# (a) Efficiency droop without Auger in InGaN LEDs

SAND2012-9643P

# (b) Laser gain in Ge-on-Si

**Weng Chow, Sandia National Labs.**

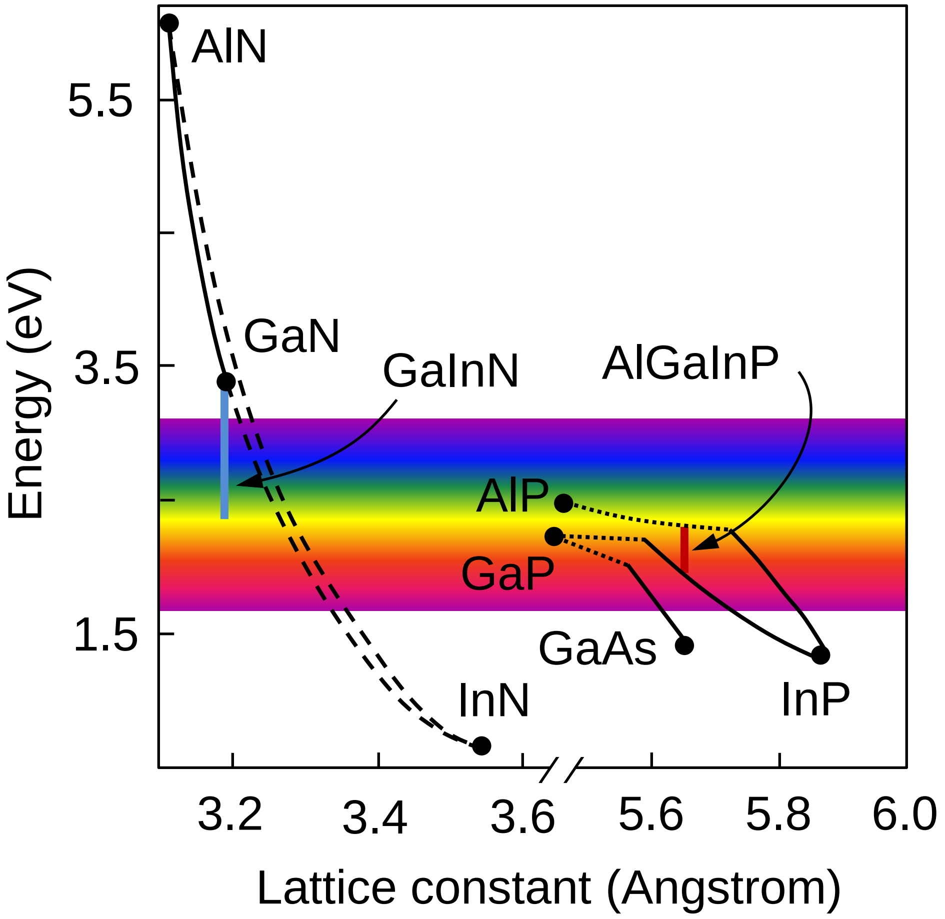
**Droop:**
**Semiconductor lights, III-N material system**
**LED model**
**Efficiency droop: intrinsic or extrinic?**

**Ge:**
**Experiment**
**Laser model**
**Results -- Required current vs. desired gain for different strain and doping densities**

Thanks to: Sandia's Energy Frontier Research Center (EFRC), DOE-Basic Energy Sciences and Sonderforschungsbereich (SFB) 787

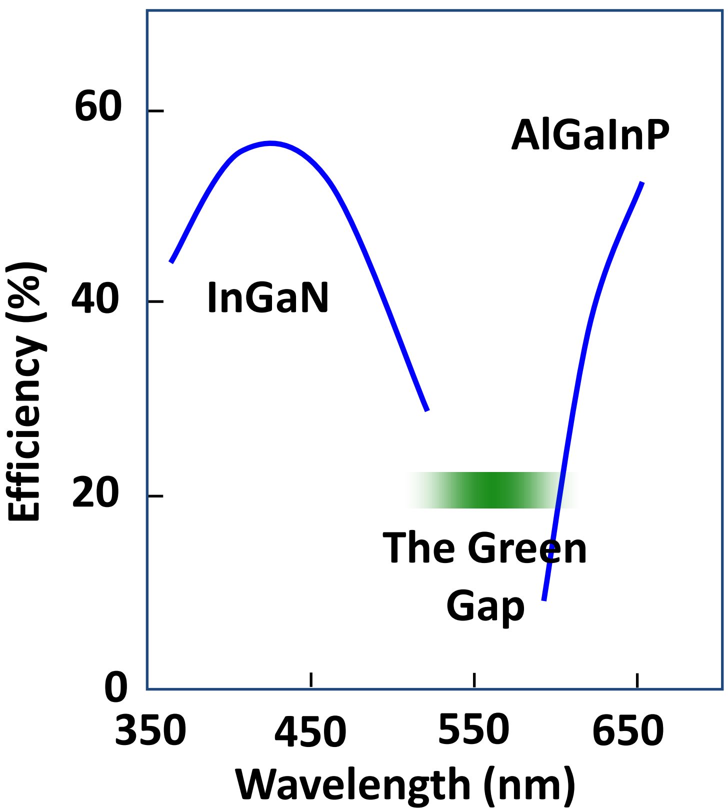
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

# Visible and ultraviolet semiconductor lasers and LEDs

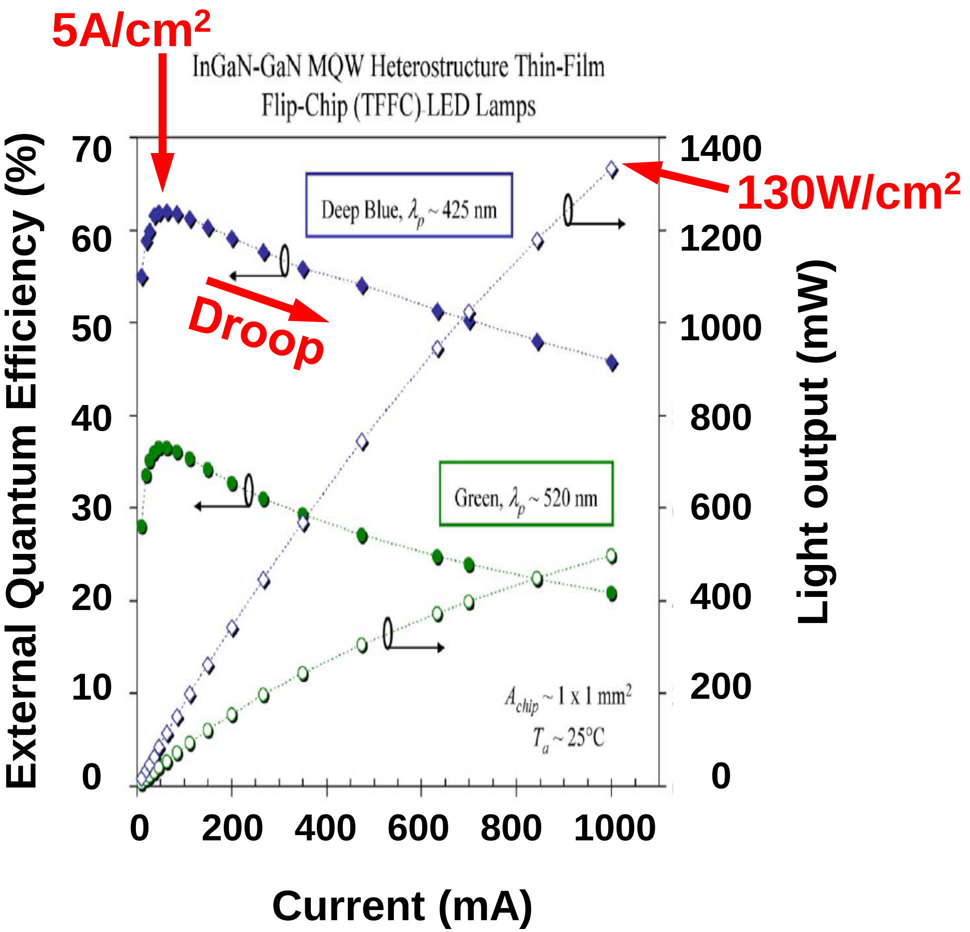


# Problems

## Green gap




## Efficiency droop




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

# LED efficiency

Internal Quantum Efficiency $\leftarrow \dfrac{\#\ \text{photons created}}{\#\ \text{electrons injected}}$

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

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

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)*

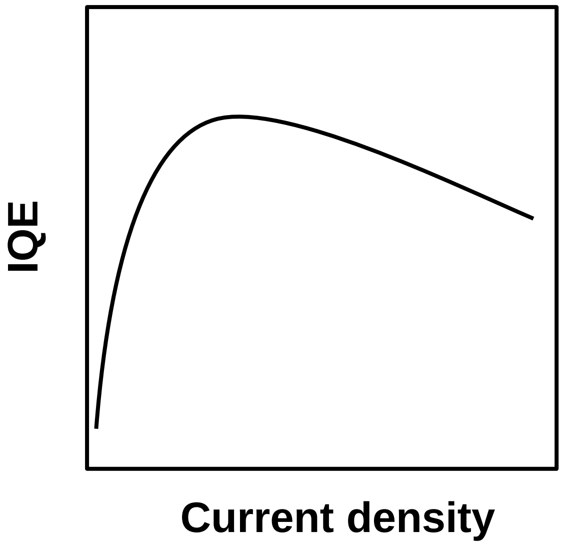
$$\frac{dN}{dt} = \frac{\eta_{inj} J}{ed} - AN - BN^2 - CN^3$$

## Steady-state

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

## Internal quantum efficiency

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



# ABC model for LED efficiency

## Carrier density rate equation

*Injection efficiency (carrier overshoot and escape)*

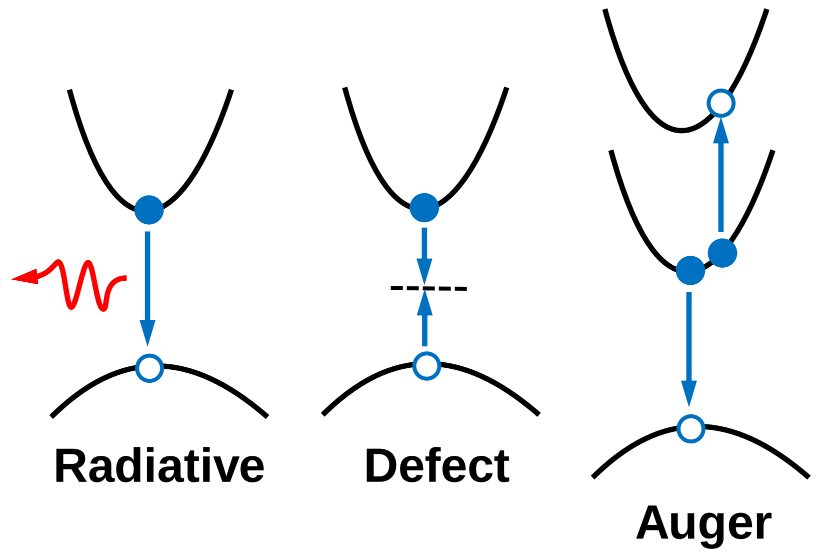
$$\frac{dN}{dt} = \frac{\eta_{inj} J}{ed} - AN - BN^2 - CN^3$$

*Defects*

*Spontaneous emission*

*Auger*

## Carrier losses

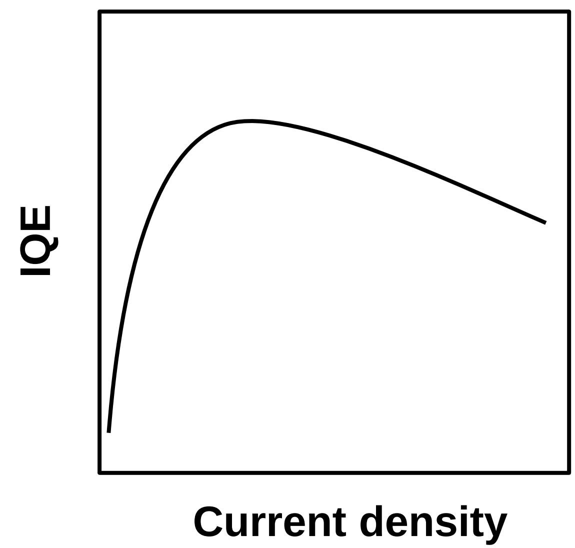



## Steady-state

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

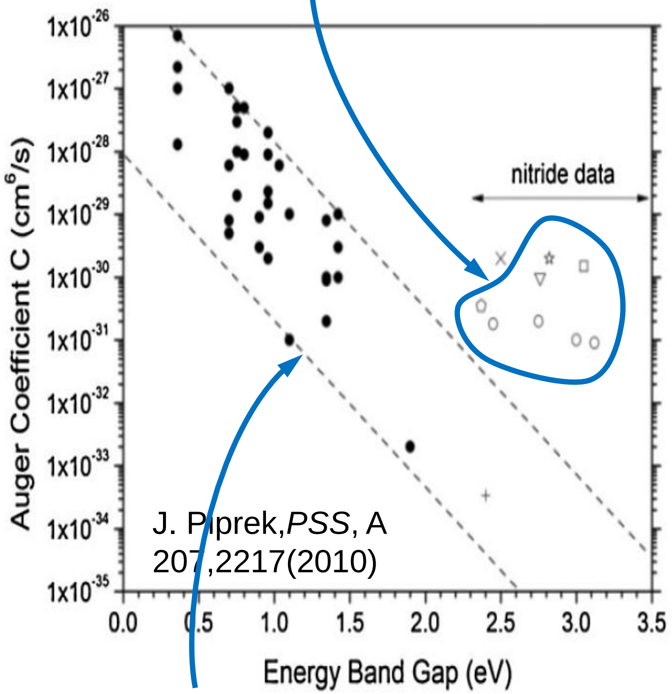
## Internal quantum efficiency

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



# Motivations for a more detailed model

**Auger coefficients needed for ABC model to reproduce experiment**

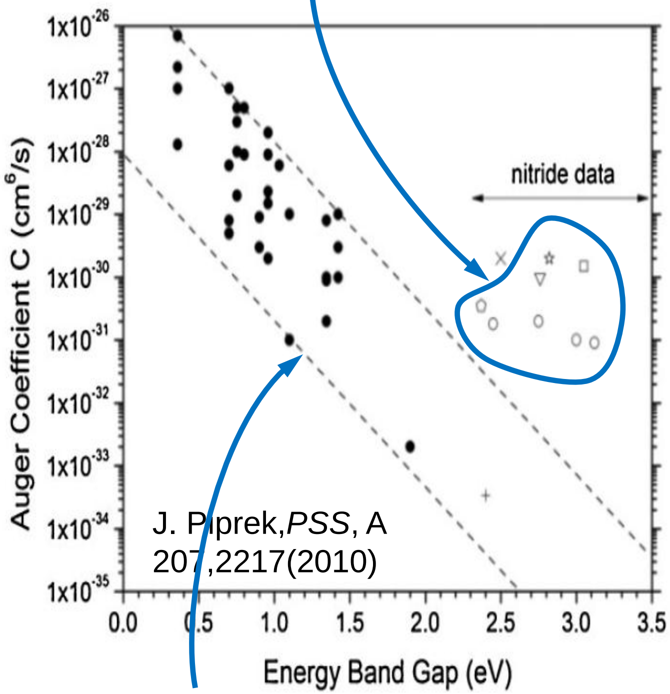



J. Piprek, *PSS*, A 207, 2217(2010)

**Generally accepted scaling of Auger coefficient with bandgap**

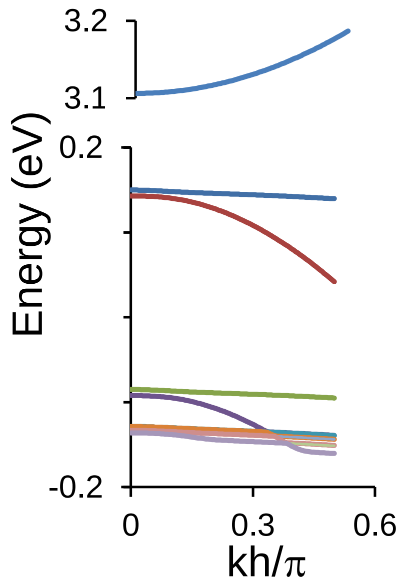
# Motivations for a more detailed model

**Auger coefficients needed for ABC model to reproduce experiment**



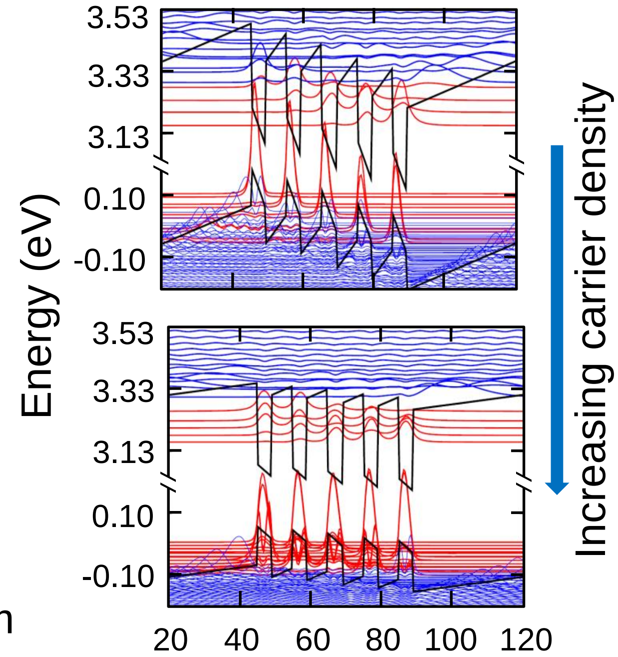

**Generally accepted scaling of Auger coefficient with bandgap**

**Energy dispersions**




In-plane momentum

**Carrier density dependent band structure changes**




Growth direction (nm)

