ECE 536 – Integrated Optics and Optoelectronics
Lecture 4 – February 4, 2021

Spring 2021
Tu-Th 11:00am-12:20pm
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Lecture 4  Outline

• Final considerations on Generation-Recombination processes
• Brief review of Quantum Mechanical concepts
The Auger-droop controversy in LED

The mechanism causing nitride LED to lose efficiency at high power (efficiency droop) was identified as Auger recombination in 2007 by Lumileds Co. However, this started a controversy since another cause, leakage of carriers out of the quantum well structure, was proposed as the responsible mechanism.

Various experimental ("Direct Measurement of Auger Electrons ...", Phys Rev Lett 110, 177406, 2013) and theoretical ("Ultrafast Hot Carrier Dynamics in GaN and Its Impact on the Efficiency Droop" Nano Letters, 2017, 17, 8, p. 5013) papers have since supported one hypothesis or the other.

IEEE Spectrum has chronicled for years the debate. The initial paper "The LED’s Dark Secret" (2009) is still interesting reading.
Radiative vs. non-radiative recombination

Even though non-radiative recombination can be reduced, it cannot be eliminated completely.

Additionally, all real crystals will always have native defects which may introduce deep levels acting as traps.

From thermodynamics considerations, if the energy to generate a defect is $E_a$, the associate probability is given by the Boltzmann factor $\exp(-E_a/k_B T)$. 
Estimate of point defect concentration

Assume a crystal with lattice constant \(a_o = 5.6\text{Å}\) and eight atoms per cubic cell. If the energy needed to move a lattice atom into interstitial position is 1.0eV, estimate the density of interstitial defects at room temperature.

\[
N_a = \frac{8}{(5.6 \times 10^{-8})^3} = 4.5 \times 10^{22} \text{ atoms/cm}^{-3}
\]

\[
N_{\text{def}} = N_a \exp\left(-\frac{1.0}{0.0256}\right) \approx 4.9 \times 10^5 \text{ cm}^{-3}
\]
Radiative vs. non-radiative recombination

Chemical purity is always an issue. The purest III-V semiconductors will still have impurity concentrations on the order of $10^{12}$ cm$^{-3}$.

Nonetheless, the internal luminescence efficiency has grown from a fraction of 1% up to 90%+ today, because of improved crystal quality and reduced defect/impurity concentrations.
Internal quantum efficiency of a semiconductor with non-radiative recombination centers

when \( n \gg (n_o + p_o) \):

\[
R = An + Bn^2 + Cn^3 = \frac{n}{\tau(n)}
\]

\( (n \approx \delta n) \)

\[
\tau(n) = \frac{1}{A + Bn + Cn^2}
\]

\[
\tau_r, \tau_{nr} = \frac{1}{\tau(n)} = \frac{1}{\tau_r} + \frac{1}{\tau_{nr}}
\]

SRH Auger

Band to Band

\[
\frac{1}{\tau_r} = Bn
\]

\[
\frac{1}{\tau_{nr}} = A + Cn^2
\]

intrinsic quantum efficiency

\[
\eta_{in} = \frac{R_r}{R_{tot}} = \frac{\delta n}{\tau(n)} = \frac{1}{\frac{\tau_r}{\tau_{nr}} + \frac{1}{\tau_{nr}}}
\]
Deep Levels

Deep levels can be caused by *native defects* (vacancies, interstitials), unwanted impurities, dislocations, impurity-defect complexes, and combinations of different defects.

Experimental analysis is often complicated by the fact that deep-levels may also be associated with radiative transitions.

For instance, Ga vacancies are common point defects in GaN, which luminesce with peak in the yellow band.
n-type GaN/sapphire

$T = 295 \text{ K}$

Band-to-band luminescence

Luminescence intensity (arb. units)

Wavelength $\lambda$ (nm)

Grieshaber et al., 1996
Stimulated Emission

An incoming photon interacts with an electron causing it to drop to a lower energy level. The energy transfers to the EM field, generating a new photon with phase, frequency, polarization, and direction of travel which are the same as those of the incident photon.

