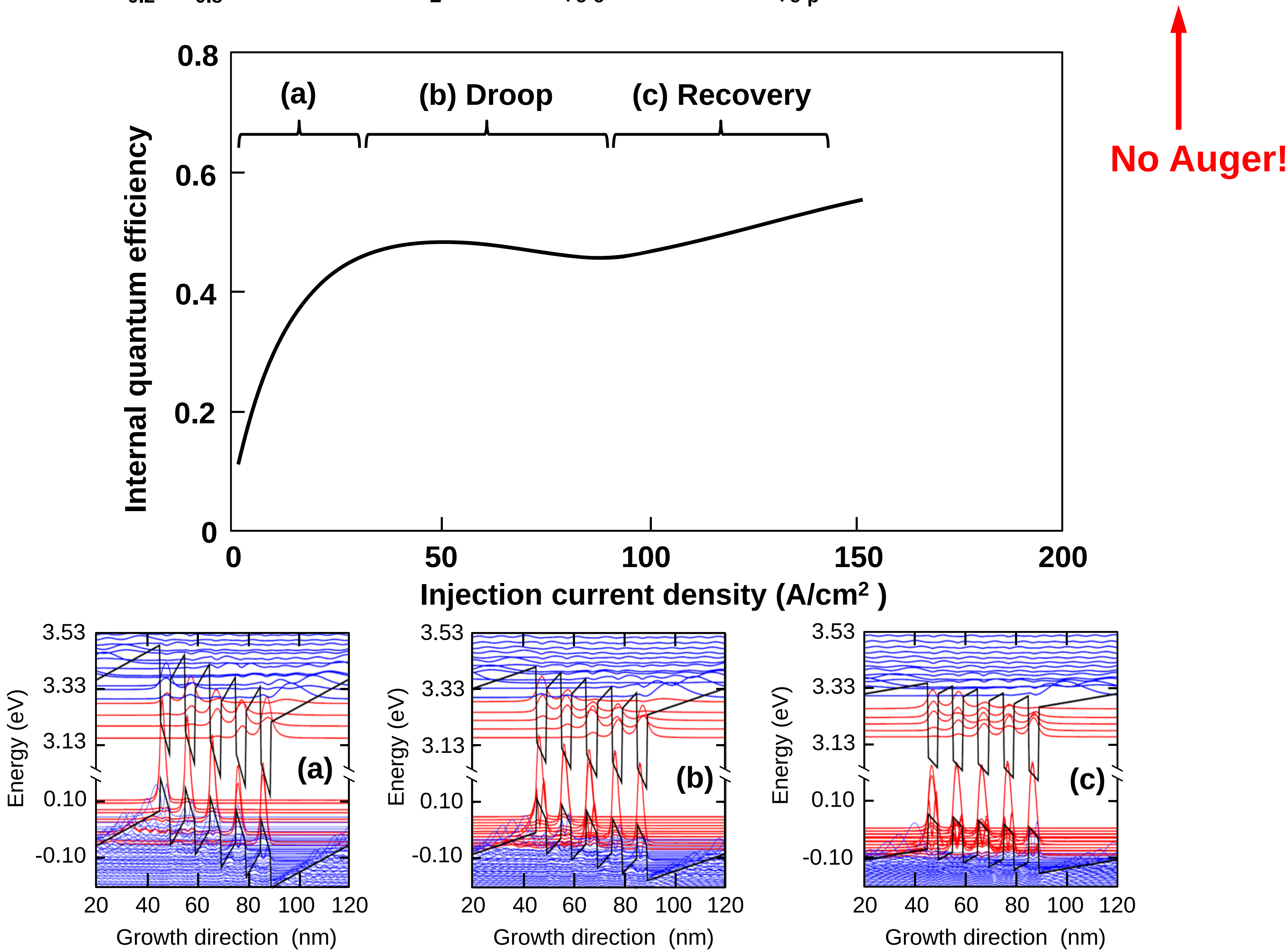

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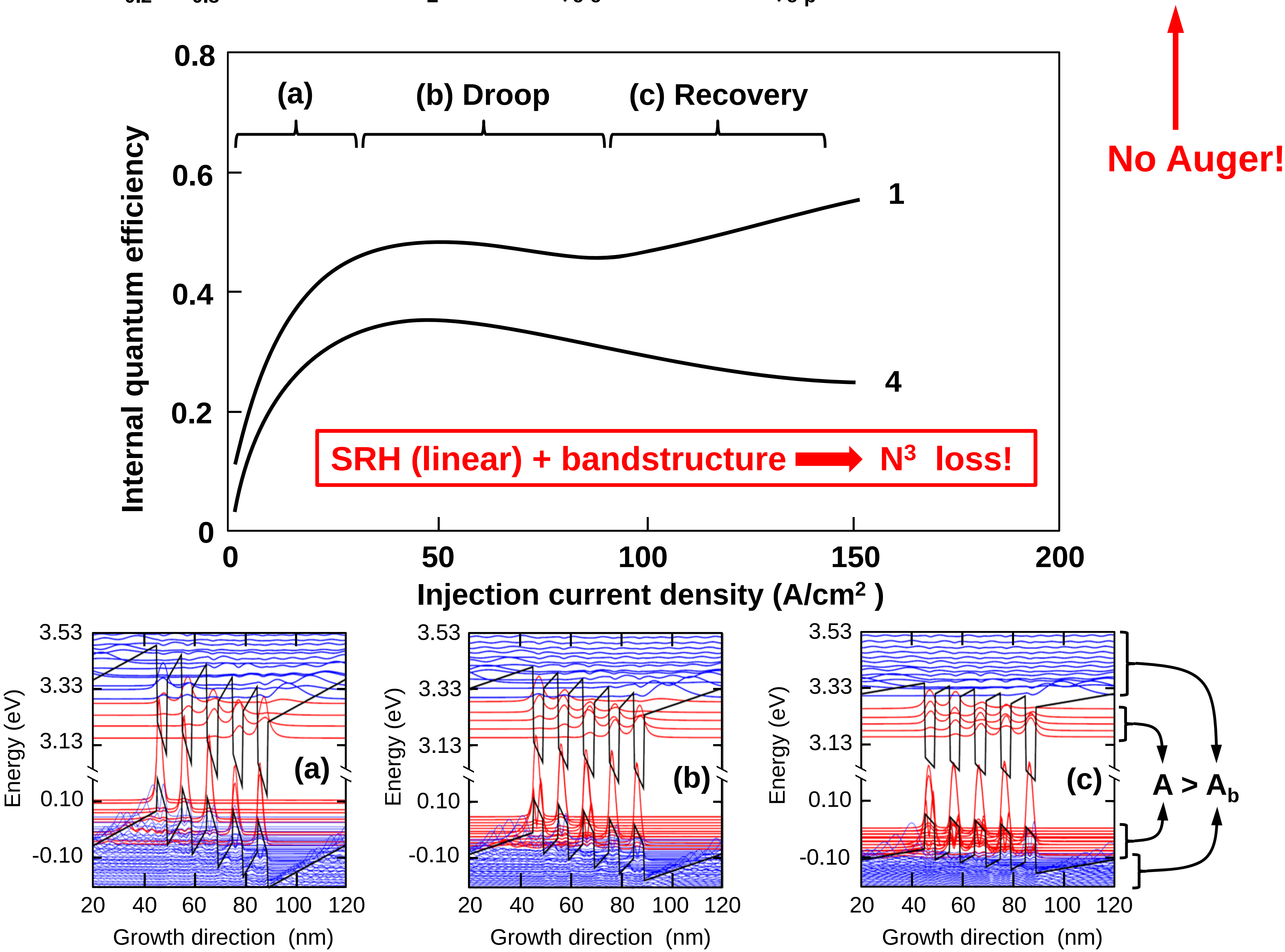