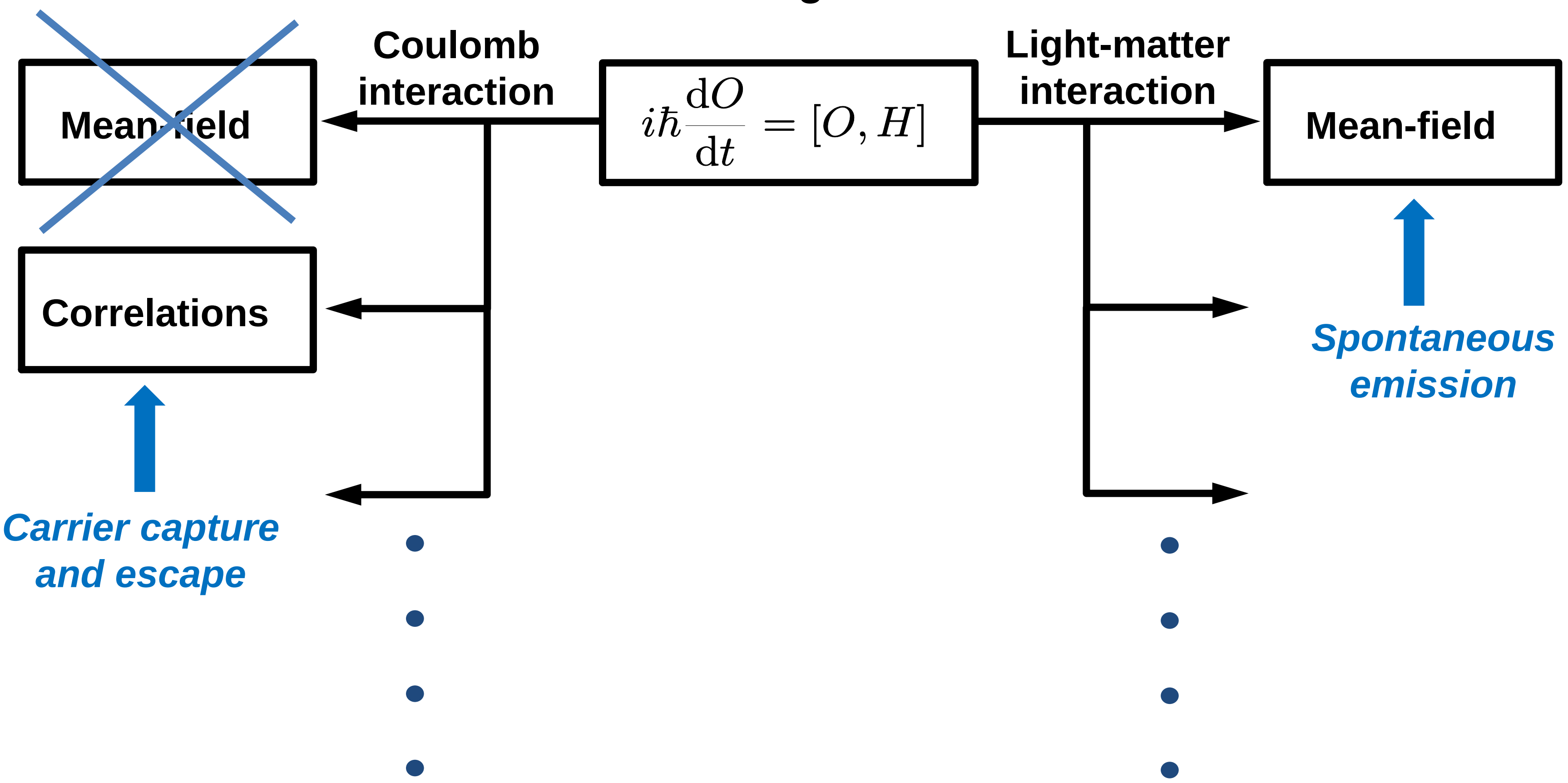
# Approach

**Hamiltonian**

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

**+ Coulomb interaction**

**Hiesenberg Picture**

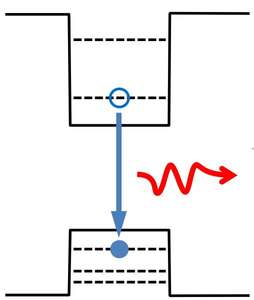


# Model

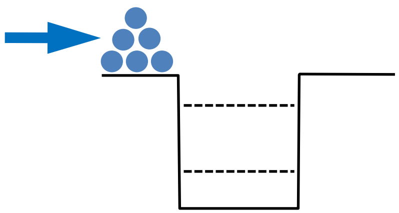
e or *h*

$$\frac{dn_{\sigma,\alpha_\sigma,k_\perp}}{dt} = -n_{\sigma,\alpha_\sigma,k_\perp}\sum_{\alpha_{\sigma'}} b_{\alpha_\sigma,\alpha_{\sigma'},k_\perp}\, n_{\sigma',\alpha_{\sigma'},k_\perp} - A n_{\sigma,\alpha_\sigma,k_\perp}$$

Spontaneous emission (>ns)



Carrier injection



$$\frac{dn^b_{\sigma,k}}{dt} = -b_k n^b_{e,k} n^b_{h,k} + \frac{J}{eN^p_\sigma} f\left(\varepsilon^b_{\sigma,k}, \mu^p_\sigma, T_p\right) - A_b n^b_{\sigma,k}$$

# Model

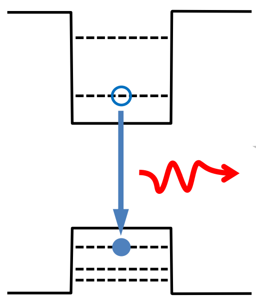
*e* or *h*

$$\frac{dn_{\sigma,\alpha_\sigma,k_\perp}}{dt} = -n_{\sigma,\alpha_\sigma,k_\perp}\sum_{\alpha_{\sigma'}} b_{\alpha_\sigma,\alpha_{\sigma'},k_\perp}\, n_{\sigma',\alpha_{\sigma'},k_\perp} - An_{\sigma,\alpha_\sigma,k_\perp}$$

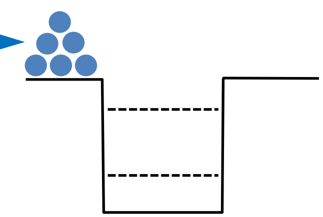
$$-\gamma_{c-c}\left[n_{\sigma,\alpha_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_\sigma,T\right)\right]$$

$$-\gamma_{c-p}\left[n_{\sigma,\alpha_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_\sigma^L,T_L\right)\right]$$

Spontaneous emission (>ns)



Carrier injection

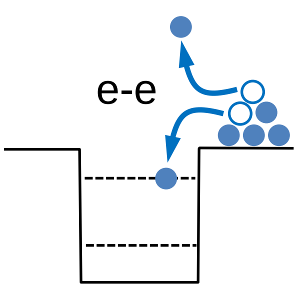


$$\frac{dn_{\sigma,k}^b}{dt} = -b_k n_{e,k}^b n_{h,k}^b + \frac{J}{eN_\sigma^p} f\left(\varepsilon_{\sigma,k}^b,\mu_\sigma^p,T_p\right) - A_b n_{\sigma,k}^b$$

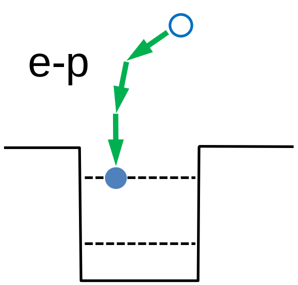
$$-\gamma_{c-c}\left[n_{\sigma,k}^b - f\left(\varepsilon_{\sigma,k}^b,\mu_\sigma,T\right)\right]$$

$$-\gamma_{c-p}\left[n_{\sigma,k}^b - f\left(\varepsilon_{\sigma,k}^b,\mu_\sigma^L,T_L\right)\right]$$

Carrier-carrier (100fs)




Carrier-phonon (<1ps)




**Similar for holes**

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

# Internal quantum efficiency

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

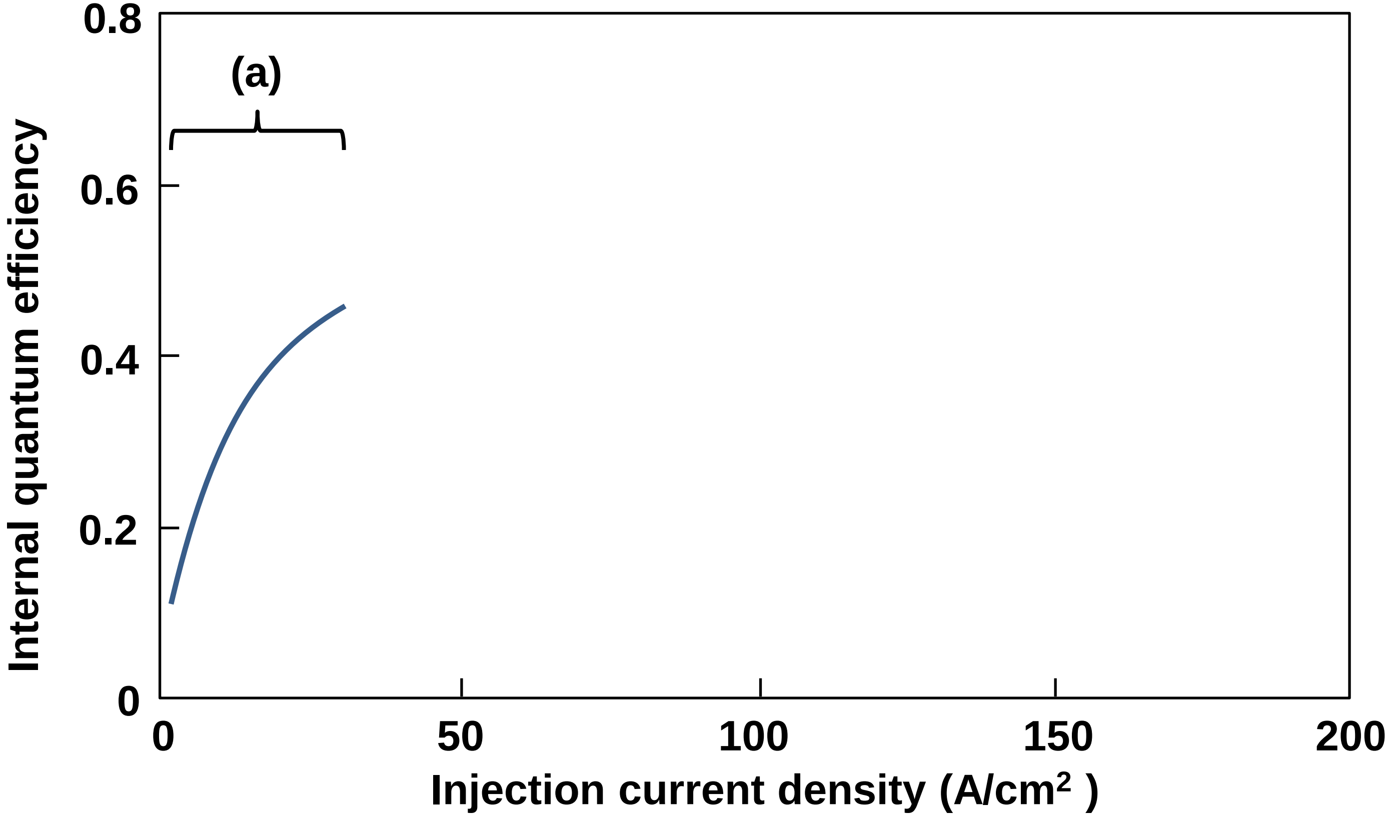
$$IQE=\frac{e}{JS}\left(\sum_{\alpha_e,\alpha_h,k_\perp} b_{\alpha_e,\alpha_h,k_\perp} n_{e,\alpha_e,k_\perp} n_{e,\alpha_e,k_\perp}+\sum_k b_k n_{e,k}^b n_{h,k}^b\right)$$

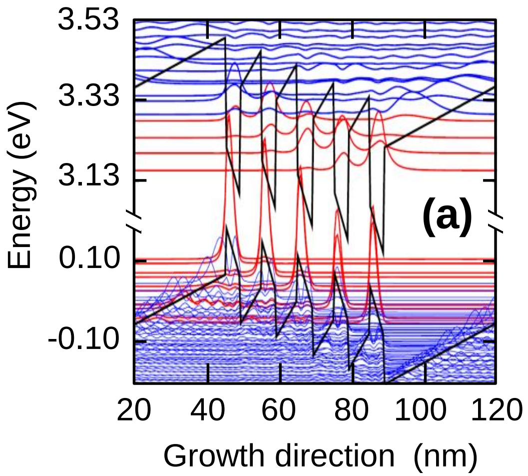
$$\frac{1}{\hbar\epsilon_b\pi c^3}\left|\wp_{\alpha_e,\alpha_h,k_\perp}\right|^2\Omega^3_{\alpha_e,\alpha_h,k_\perp}$$

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

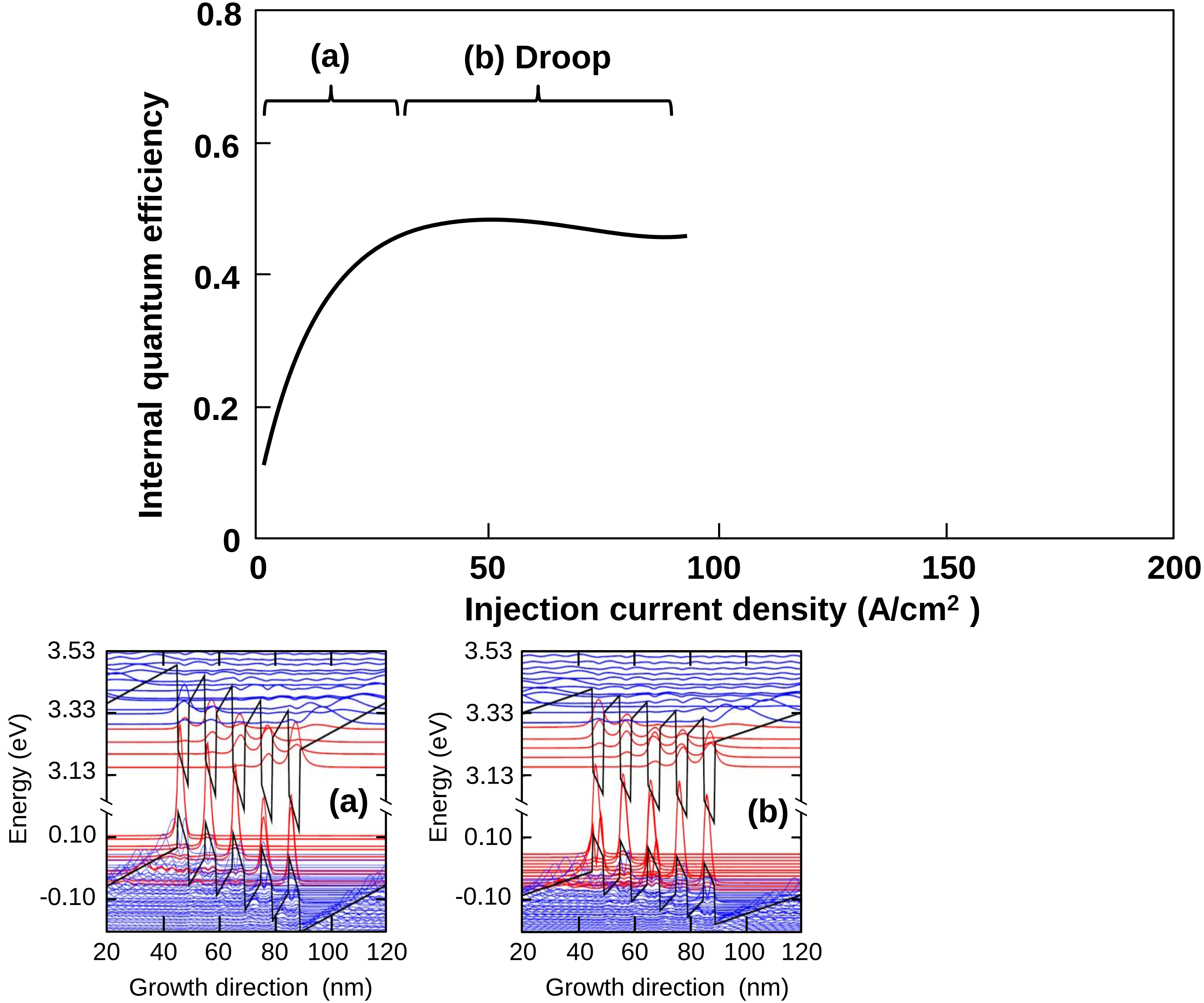
$$\frac{1}{4}\left|\sum_{\beta_e}\sum_{\beta_h}\sum_{m_e}\sum_{m_h} A_{\beta_e,\alpha_e,k_\perp} A_{\beta_h,\alpha_h,k_\perp}\int_{-\infty}^{\infty} dz\, u_{m_e,\beta_e}(z)\, u_{m_h,\beta_h}(z)\right|^2$$