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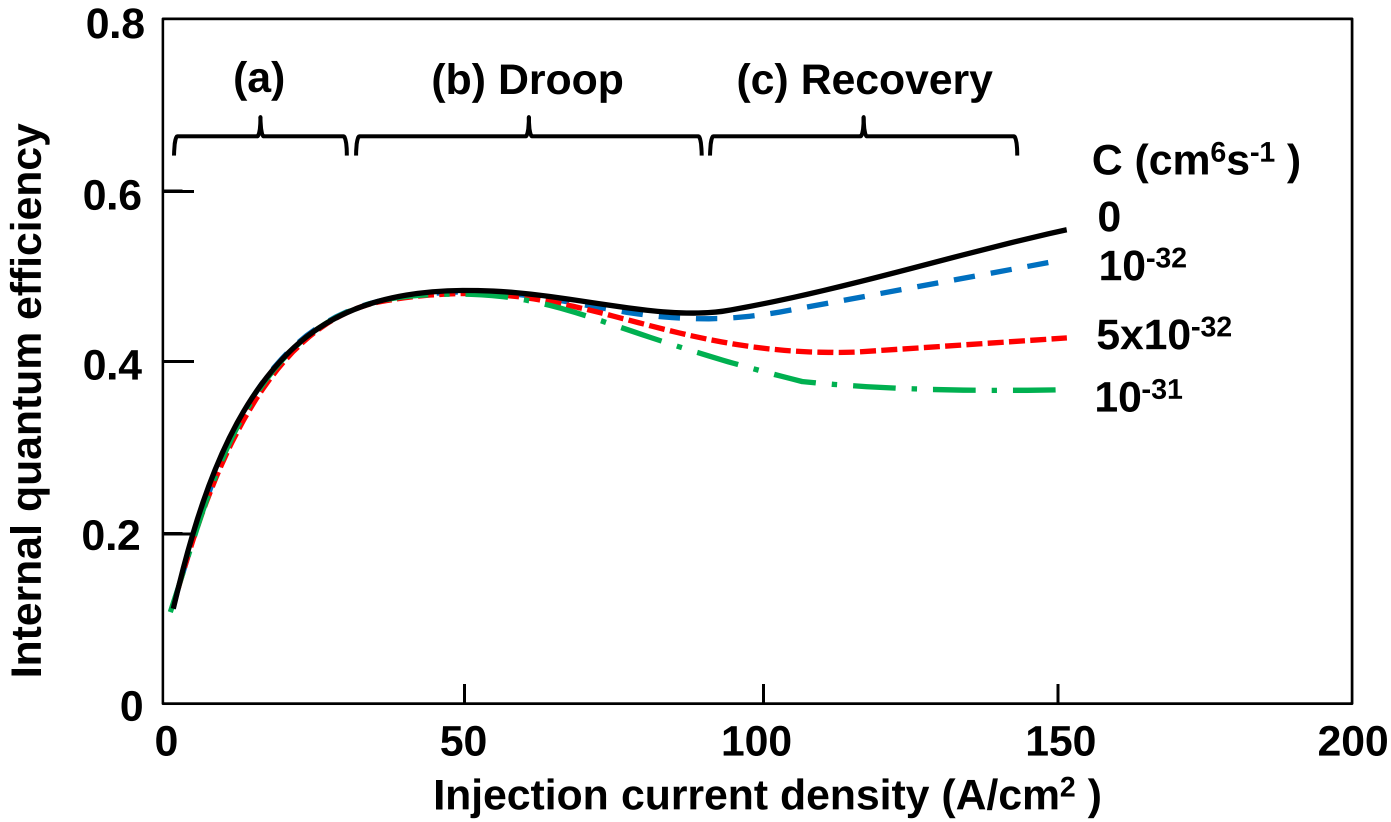
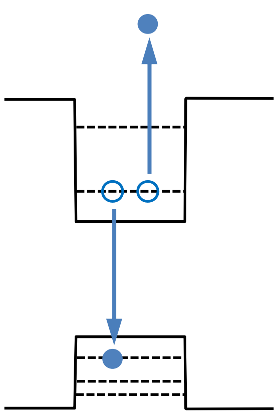
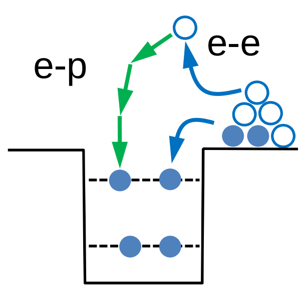


Auger



Carrier-phonon



- Auger loss prevents recovery of IQE
- Required coefficient

  --- smaller than ABC model estimation

  --- consistent with microscopic calculations

Summary

Can fit experiment with :

$$\text{IQE} = \frac{BN^2}{AN + BN^2 + CN^3}$$

Extrinsic ?

Localization

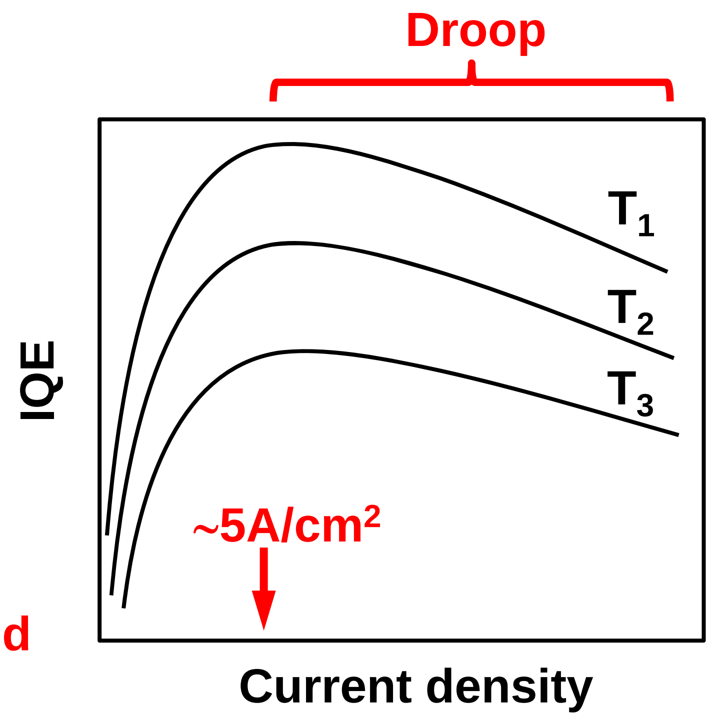
Current leakage

Defect loss

Intrinsic ?

Auger

Screening of piezoelectric field



Talk --- describes k-resolve carrier population model

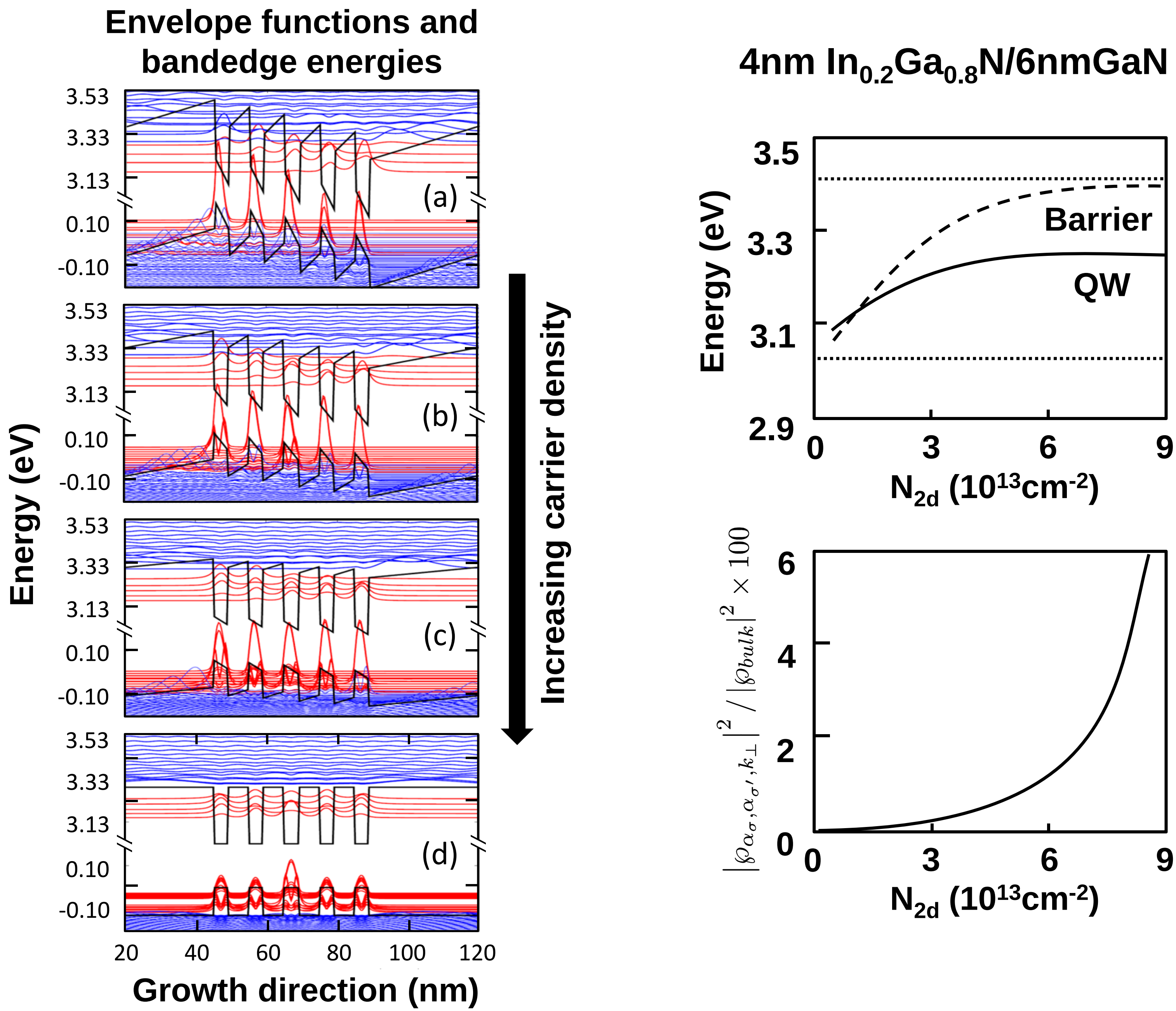
--- systematic description of above effects at microscopic level