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

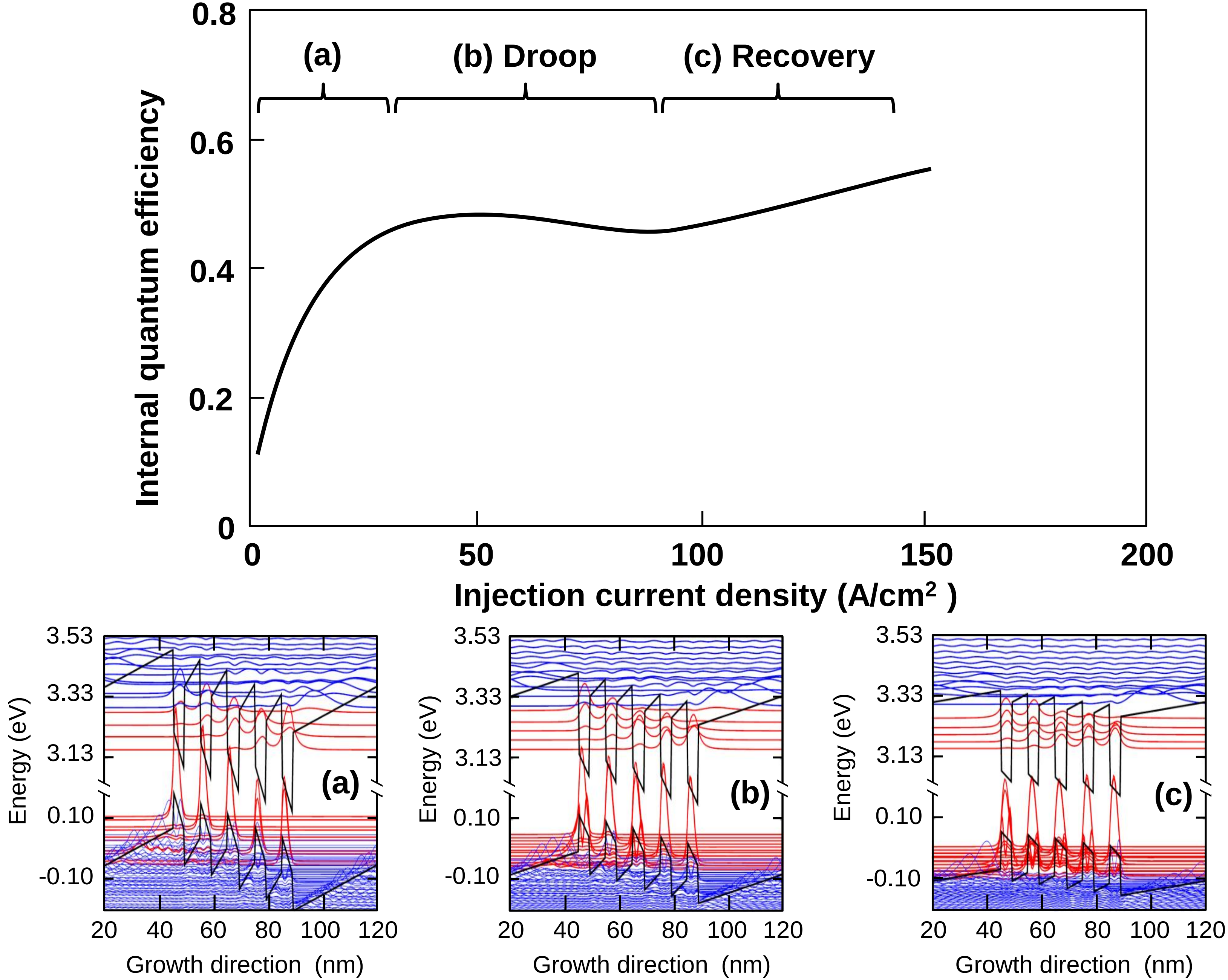


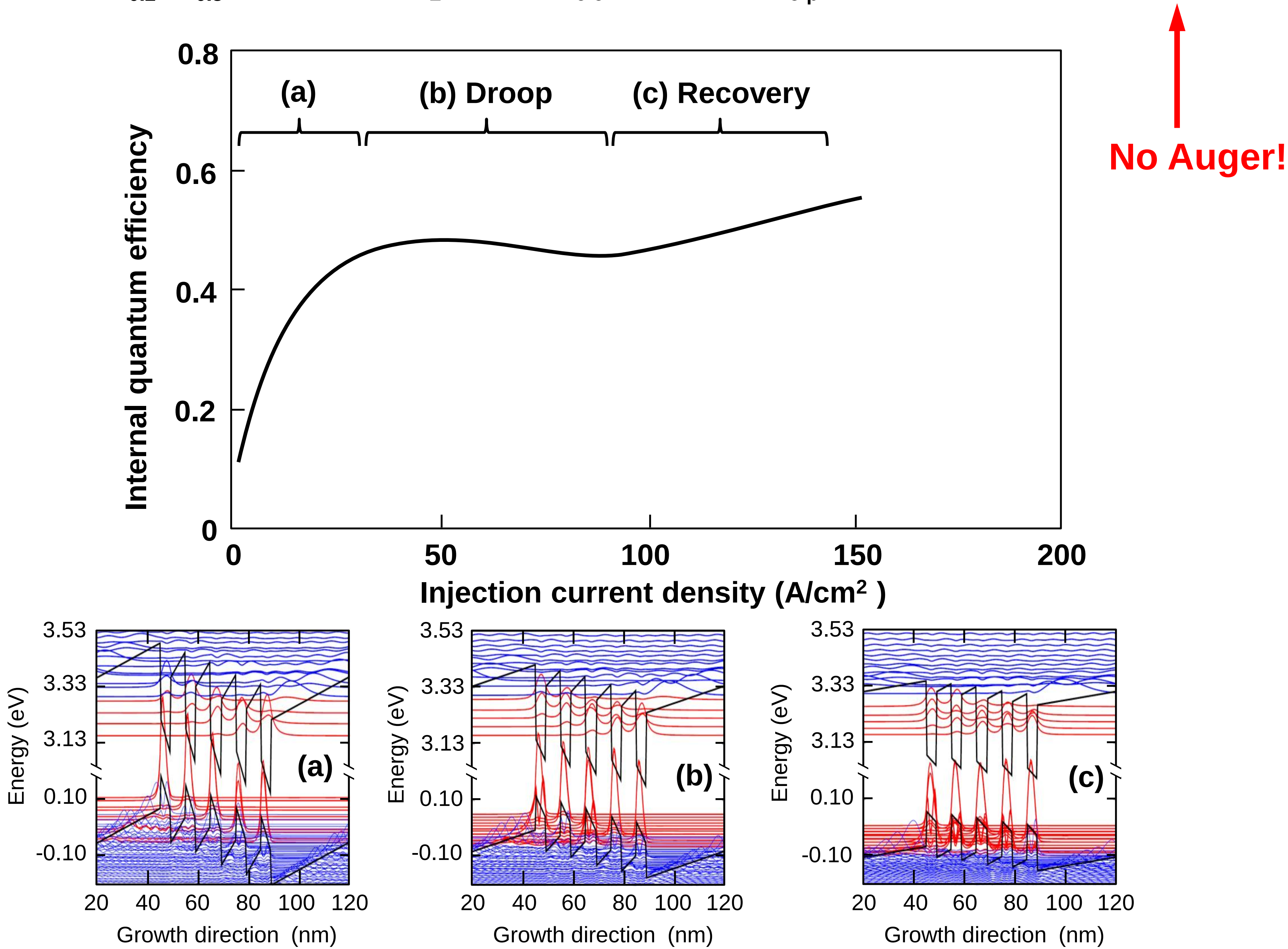
4nm $In_{0.2}Ga_{0.8}N$/6nmGaN, $T_L$ = 300K, $\gamma_{c\text{-}c} = 5 \times 10^{13} s^{-1}$, $\gamma_{c\text{-}p} = 10^{13} s^{-1}$, $A = 10^{-7} s^{-1}$, C = 0

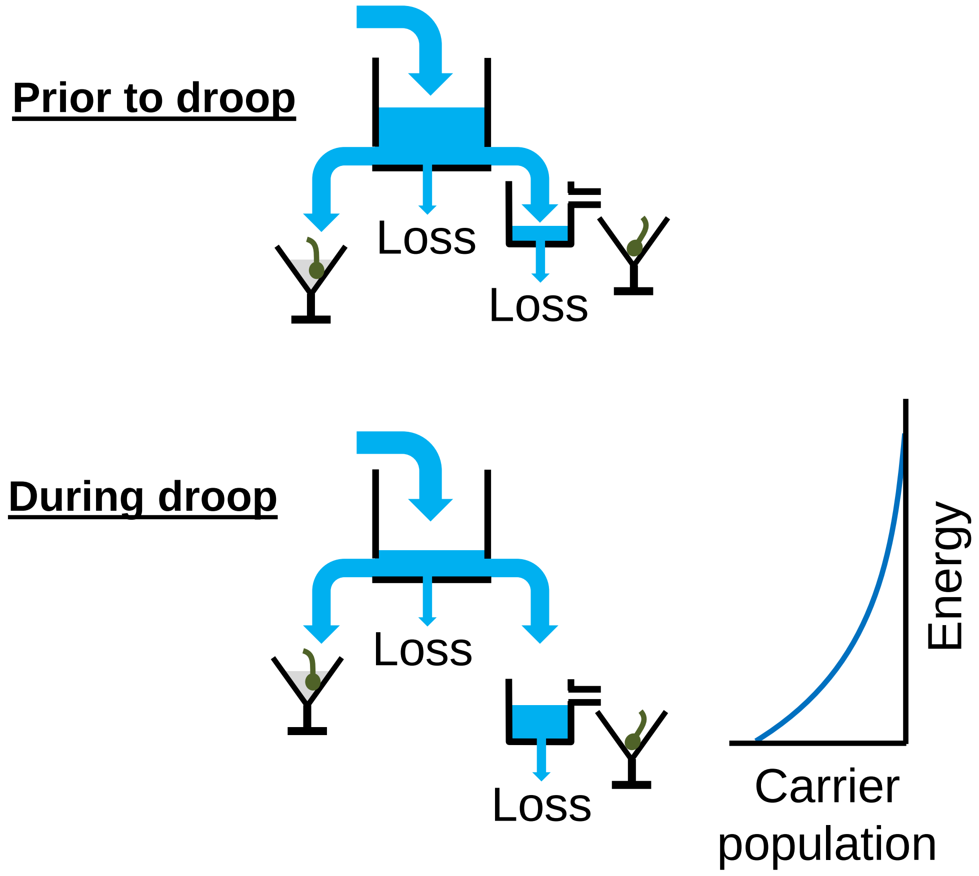


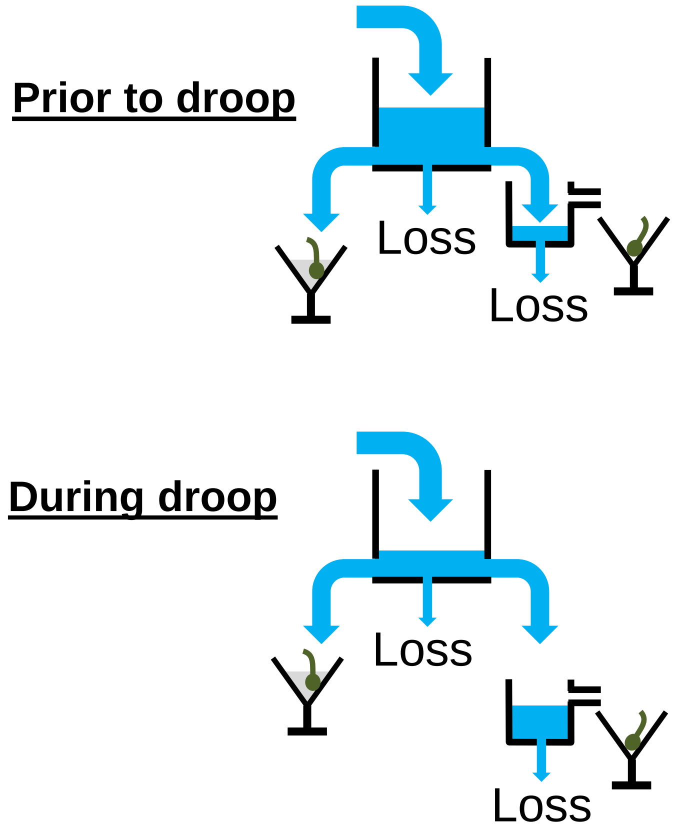
4nm $In_{0.2}Ga_{0.8}N$/6nmGaN, $T_L$ = 300K, $\gamma_{c\text{-}c} = 5\times10^{13}s^{-1}$, $\gamma_{c\text{-}p} = 10^{13}s^{-1}$, $A = 10^{-7}s^{-1}$, C = 0



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




Prior to droop
Loss
Loss
During droop
Loss
Loss
Energy
Carrier population



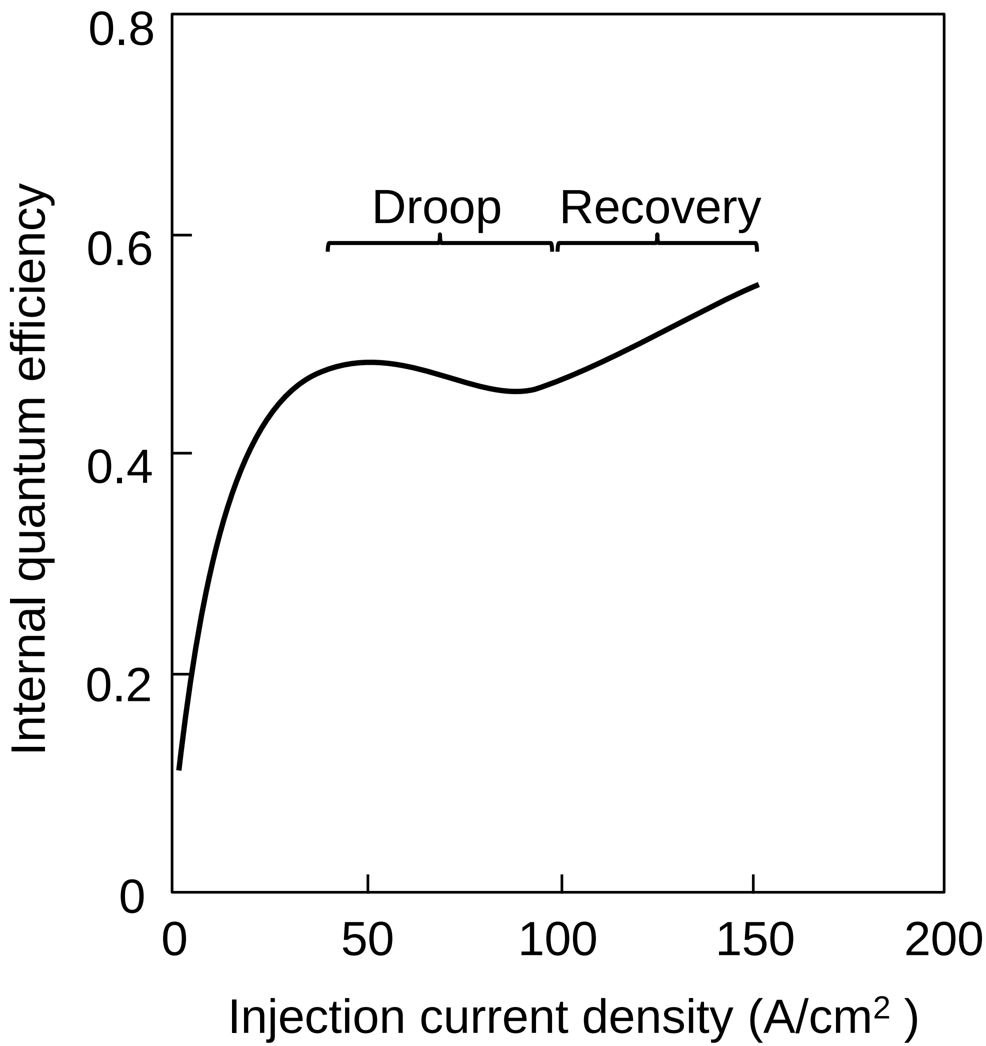

4nm $In_{0.2}Ga_{0.8}N$/6nmGaN

$T_L$ = 300K

$\gamma_{c\text{-}c} = 5\mathrm{x}10^{13}\mathrm{s}^{-1}$, $\gamma_{c\text{-}p} = 10^{13}\mathrm{s}^{-1}$