--- droop can arise from --- screening of QCSE

--- localization of SRH losses

--- Auger loss (with small necessary C)

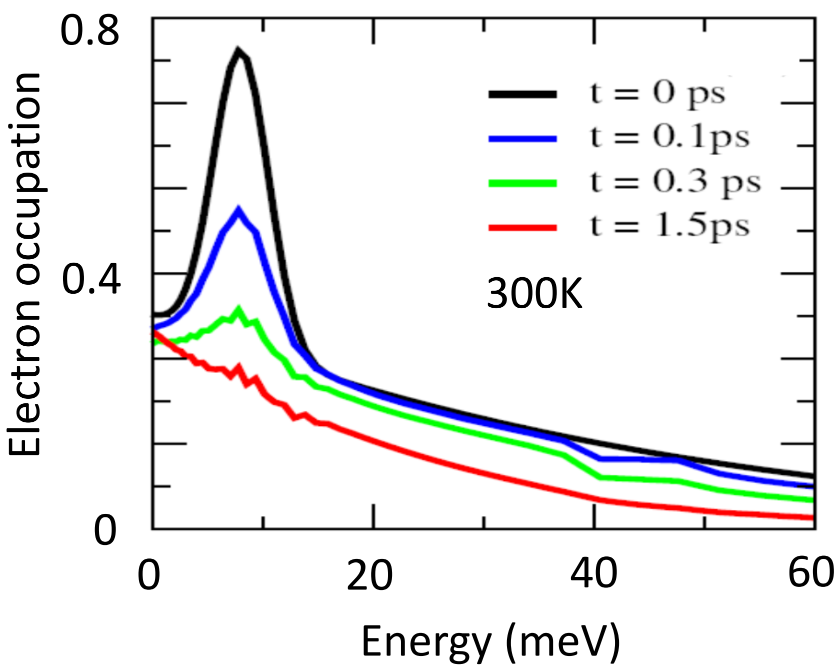
Excitation dependent band-structure effects



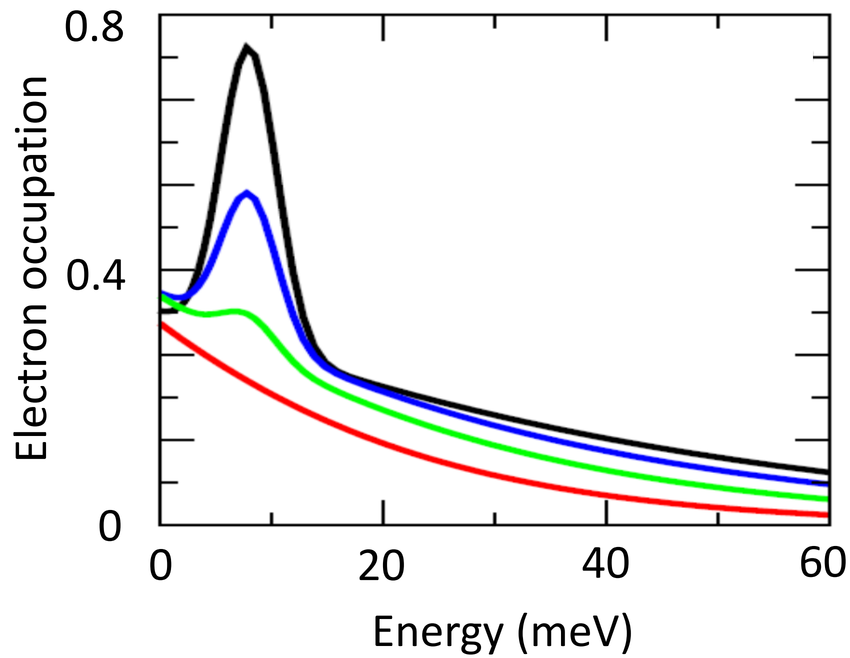
Carrier population relaxation

$$H_{Coul} = \frac{1}{2}\sum_{\alpha,\beta,\alpha',\beta'} V_{\alpha,\beta,\alpha',\beta'}\left[a^\dagger_{\alpha'}a^\dagger_{\beta'}a_\beta a_\alpha + b^\dagger_{\alpha'}b^\dagger_{\beta'}b_\beta b_\alpha - 2a^\dagger_{\alpha'}b^\dagger_{\beta'}b_\beta a_\alpha\right]$$
$$+\sum_{\alpha,\beta,\vec{q}} \hbar G_q a^\dagger_\beta a_\alpha \left(b_{\vec{q}} + b^\dagger_{-\vec{q}}\right)$$

Quantum kinetic calculation



(Our) Rate equation approximation



IEEE JQE **42**, 292 (2006)

Internal quantum efficiency

$$\frac{1}{\hbar\epsilon_b\pi c^3}\left|\wp_k\right|^2\Omega_k^3,$$

$$IQE = \frac{e}{JS}\left(\sum_{\alpha_e,\alpha_h,k_\perp} b_{\alpha_e,\alpha_h,k_\perp} n_{e,\alpha_e,k_\perp} n_{h,\alpha_h,k_\perp} + \sum_k b_k n^b_{e,k} n^b_{h,k}\right)$$

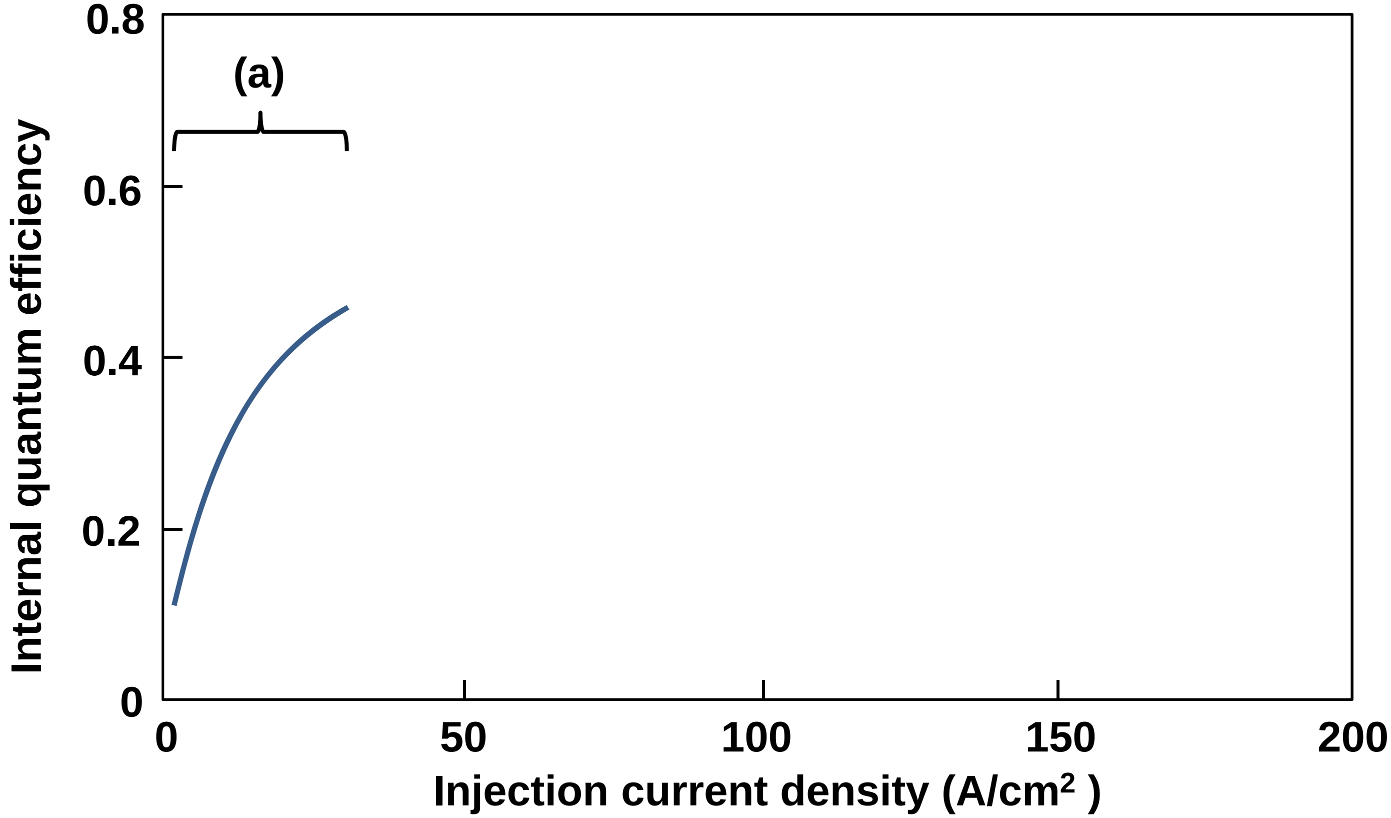
$$\frac{1}{\hbar\epsilon_b\pi c^3}\left|\wp_{\alpha_\sigma,\alpha_{\sigma'},k_\perp}\right|^2\Omega^3_{\alpha_\sigma,\alpha_{\sigma'},k_\perp}$$

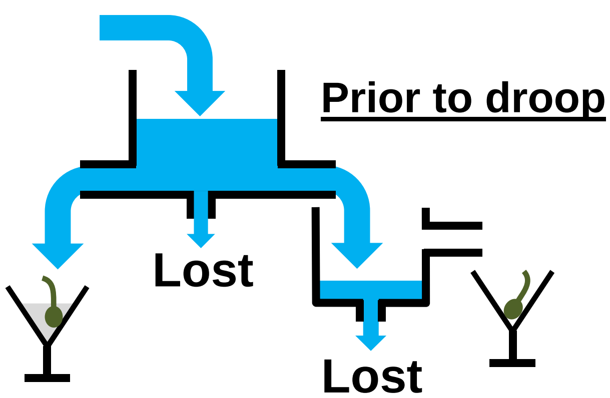
$$\left|\wp_{bulk}\right|^2\xi_{\alpha_e,\alpha_h,k_\perp}$$

$$\frac{1}{4}\left|\sum_{\beta_e}\sum_{\beta_h}\sum_{m_e}\sum_{m_h} A_{\beta_e,\alpha_e,k_\perp} A_{\beta_h,\alpha_h,k_\perp}\int_{-\infty}^{\infty} dz\ u_{m_e,\beta_e}(z) u_{m_h,\beta_e}(z)\right|^2$$

4nm $In_{0.2}Ga_{0.8}N$/6nmGaN, T_L = 300K, $\gamma_{c\text{-}c} = 5\text{x}10^{13}s^{-1}$, $\gamma_{c\text{-}c} = 10^{13}s^{-1}$, $A = 10^{-7}s^{-1}$, $C = 0$

No Auger!