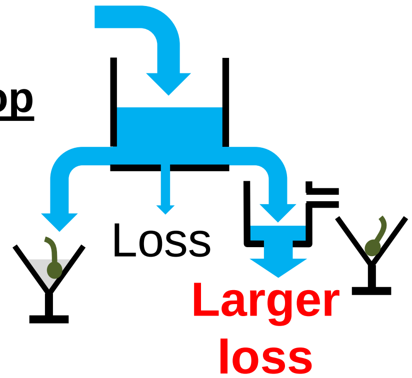
$A = 10^{-7}\mathrm{s}^{-1}$

C = 0 **No Auger!**

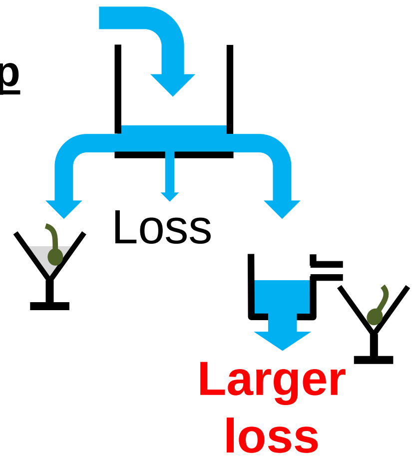


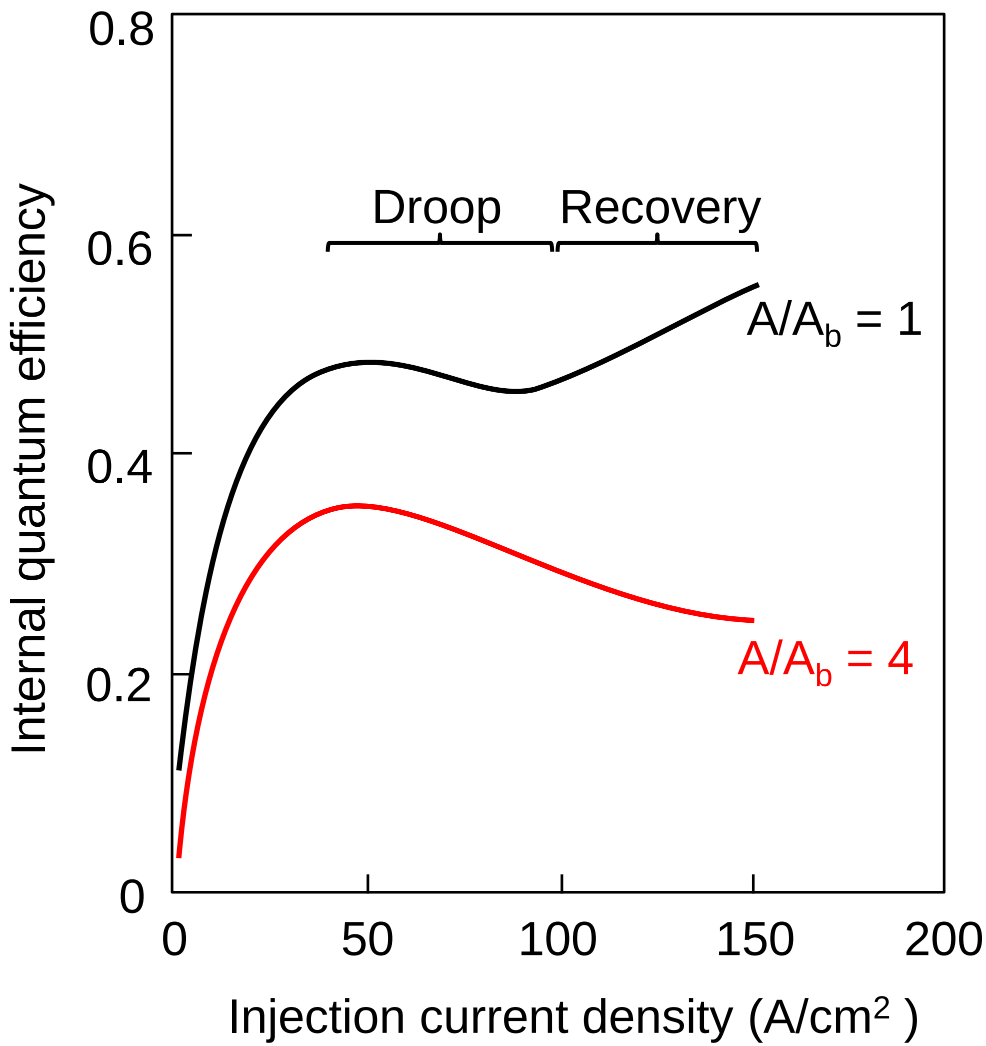
# Localized defects

**Prior to droop**




**During droop**




4nm $In_{0.2}Ga_{0.8}N$/6nmGaN

$T_L$ = 300K

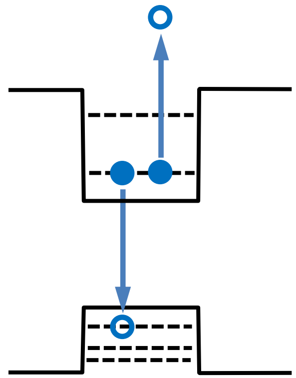
$\gamma_{c\text{-}c} = 5\times10^{13}s^{-1}$, $\gamma_{c\text{-}p} = 10^{13}s^{-1}$

$A = 10^{-7}s^{-1}$

C = 0 ← **No Auger!**

**SRH (linear) + bandstructure ➡ $N^3$ loss!**

# Auger loss



Auger

e or h

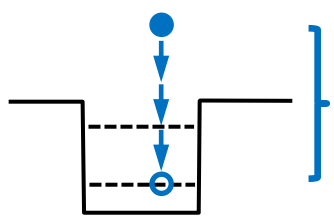
$$\left.\frac{dn_{\sigma,\alpha_\sigma,k_\perp}}{dt}\right|_{ag} = \overbrace{-\gamma_{ag}\left[n_{\sigma,\alpha_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_{ag},T_{ag}\right)\right]}^{\text{Auger}}$$

$CN^2$

Chemical potential for intrinsic semiconductor

$$\underbrace{-\gamma_{c-p}\left[n_{\sigma,\alpha_\sigma,k_\perp} - f\left(\varepsilon_{\sigma,k_\perp},\mu_\sigma^L,T_L\right)\right]}_{\text{Carrier-phonon}}$$

Carrier-phonon



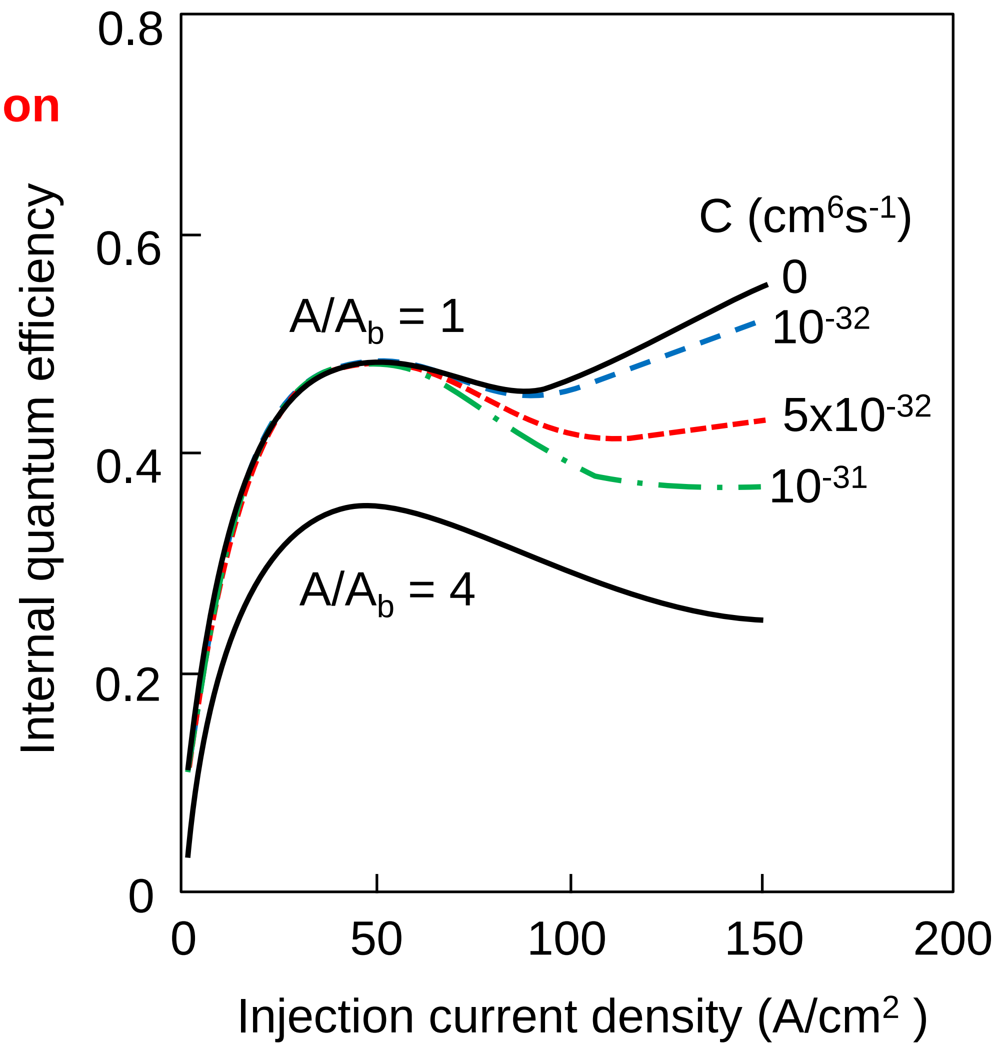
Heat

APL **97**, 121105, 2010

# Auger loss

**Auger prevents IQE recovery**

**Required C << ABC model estimation**




4nm $In_{0.2}Ga_{0.8}N$/6nmGaN

$T_L$ = 300K

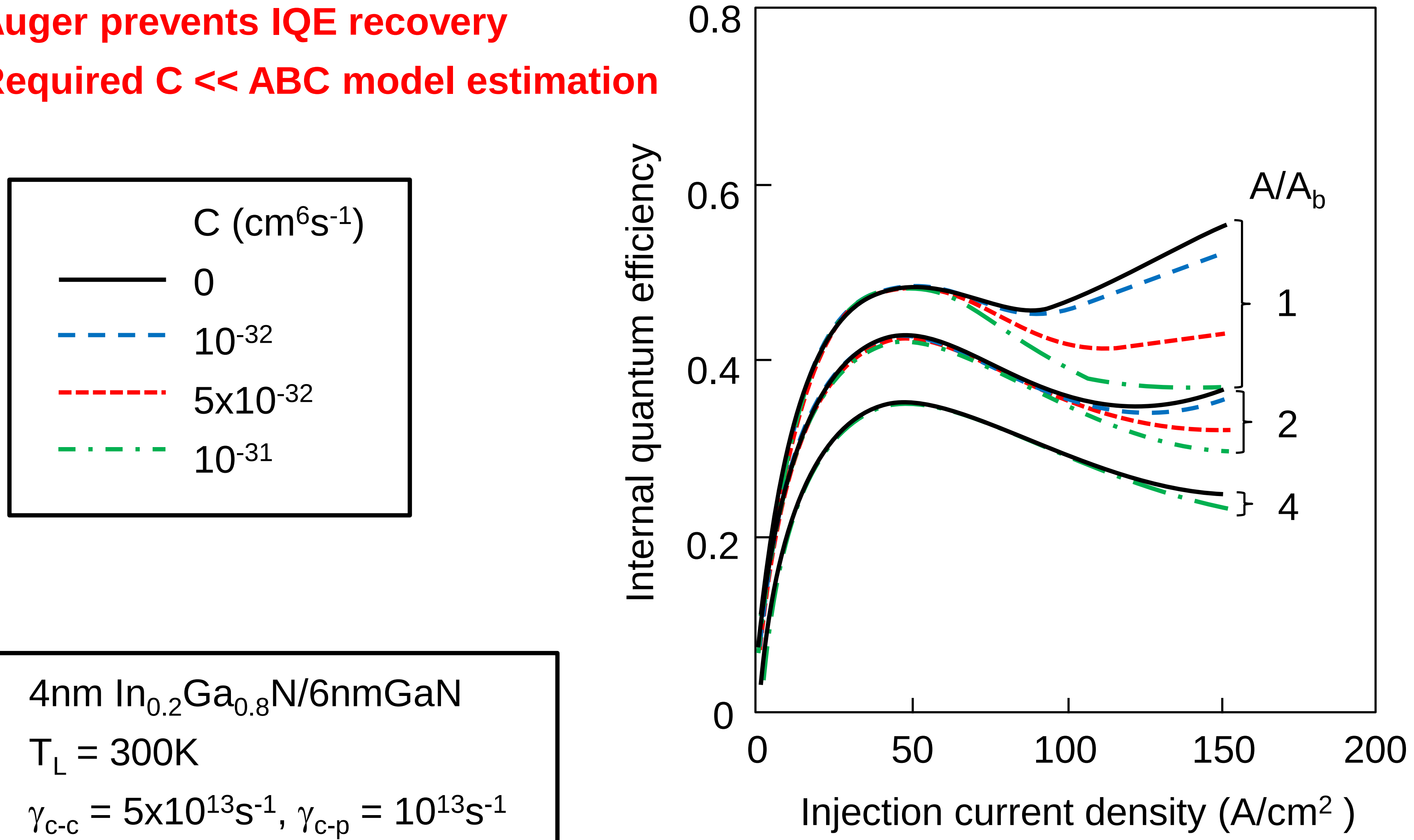
$\gamma_{c\text{-}c} = 5\times10^{13}s^{-1}$, $\gamma_{c\text{-}p} = 10^{13}s^{-1}$

$A = 10^{-7}s^{-1}$

# Combination of localized defects and Auger loss

**Auger prevents IQE recovery**

**Required C << ABC model estimation**




4nm $In_{0.2}Ga_{0.8}N$/6nmGaN

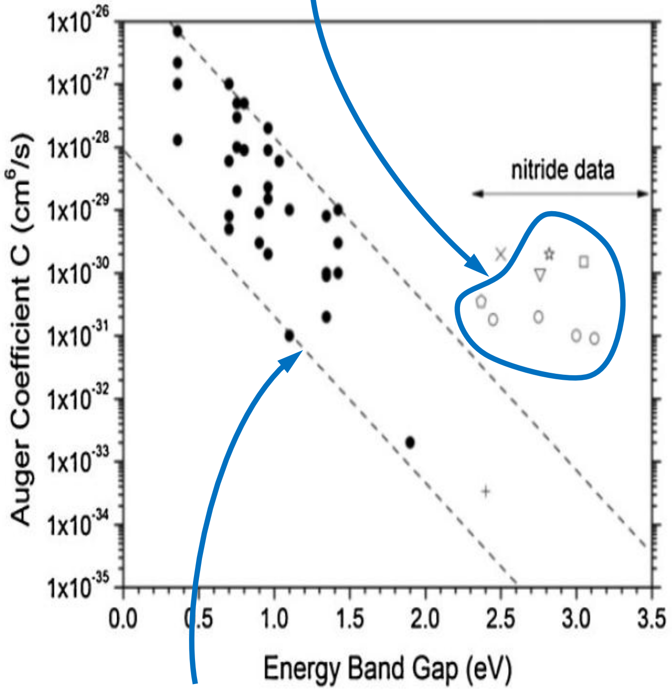
$T_L$ = 300K

$\gamma_{c\text{-}c} = 5x10^{13}s^{-1}$, $\gamma_{c\text{-}p} = 10^{13}s^{-1}$

$A = 10^{-7}s^{-1}$

# Motivations for a more detailed model

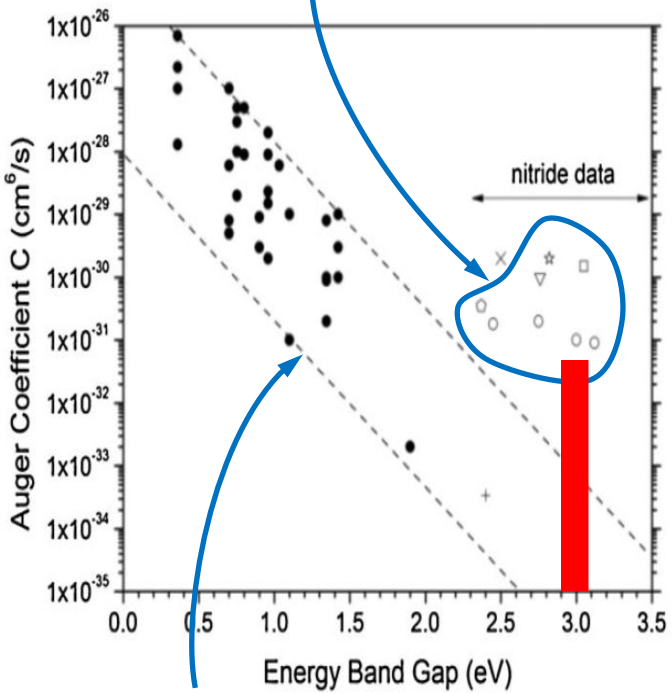
Auger coefficients needed for ABC model to reproduce experiment




Generally accepted scaling of Auger coefficient with bandgap

# Motivations for a more detailed model

Auger coefficients needed for ABC model to reproduce experiment

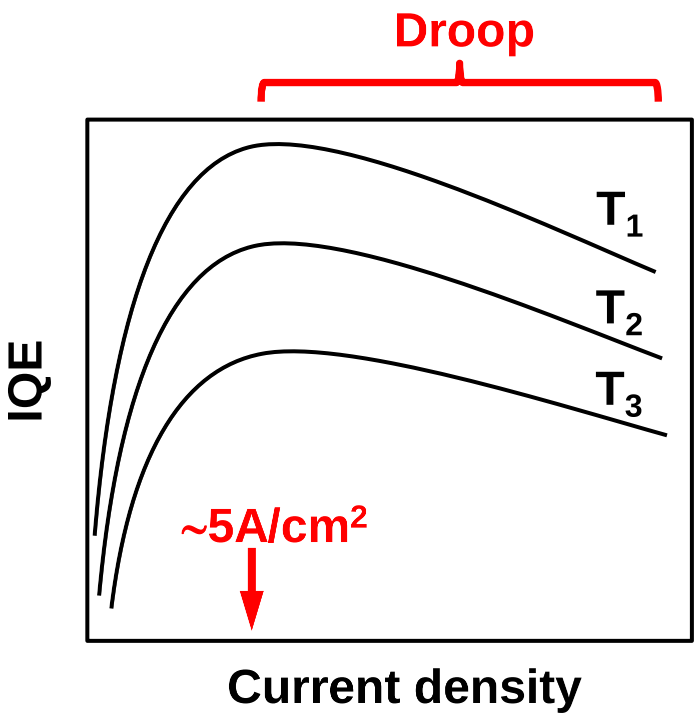



Generally accepted scaling of Auger coefficient with bandgap

Range of Auger coefficients producing efficiency droop according to present LED model