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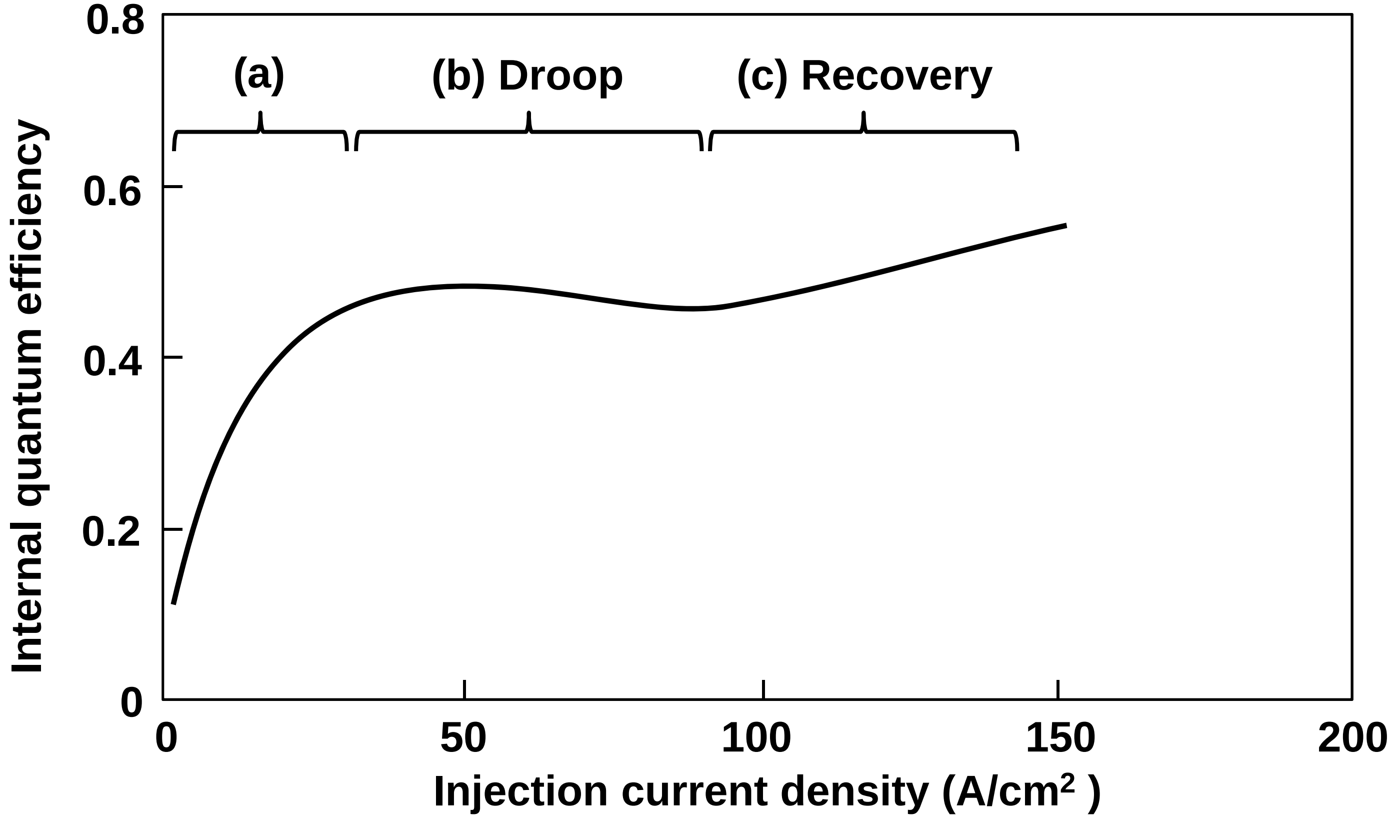

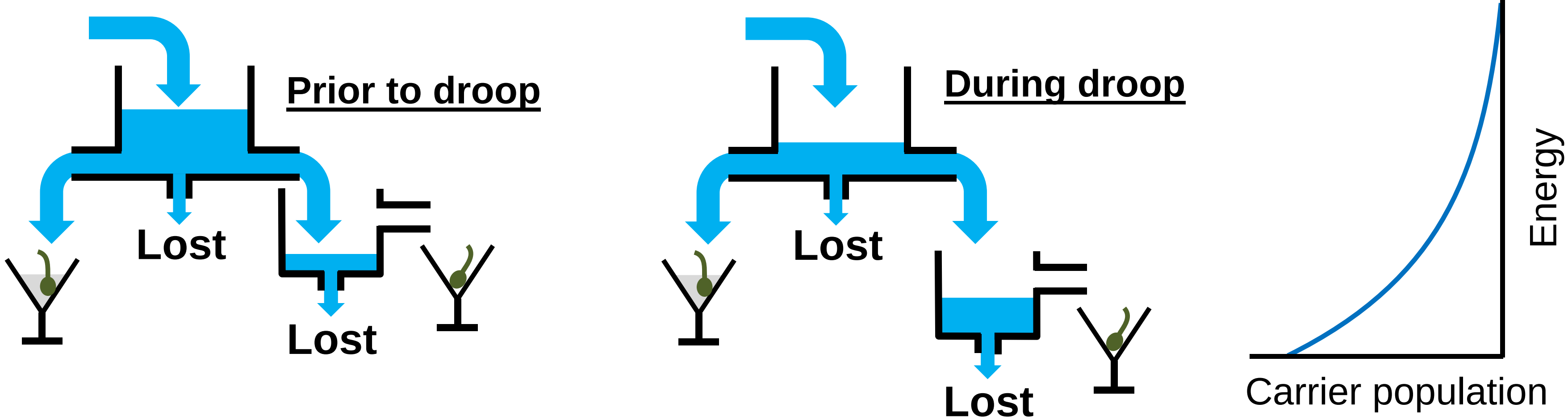

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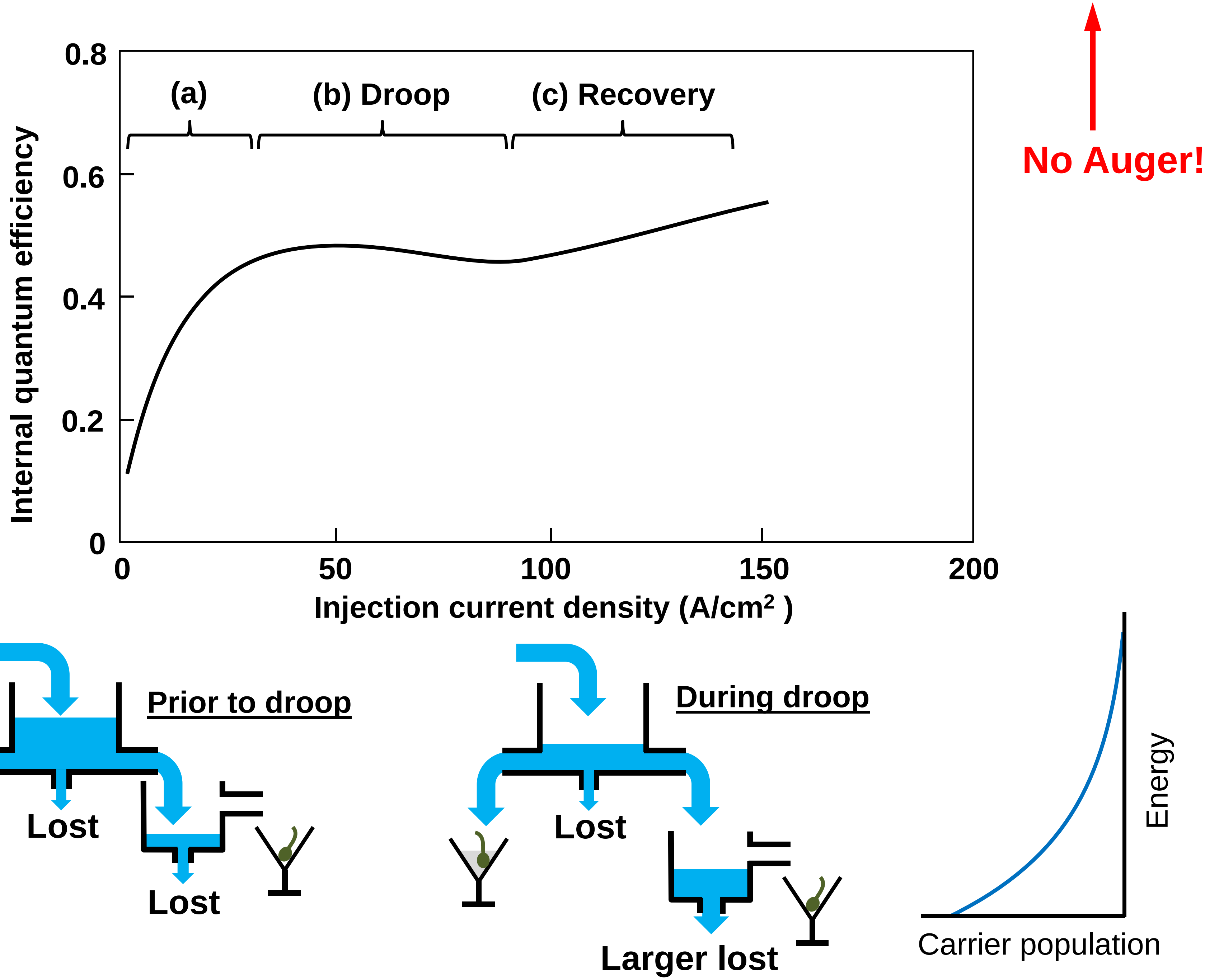