<u>Agreement between droop observation and 1st principle theory</u>

# Summary




**Can fit experiment with :**

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

| | |
|---|---|
| **Extrinsic ?** | **Intrinsic ?** |
| Localization | Auger |
| Current leakage | Screening of piezoelectric field |
| Defect loss | |

**Talk --- describes k-resolve carrier population model**

**--- systematic description of above effects at microscopic level**

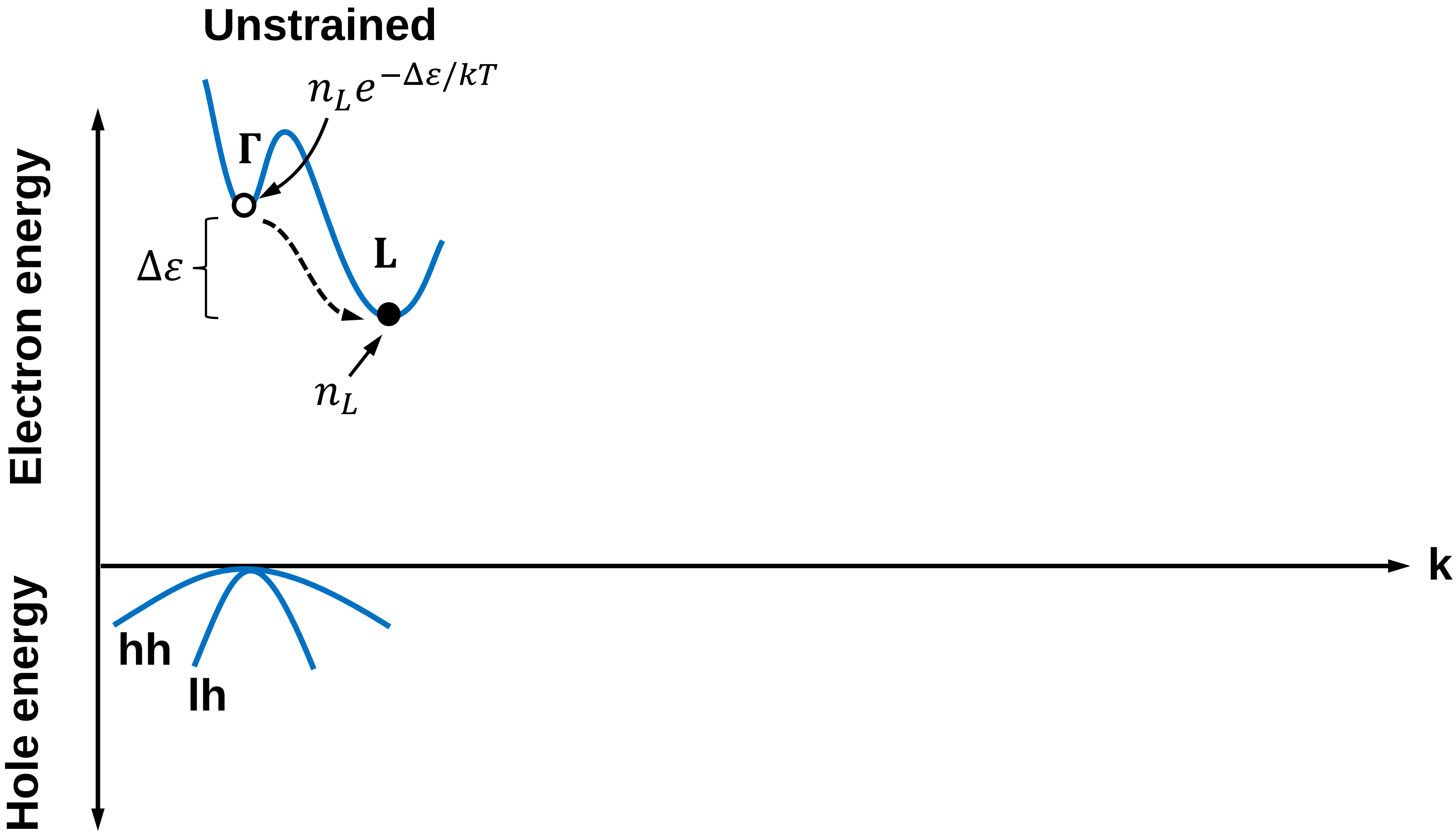
**--- droop can arise from --- screening of QCSE**

**--- localization of SRH losses**

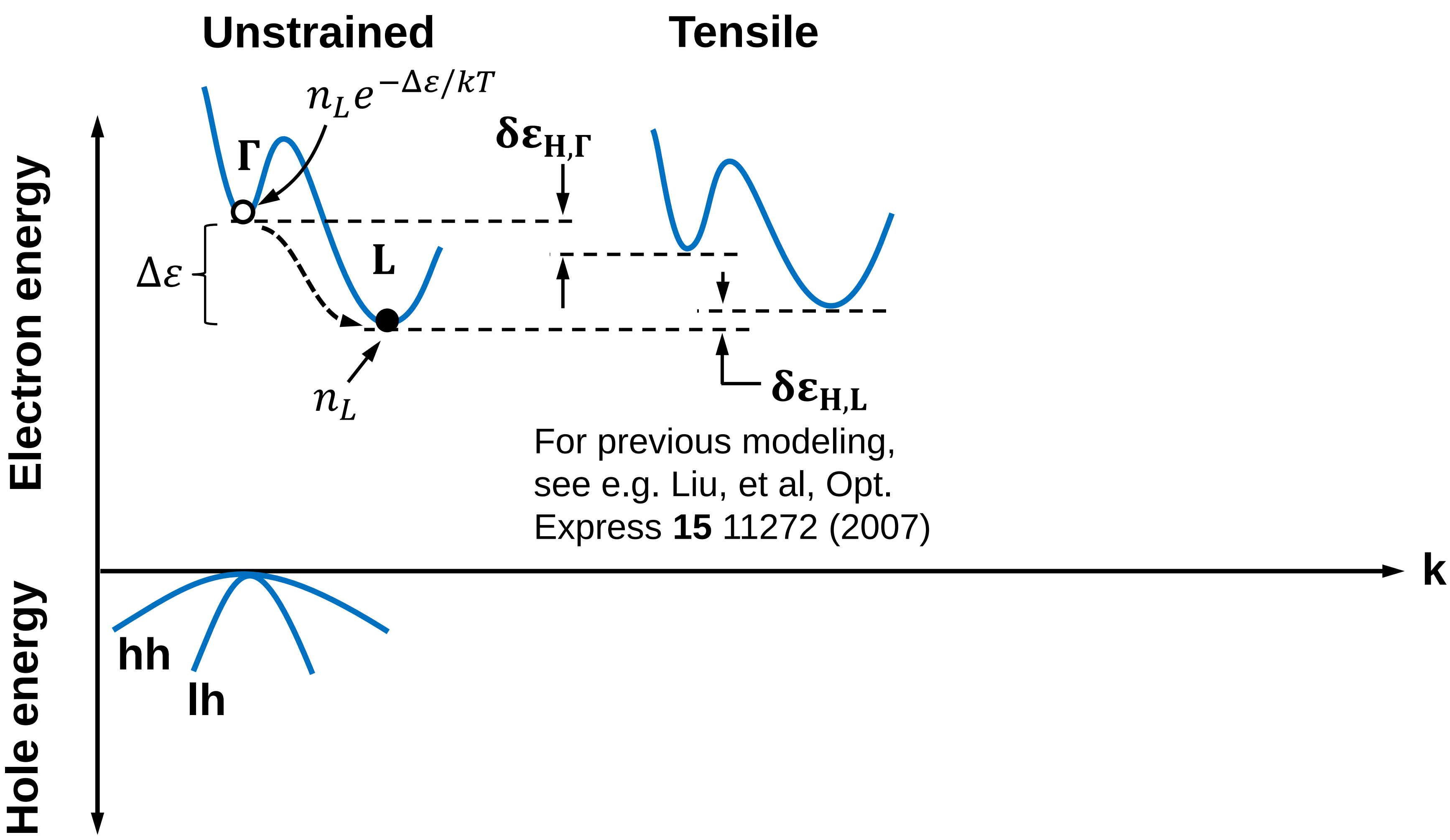
**--- Auger loss (with small necessary C)**

# Ge-on-Si Laser

# Effects of strain and doping on Ge

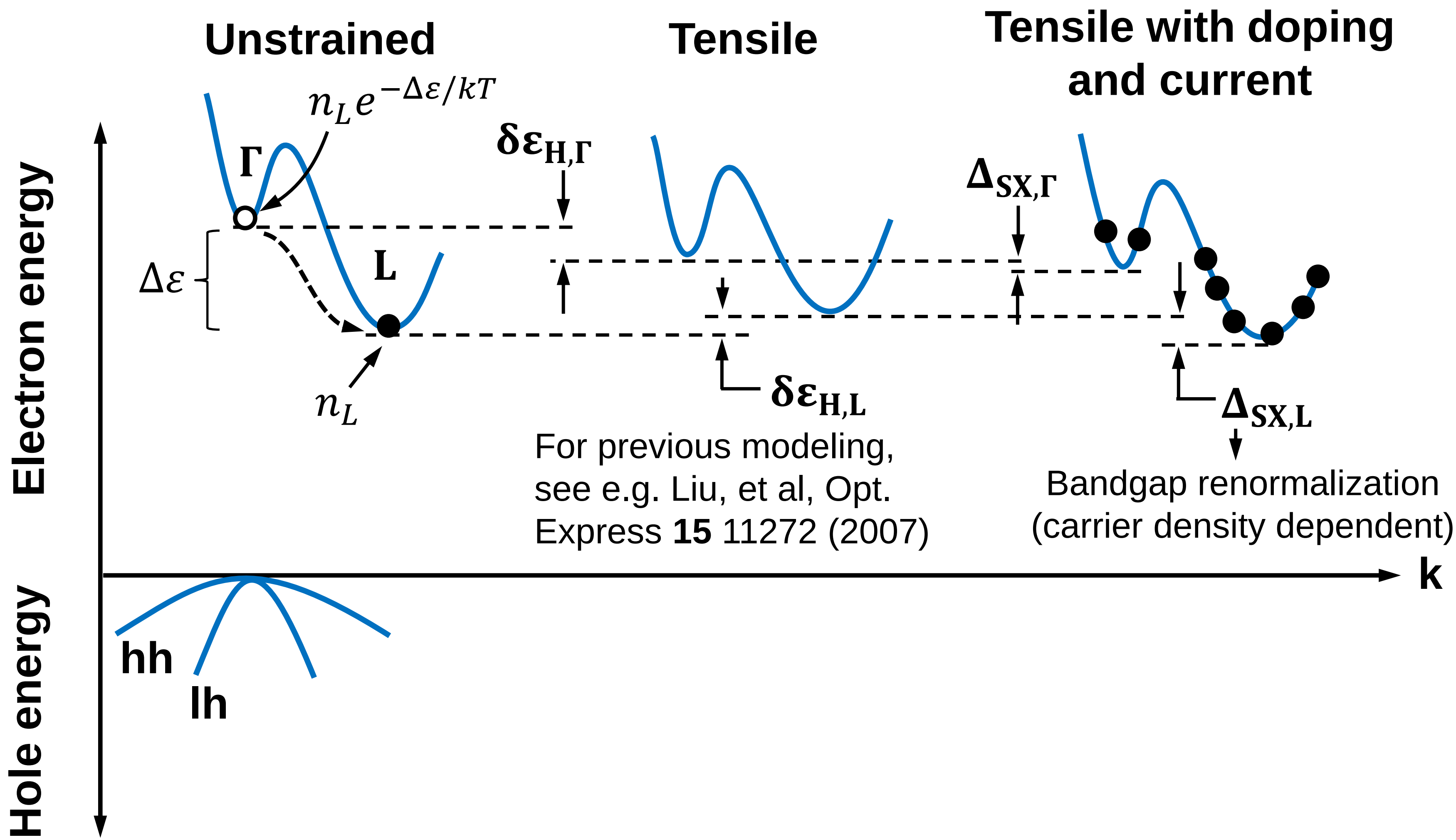


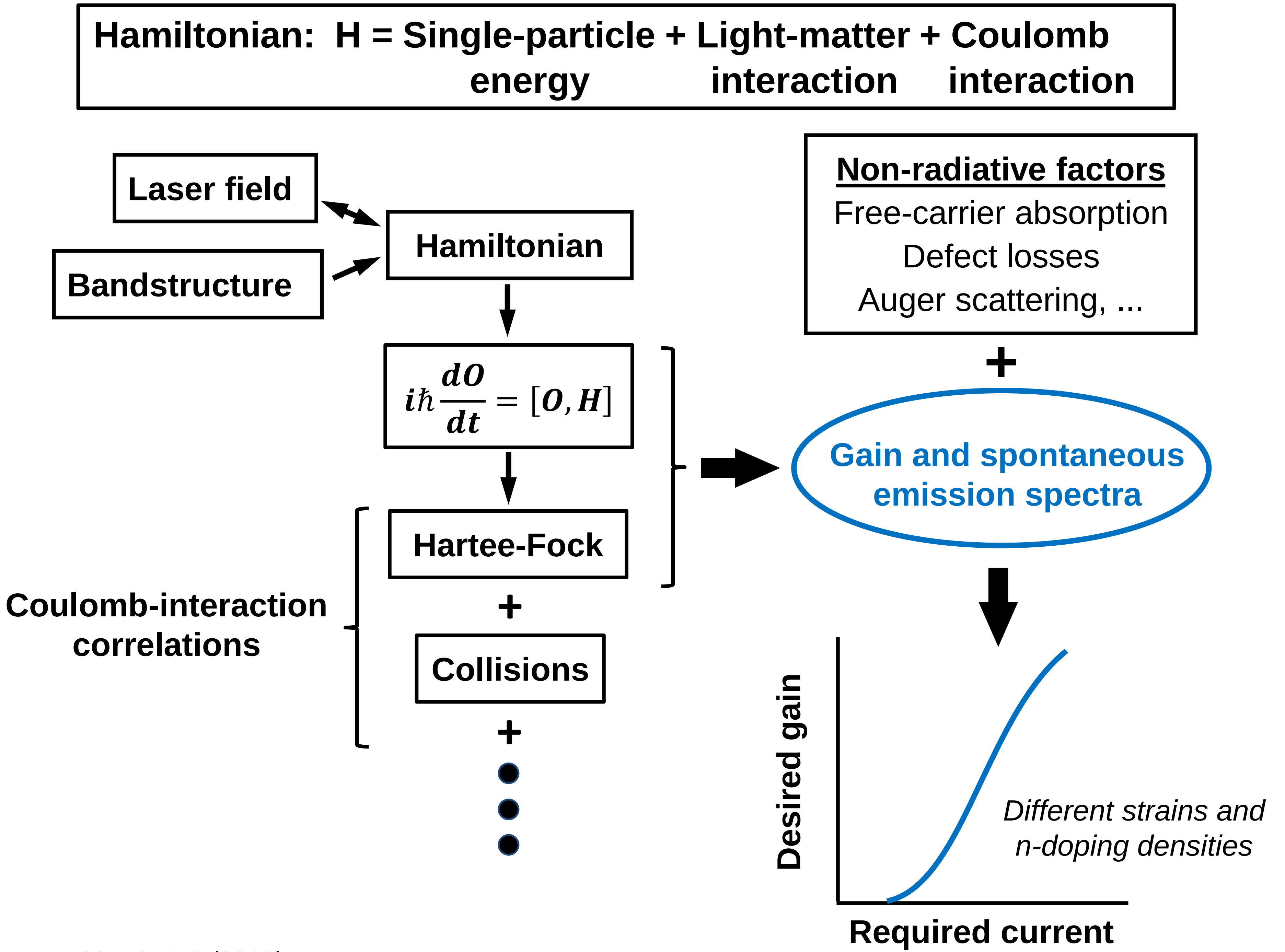
# Effects of strain and doping on Ge




For previous modeling,
see e.g. Liu, et al, Opt.
Express **15** 11272 (2007)