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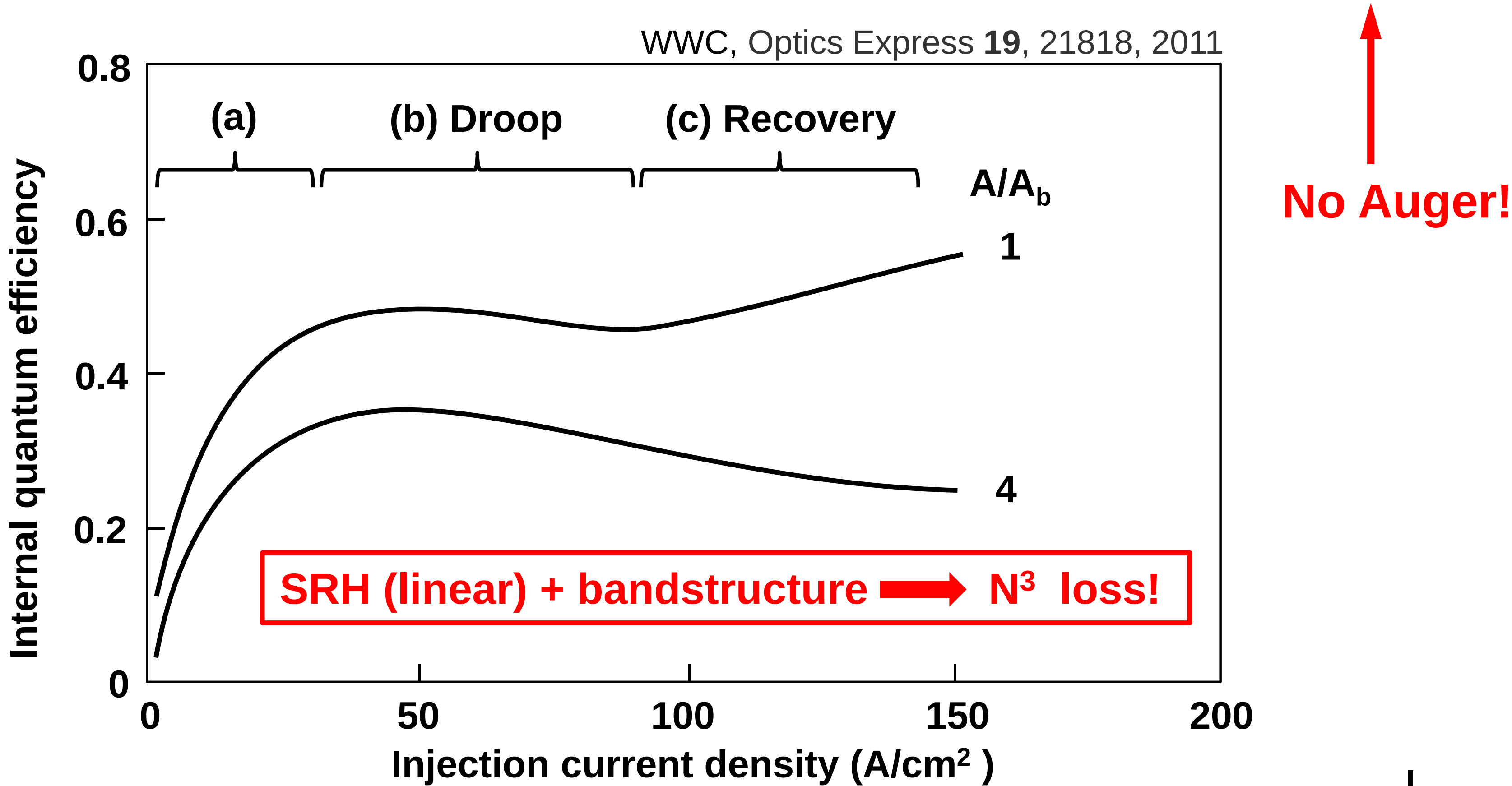
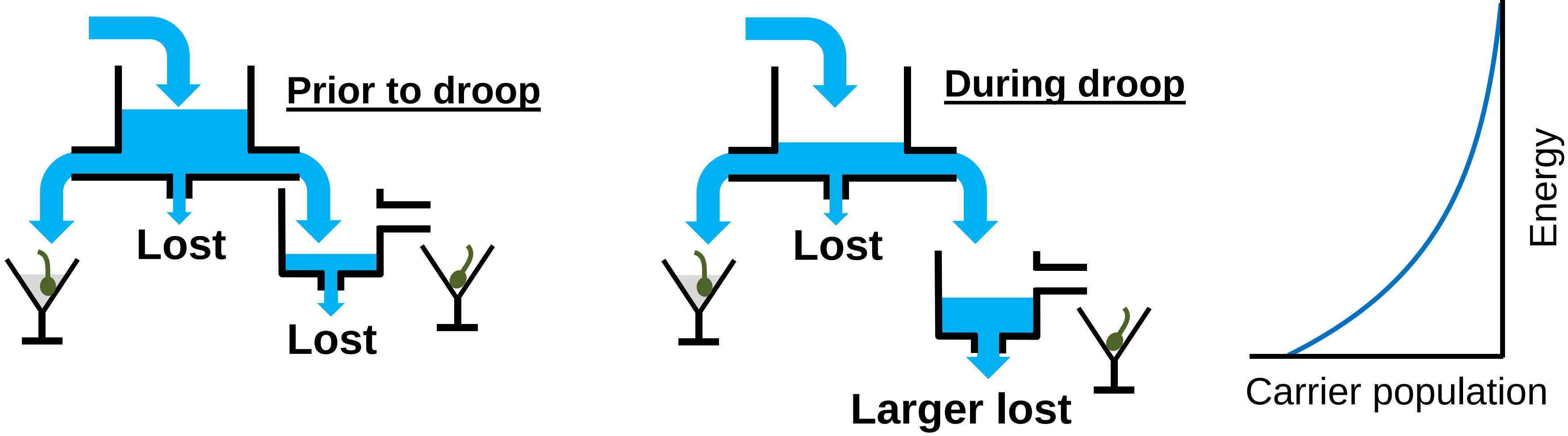
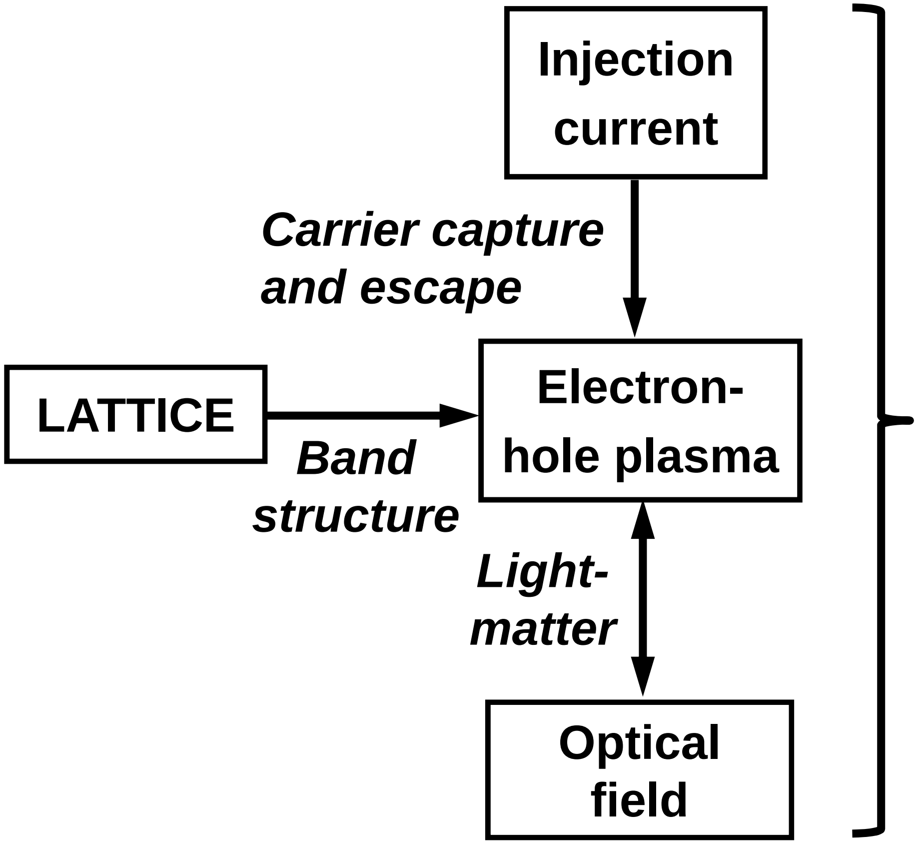




k-resolved LED model



Present model

Next step:
Model/Expt comparison (esp. IQE vs. J and T)

Efficiency droop is observed under a wide range of experimental conditions – involving different LED emitting wavelengths, polar versus non polar substrates, with or without electron blocking layers, etc

It is possible that the differences in observed droop behavior (involving different LED emitting wavelengths, polar versus non polar substrates, with or without electron blocking layers, etc.) arise from differences in the relative importance of various mechanisms.