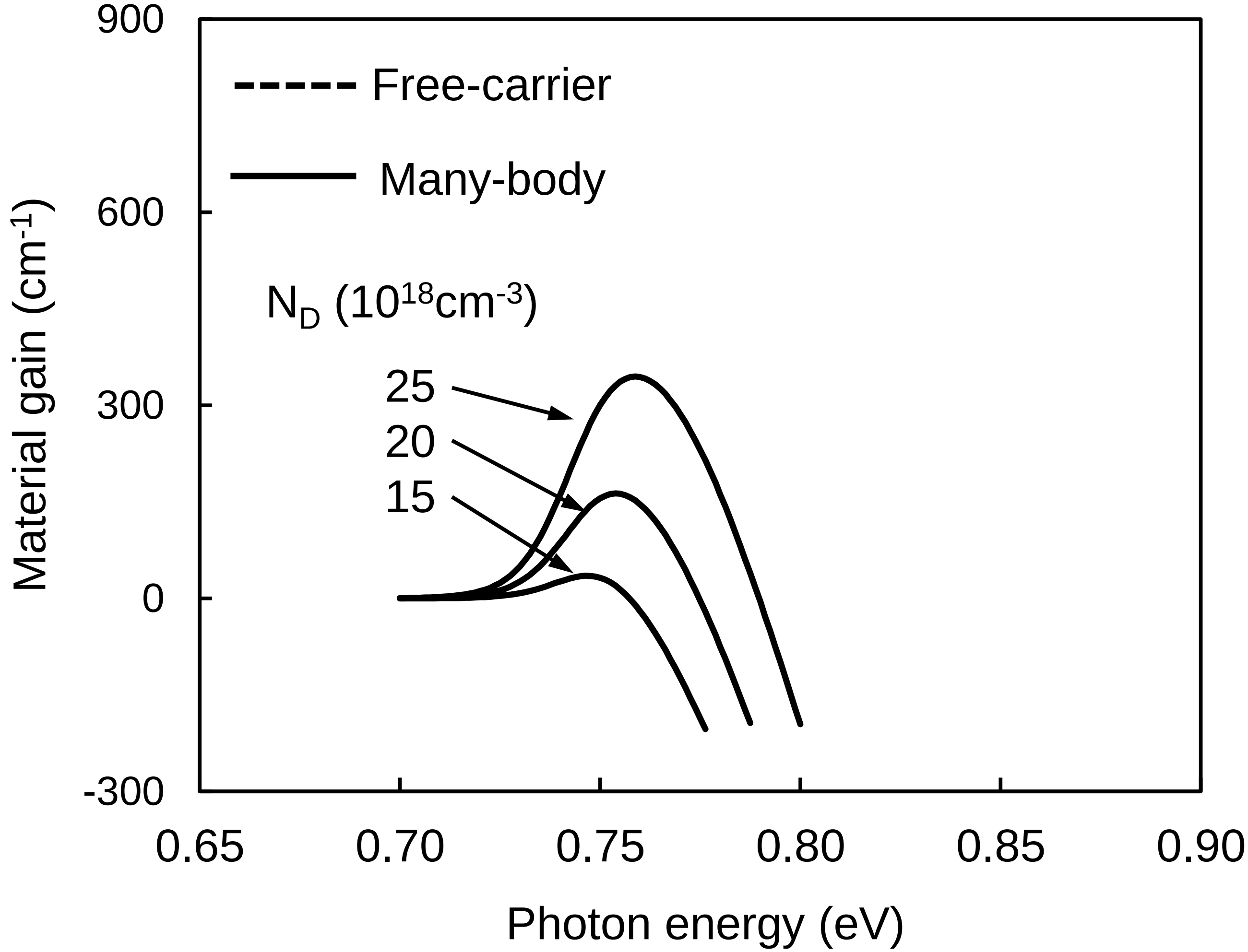
# Effects of strain and doping on Ge





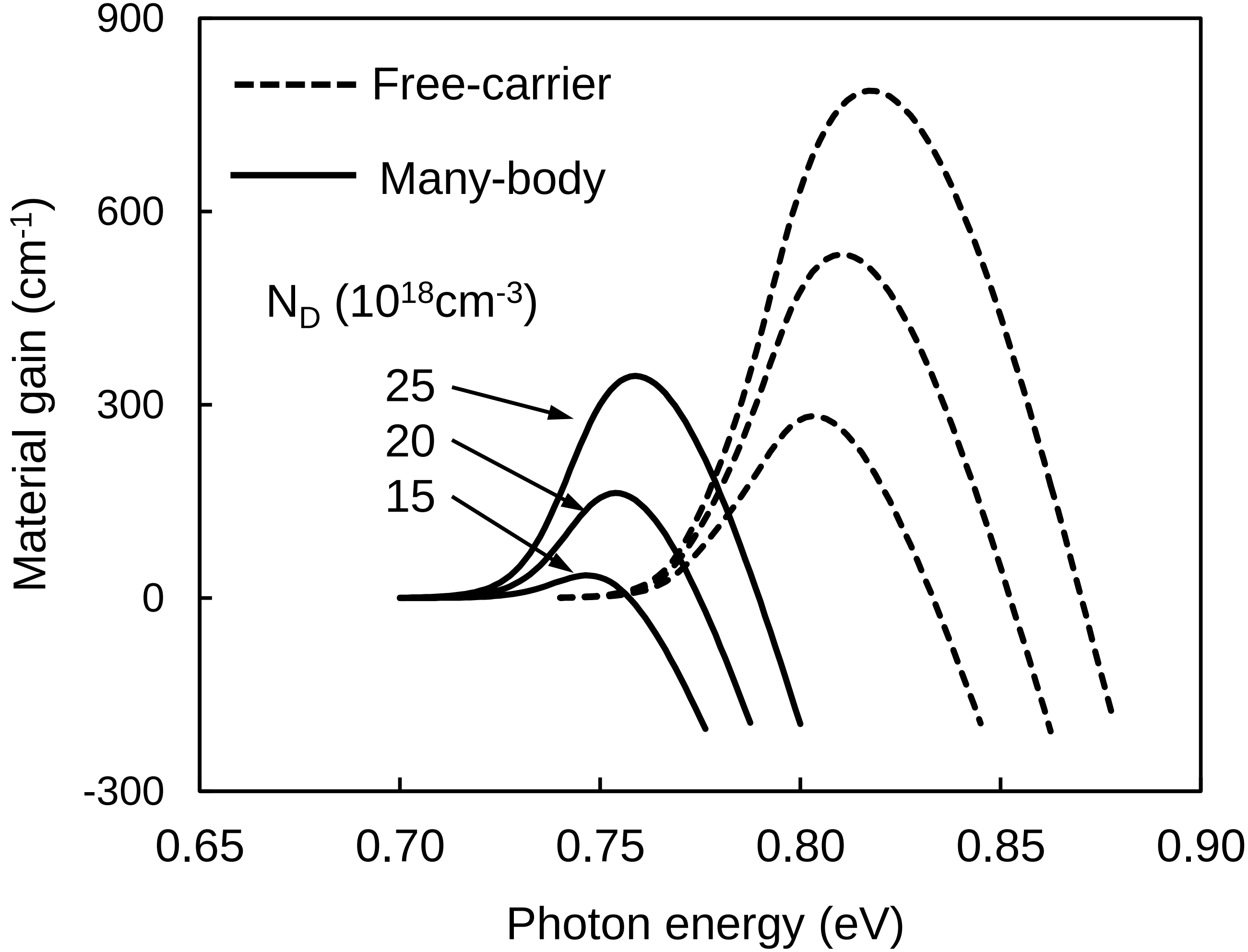

APL 100, 191113 (2012)

# Gain spectrum




T = 300K, 0.2% tensile strain, $\gamma = 10^{13} s^{-1}$, $N_I = 8 \times 10^{18} cm^{-3}$

# Gain spectrum



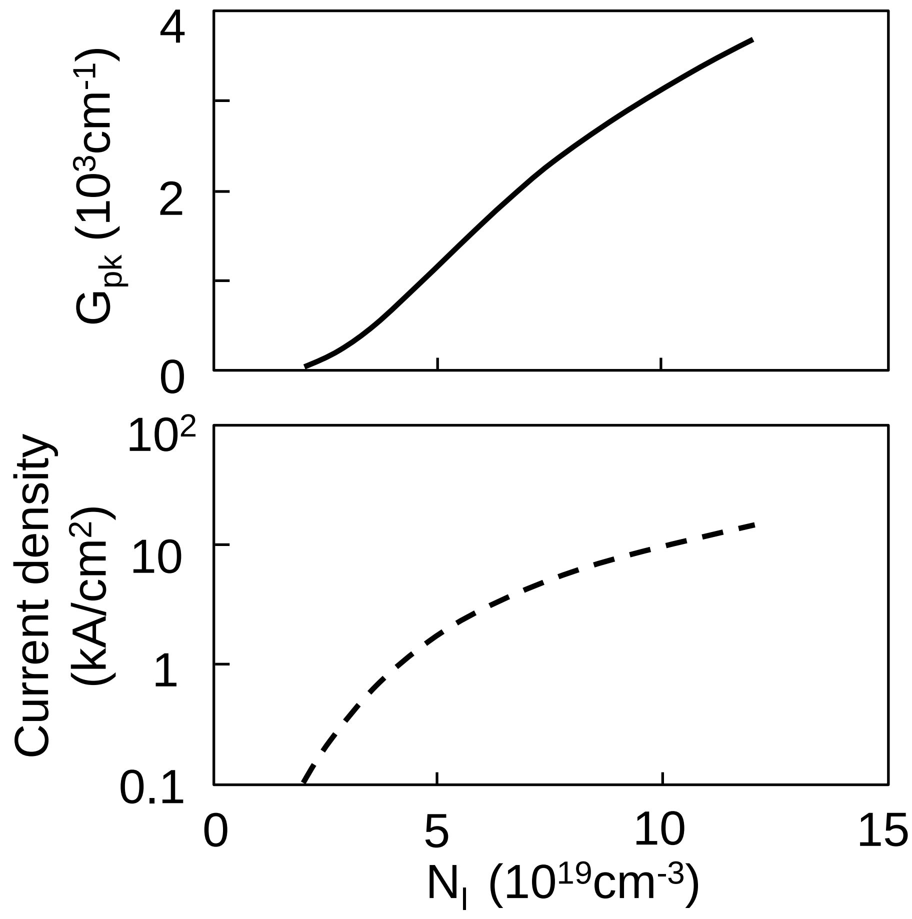

T = 300K, 0.2% tensile strain, $\gamma = 10^{13}s^{-1}$, $N_I = 8 \times 10^{18}cm^{-3}$

From gain spectrum:

1) Peak gain versus injected carrier density
2) Spontaneous emission contribution to current density:

$$J_{sp} = \frac{ed}{\hbar}\left(\frac{n}{\pi c}\right)^2 \int_0^\infty d\nu\, \nu^2 \frac{G(\nu)}{e^{\frac{\hbar\nu-\mu_{eh}}{k_B T}} - 1}$$

Unstrained, undoped



From gain spectrum:

1) Peak gain versus injected carrier density
2) Spontaneous emission contribution to current density:

$$J_{sp} = \frac{ed}{\hbar}\left(\frac{n}{\pi c}\right)^2 \int_0^{\infty} d\nu\, \nu^2 \frac{G(\nu)}{e^{\frac{\hbar\nu-\mu_{eh}}{k_B T}} - 1}$$

Free-carrier absorption:

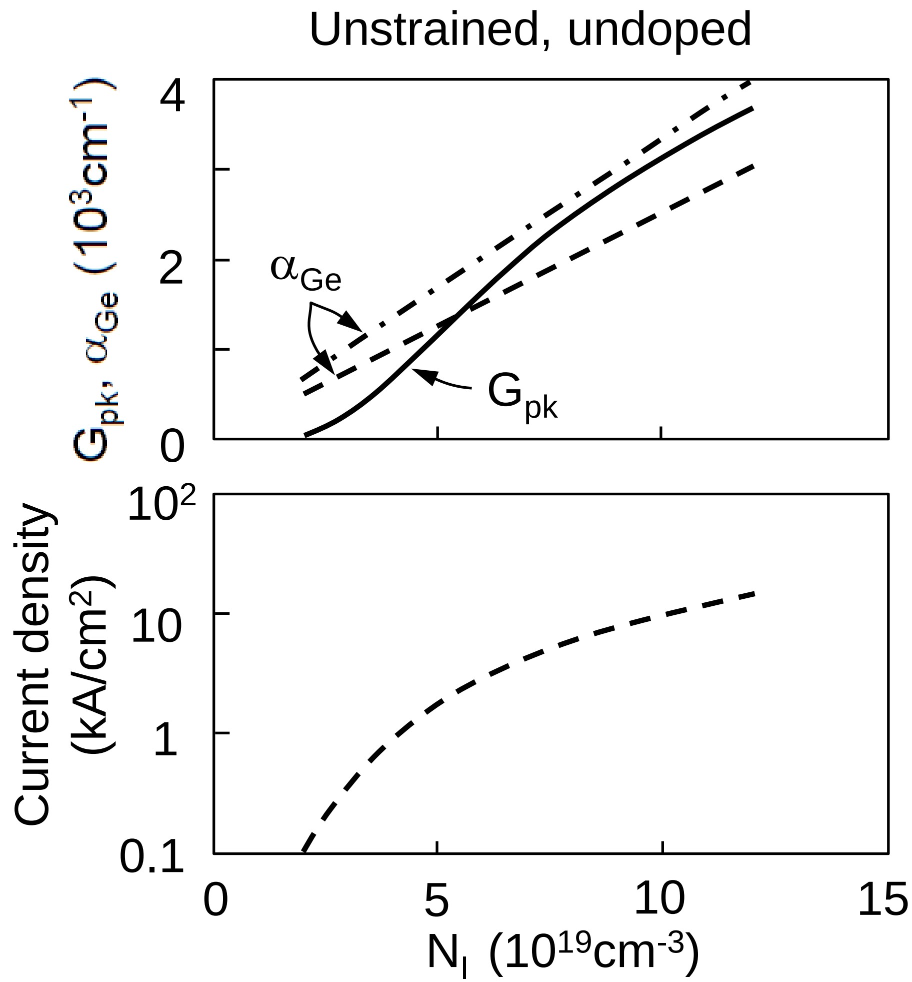
$$\alpha_{Ge} = \alpha_1(N_D + N_I) + \alpha_2 N_I$$

$\alpha_1(10^{-18} cm^2) = 5.54$ [1] $or$ $3.17$ [2]

$\alpha_2(10^{-17} cm^2) = 1.969$ [1] $or$ $3.8$ [2]

[1] Liu, et al, Opt. Exp. 15, 11272, 2007
[2] Carroll, et al, PRL 109, 057402, 2012

Net (available) gain: $G_{net} = G_{pk} - \alpha_{Ge}$



From gain spectrum:

1) Peak gain versus injected carrier density
2) Spontaneous emission contribution to current density:

$$J_{sp} = \frac{ed}{\hbar}\left(\frac{n}{\pi c}\right)^2 \int_0^\infty d\nu\, \nu^2 \frac{G(\nu)}{e^{\frac{\hbar\nu-\mu_{eh}}{k_B T}} - 1}$$

Free-carrier absorption:

$$\alpha_{Ge} = \alpha_1(N_D + N_I) + \alpha_2 N_I$$

$$\alpha_1(10^{-18} cm^2) = 5.54\ [1]\ or\ 3.17\ [2]$$

$$\alpha_2(10^{-17} cm^2) = 1.969\ [1]\ or\ 3.8\ [2]$$

[1] Liu, et al, Opt. Exp. 15, 11272, 2007

[2] Carroll, et al, PRL 109, 057402, 2012

Net (available) gain: $G_{net} = G_{pk} - \alpha_{Ge}$

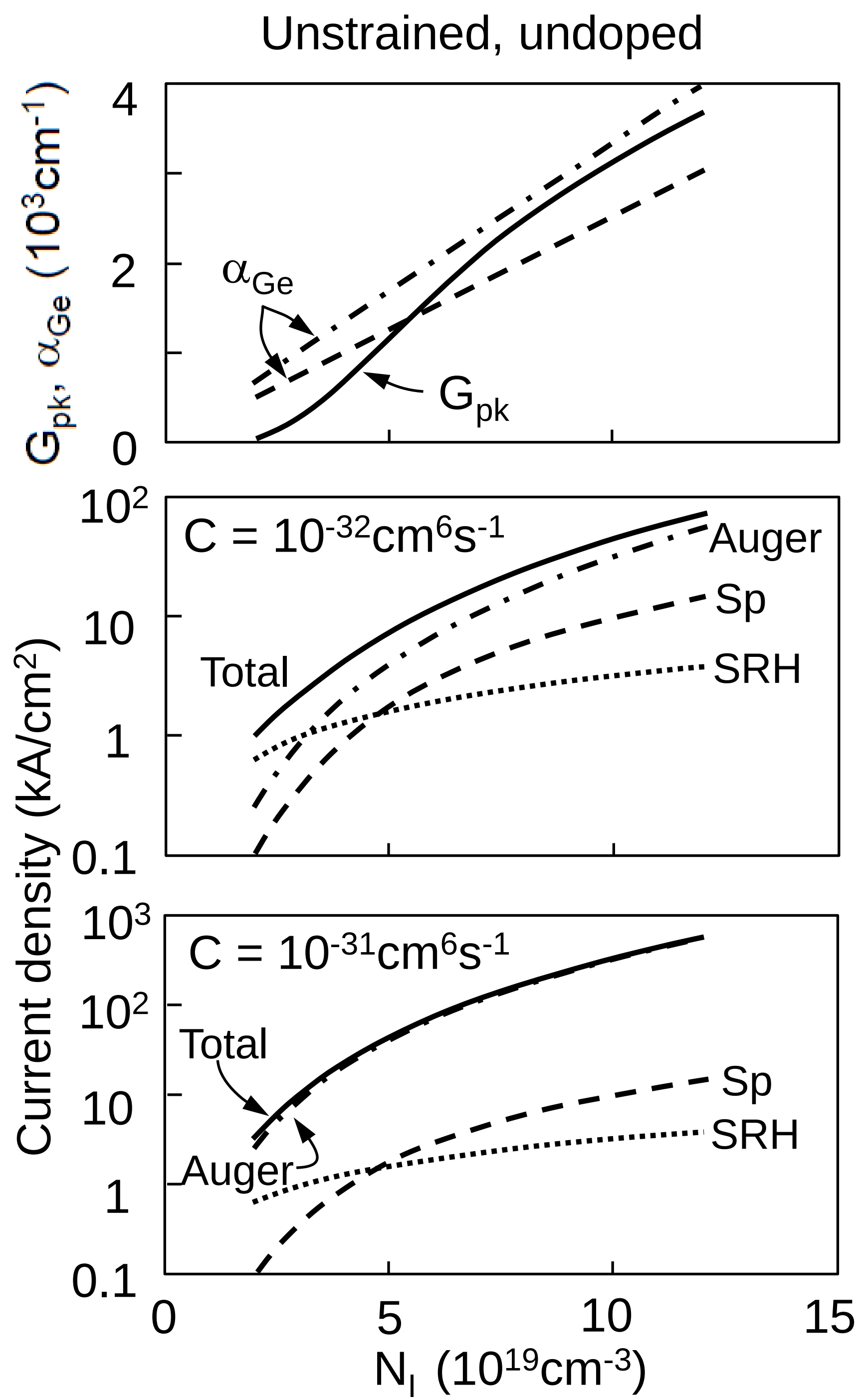
Non-radiative contributions to current density:

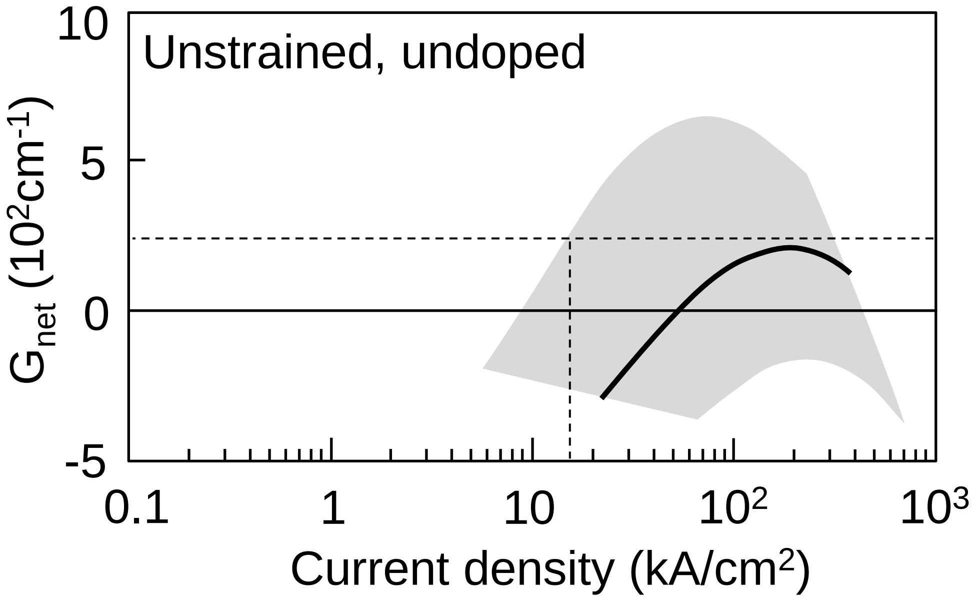
Defect (Shockley-Read-Hall) loss

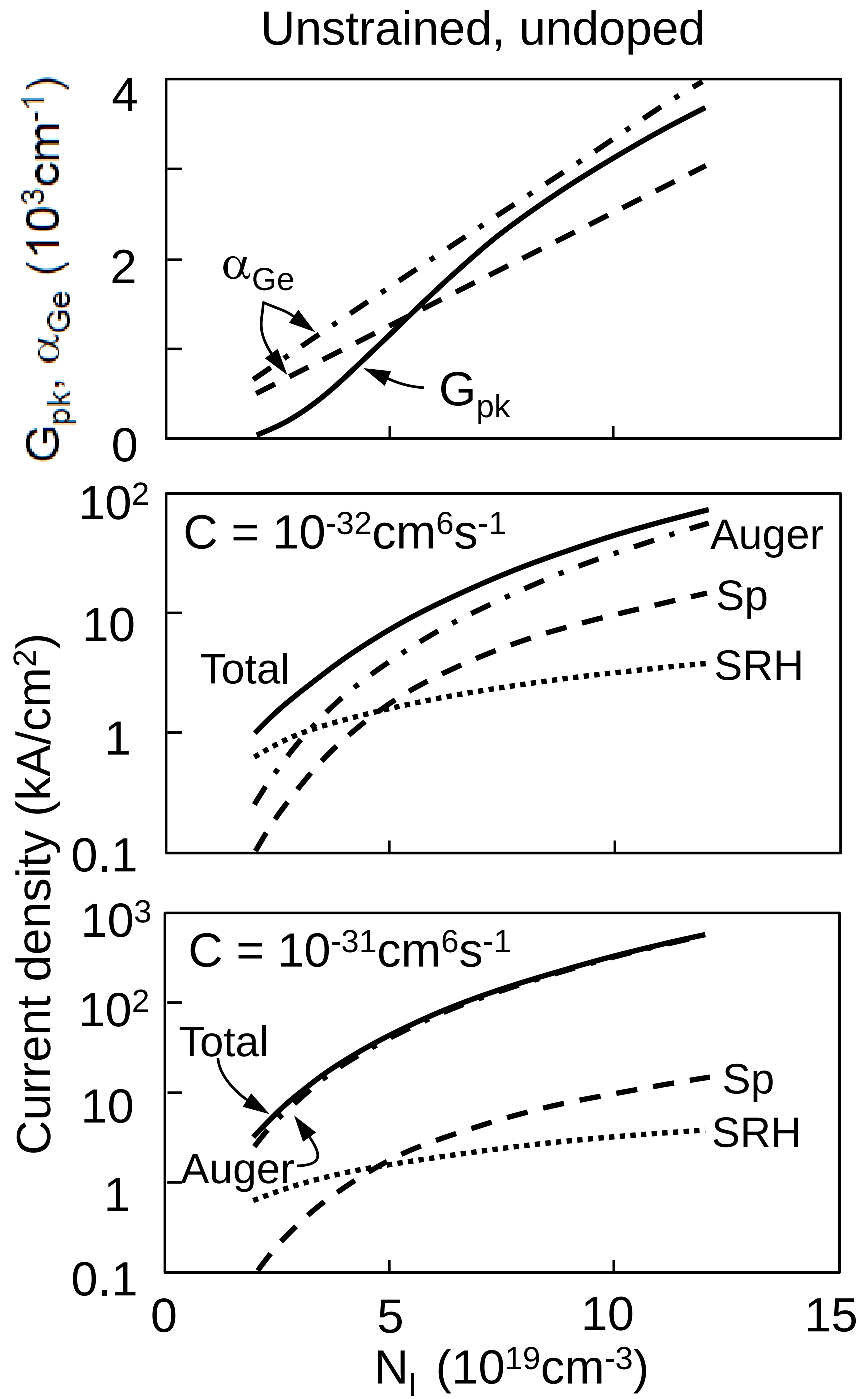
Auger scattering

Total current density:

$$J = J_{sp} + ed(\gamma_{SRH} N_I + C N_I^3)$$





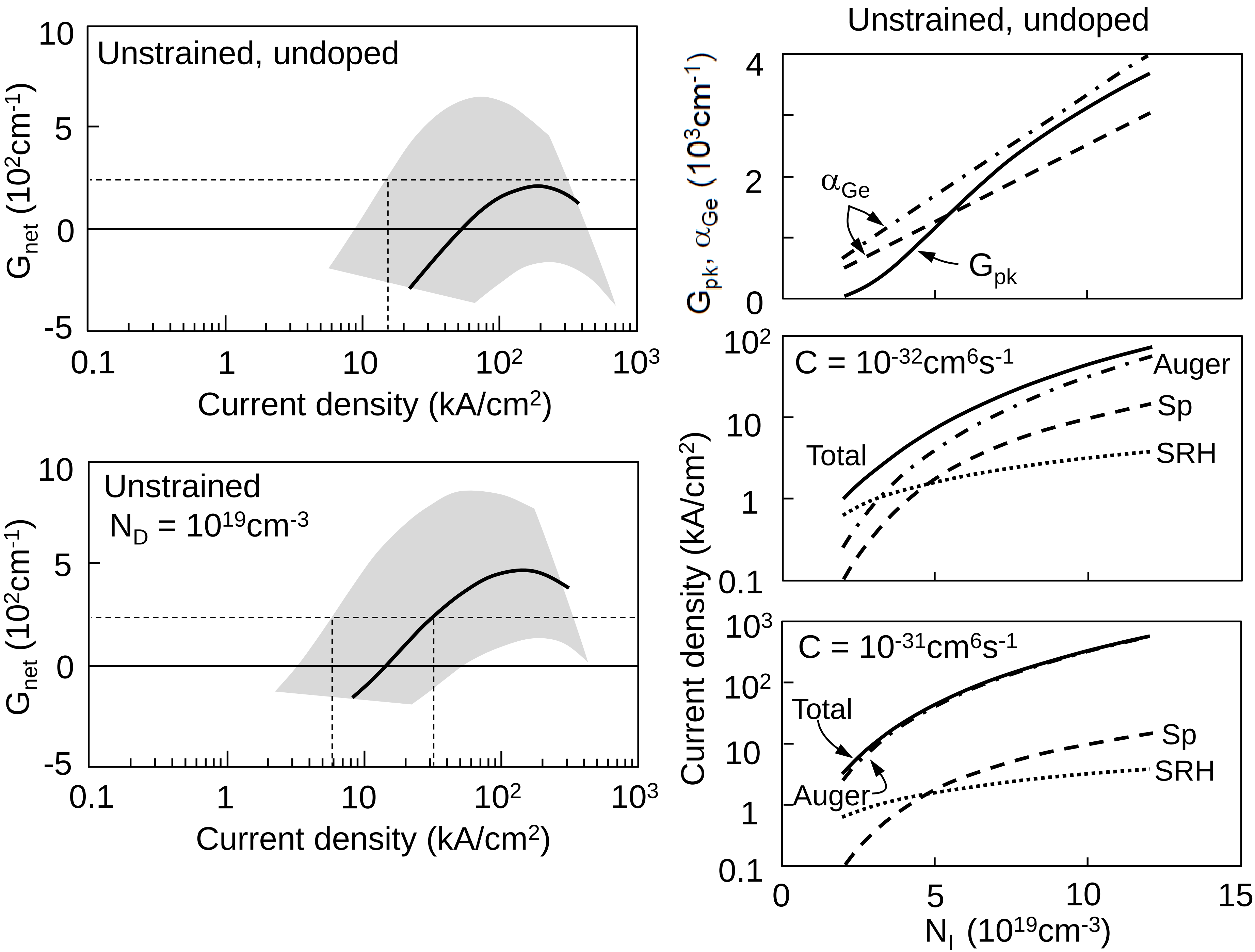




Required threshold gain

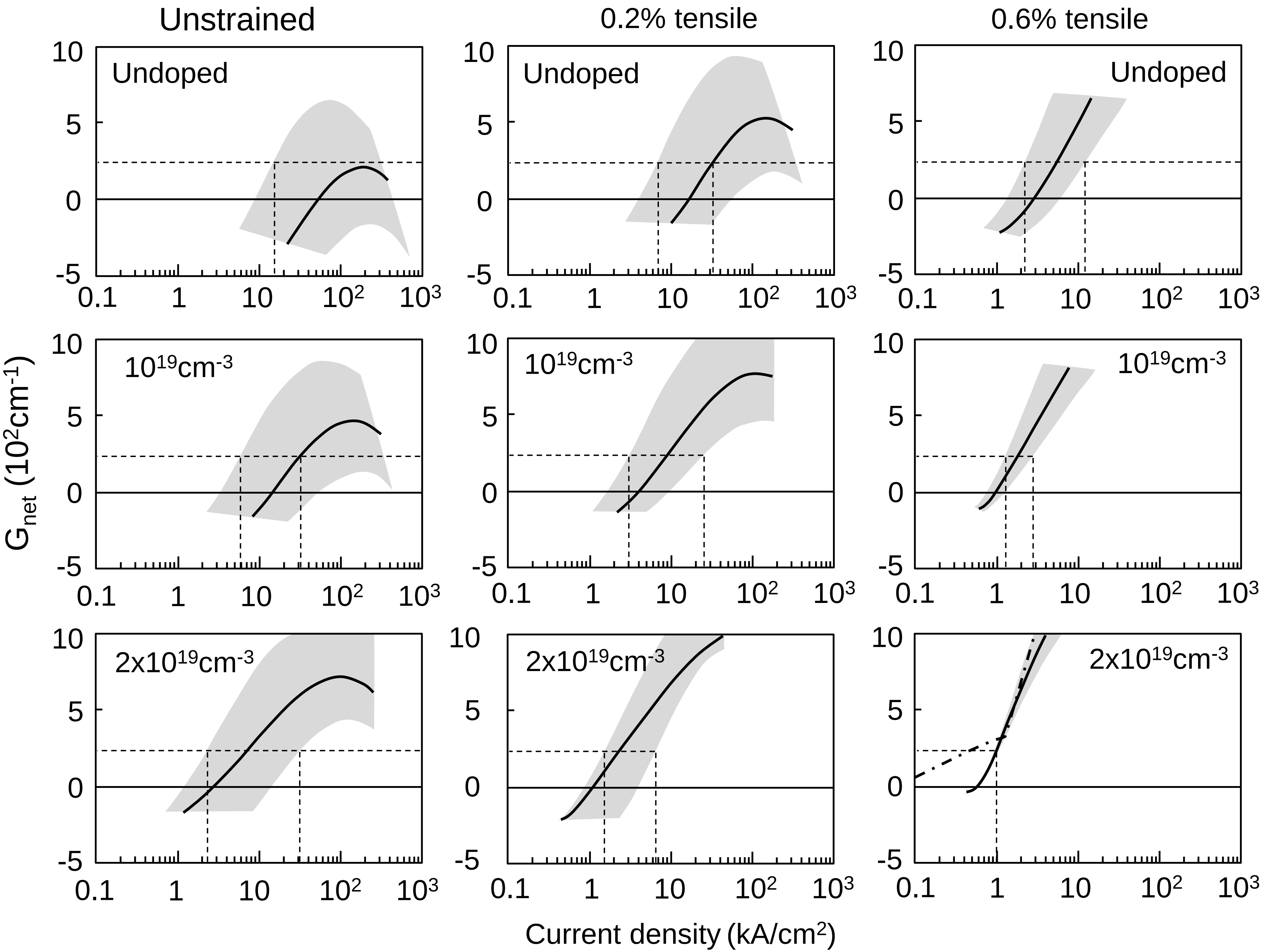
$$R_1 R_2 e^{2[\Gamma G_{net} - (1-\Gamma)\alpha_{Si}]L} = 1$$

Uncoated facets, $\Gamma$ = 0.4

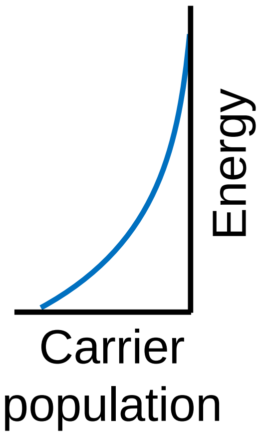
| L | $G_{net}$ |
|---|---|
| 1mm | 235cm$^{-1}$ |
| 500μm | 291cm$^{-1}$ |
| 200 μm | 457cm$^{-1}$ |

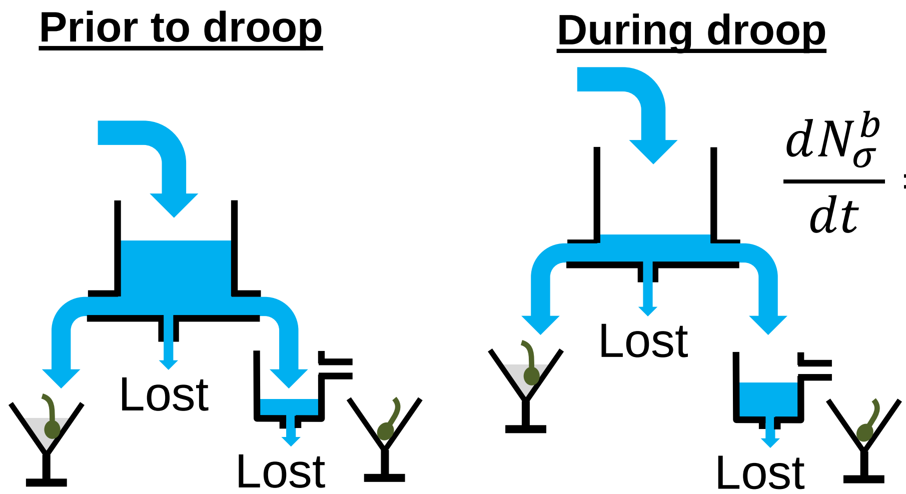


Unstrained, undoped
$G_{net}$ ($10^2$cm$^{-1}$)
10
5
0
-5
0.1
1
10
$10^2$
$10^3$
Current density (kA/cm$^2$)
Unstrained
$N_D = 10^{19}$cm$^{-3}$
$G_{net}$ ($10^2$cm$^{-1}$)
Current density (kA/cm$^2$)
Unstrained, undoped
$G_{pk}$, $\alpha_{Ge}$ ($10^3$cm$^{-1}$)
4
2
0
$\alpha_{Ge}$
$G_{pk}$
$C = 10^{-32}$cm$^6$s$^{-1}$
Auger
Sp
SRH
Total
Current density (kA/cm$^2$)
$C = 10^{-31}$cm$^6$s$^{-1}$
Total
Auger
Sp
SRH
0
5
10
15
$N_I$ ($10^{19}$cm$^{-3}$)


Unstrained
0.2% tensile
0.6% tensile
Undoped
Undoped
Undoped
10^19cm^-3
10^19cm^-3
10^19cm^-3
2x10^19cm^-3
2x10^19cm^-3
2x10^19cm^-3
G_net (10^2cm^-1)
Current density (kA/cm^2)
10
5
0
-5
0.1
1
10
10^2
10^3

# Droop from screening of quantum-confined Stark effect



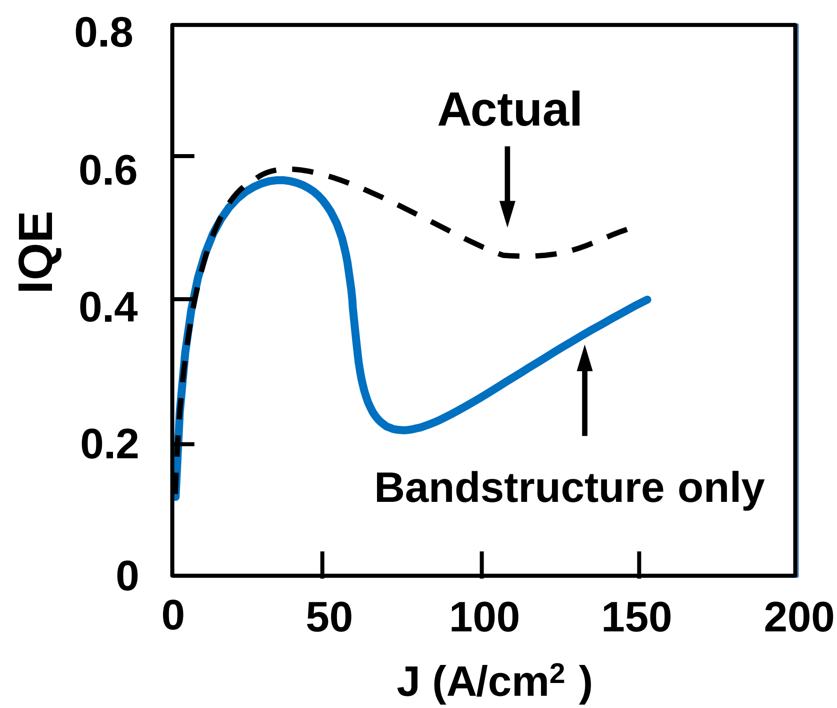

$$\frac{dN_\sigma^b}{dt} = -B_b N_e^b N_h^b - A_b N_\sigma^b + \frac{J}{eh_b}$$

$$\frac{dN_\sigma}{dt} = -BN_eN_h - AN_\sigma$$

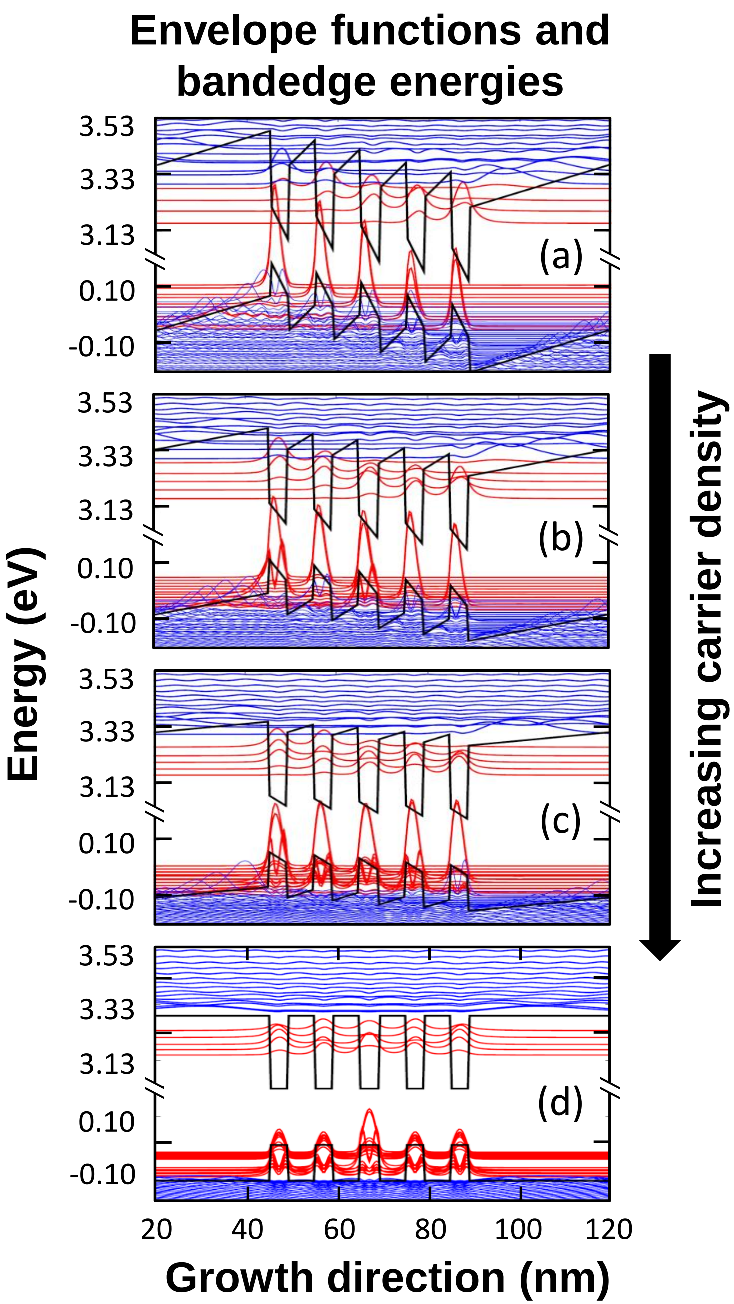
$$eA_b^2(4\beta)^{-1}$$

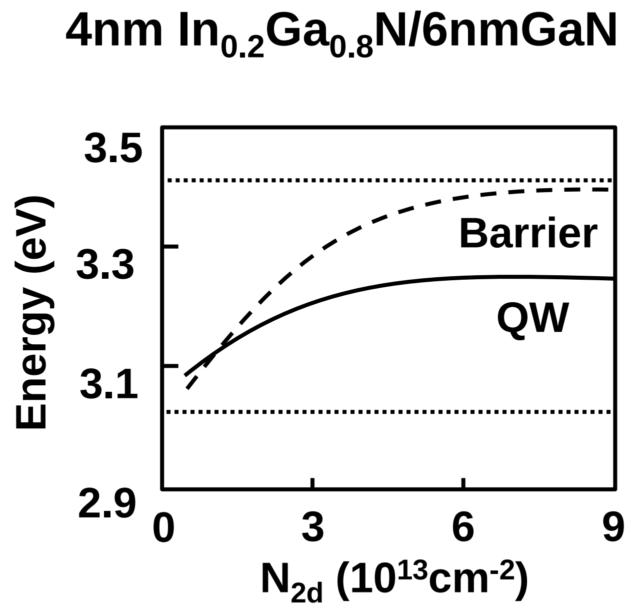
$$\boxed{IQE = 1 - 2\frac{J_0}{J}\left[\sqrt{\frac{J_0}{J}+1} - 1\right]}$$

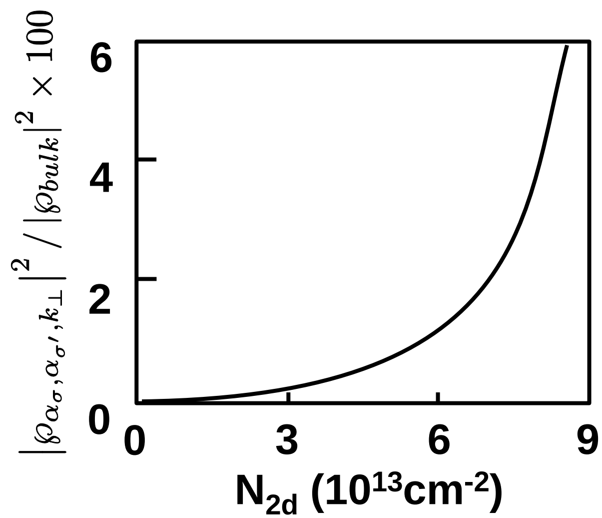
$$\beta = \frac{\frac{h}{h_b}N_{qw}B + B_b\exp\left(\frac{\Delta_e+\Delta_h}{k_BT}\right)}{\left[1+\exp\left(\frac{\Delta_e}{k_BT}\right)\right]\left[1+\exp\left(\frac{\Delta_h}{k_BT}\right)\right]}$$



# Excitation dependent band-structure effects



# Summary: Theory of Laser Gain in a Ge-on-Si Laser

**Motivation**

**Have computation tool for parametric studies of gain in Ge-on-Si lasers**

**Design parameters: strain and n-doping density**

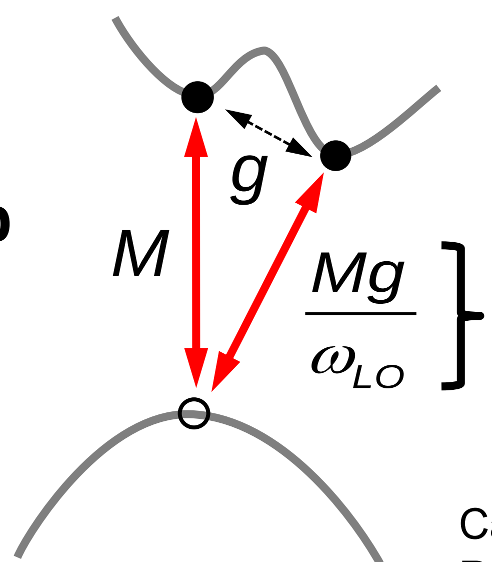
**Nonradiative factors: defect and Auger losses, free-carrier absorption**

**Environmental factors: temperature**

---

## ?Interesting dynamics or quantum optics?

**Indirect bandgap systems**



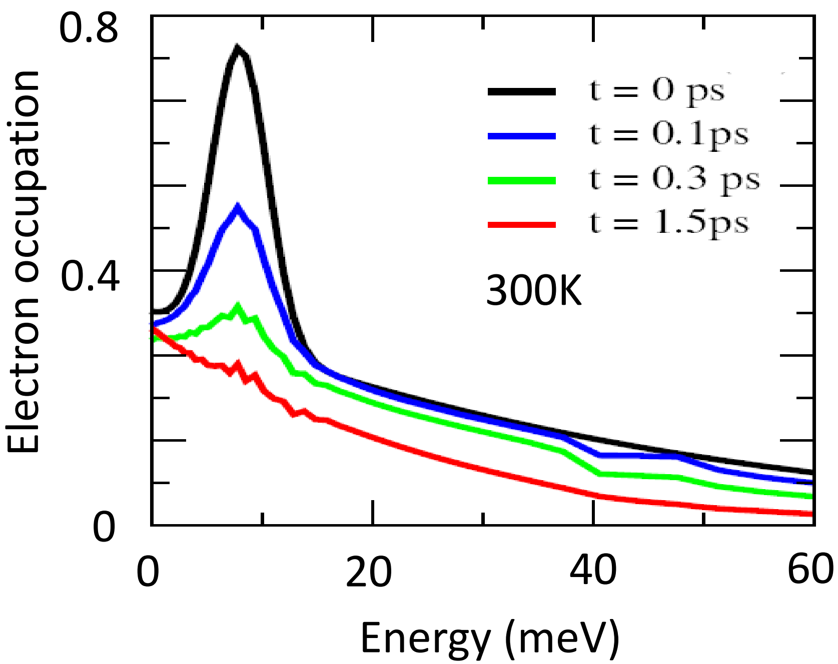

**Phonon assisted light-matter coupling**

Carmele, Kabuss and Chow, “Highly-detuned Rabi oscillations in a quantum-dot-microcavity system”, PRB rapid comm. (TBR)

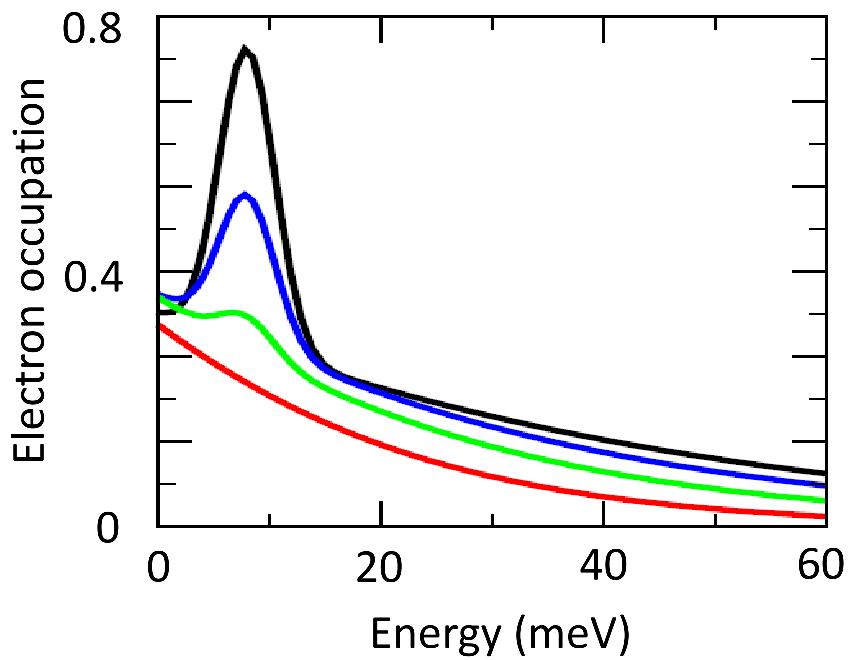
# Carrier population relaxation

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

**Quantum kinetic calculation**




**(Our) Rate equation approximation**




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

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.

# Summary of results

<u>Distinguishing feature</u>: **tracks k-resolved carrier populations instead of total carrier density**

- **Accounts for band-structure details esp. excitation dependences**
- **Computes radiative rate instead of using phenomenological $BN^2$**
- **Describes carrier capture and escape in terms of carrier-carrier and carrier-phonon relaxation rates – accounts for nonequilibrium carrier distributions and plasma heating**

## Preliminary simulations: bandstructure influence on droop description

- **For higher defect density in QWs then barriers ($A > A_b$ ):**

**SRH (linear) + excitation dependent band structure ➡ $N^3$ loss!**

➡ **Droop can be totally extrinsic**

- **For defect density in QW comparable or less than barriers :**

**Present experimental droop can be explained with $\underbrace{C > 5 \times 10^{-32}\ cm^6 s^{-1}}$**

**Needed Auger coefficient is smaller and consistent with microscopic calculations**

# Other reasons

**<u>Eliseev, Osinski, Li, APL 75, 3838 (1999)</u>**

"Sublinearity of light-current characteristics ...Auger coefficient C may be much smaller since higher-order nonradiative processes may also behaves like $N^3$"

**<u>Pope, Smowton, Blood, Thomson, Kappers, Humphreys, APL 82, 2755 (2003)</u>**

"... L-I curves are sublinear ... characteristic of localized states."

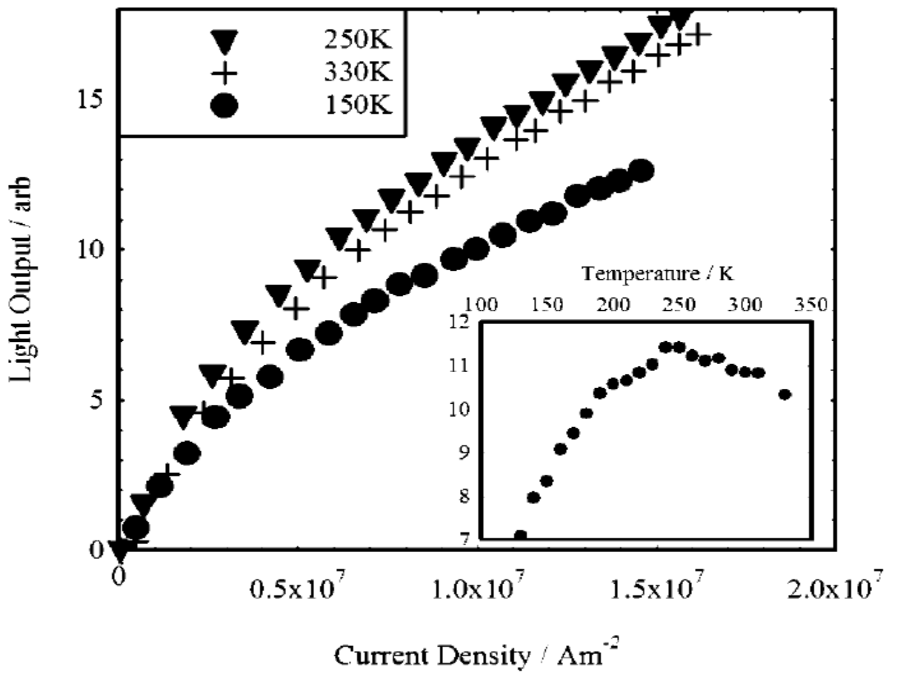



FIG. 1. Experimental $L-I$ characteristics over the temperature range 150–330 K. The inset shows the light output at a fixed current density of $10^7$ A $m^{-2}$ as a function of temperature.