In contrast, spontaneous emission occurs randomly without particular correlation with the ambient EM field.
Stimulated Emission

\[ R = v_g g(n)S \]

where:

- \( S \) is the photon density (units cm\(^{-3}\))
- \( v_g \) is the group velocity (units cm/s):
  \[ v_g = \frac{c}{n_g} \]
- \( g(n) \) is the optical gain (units cm\(^{-1}\))
- \( n_g \) is the group index
- \( v_g g(n) \) is the "rate of growth"
Impact Ionization

It is essentially the reverse of an Auger recombination process, but the rate depends upon current densities as opposed to carrier concentrations.

Detailed theoretical analysis is quite difficult because of the need for a full band structure and it has been addressed with Monte Carlo simulation in some materials. Physics of threshold remains fuzzy.

Models are typically semi-empirical with calibration from measurements.
\[ G_n = \alpha_n \frac{|J_n|}{q} \]

Hot electron

\[ E_c \]

\[ E_v \]

particle flow

electron ionization coefficient
\[ G_p = \beta_n \frac{|J_p|}{q} \]

- \( G_p \): Hole ionization coefficient
- \( \beta_n \): Particle flow
- \( J_p \): Hole ionization coefficient
Net Generation-Recombination rate

\[ R = R_{n,p} - G_n - G_p = -\alpha_n \frac{|J_n|}{q} - \beta_p \frac{|J_p|}{q} \]

can be neglected

Empirical form of ionization coefficients. Both measure the number of generated electron-hole pairs per unit distance.

\[ \alpha_n (E) = \alpha_n^\infty e^{-(E_{nc}/E)\gamma} \]

\[ \beta_p (E) = \beta_p^\infty e^{-(E_{pc}/E)\gamma} \]

\( E_{nc} \) and \( E_{pc} \) are critical fields

\( 1 \leq \gamma \leq 2 \)
Brief Review of
Quantum Mechanical concepts
Discovery of the electron

Thomson’s experiments with cathode rays (1897) and “plum-pudding” model of the atom
The atom is still believed to be a uniformly distributed substance, with electrons stuck in a mass of positive charges

Rutherford’s experiments on gold foil (1909) and first planetary model of the atom (1911)
The atom is described as a mostly empty volume, including a core of protons at the center and orbiting electrons.
Quantization

Planck’s hypothesis (1901): Explains black body radiation assuming that the energy of an atomic oscillator vibrating at frequency $\nu$ is restricted to quantized values

$$E_n = n\hbar\nu = n\hbar\omega, \quad n = 0, 1, 2, 3 \ldots$$

Planck’s constant

$$h = 6.628 \times 10^{-34} \text{ J/s (}\hbar = h/2\pi)$$

Einstein’s model (1905): Provides an explanation of the photoelectric effect using Planck’s quantization
Light quanta

Einstein’s “heuristic point of view toward the emission and transformation of light” (1905): introduces the concept of elementary light quanta as indivisible packets.

The term “photon” was introduced in 1926 by Gilbert Lewis.
Simple model of the atom

Bohr’s model (1913): Electrons in a planetary atom are restricted to well-defined orbits assuming only quantized values of the angular momentum $L$ and of the energy $E$. For the hydrogen atom

$$L_n = m_0 v r_n = n \hbar, \quad n = 1, 2, 3 \ldots$$

$$E_n = -\frac{m_0 q^4}{2(4\pi \varepsilon_0 n \hbar)^2} = \frac{-13.6}{n^2} \text{ (eV)}$$
Wave-Particle Duality

debroglie’s hypothesis (1925): Since electromagnetic radiation (waves) exhibit particle-like (photon) properties, particles should also exhibit wave like properties. The momentum of a particle (or wave) can be written as:

\[ p = m_0 v = \hbar k \]

This parallel between electrons and photons is at the basis of optoelectronics, with the distinction that electrons obey the Fermi-Dirac statistics and photons the Bose-Einstein statistics
Schrödinger equation

Wave mechanics (1927): A complex wave function $\Psi(r, t)$ describes elementary particles according to the evolution equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + V(r)\Psi$$

Volume Normalization

$$\int_v \Psi^* \Psi \, dr^3 = 1$$

probability to find particle in volume $dr^3$

Expectation value of observables

$$\langle \alpha \rangle = \int \Psi \alpha \Psi^* \, dr^3$$
Particles in crystalline solid

The Schrödinger equation is used to solve the electron wave functions and energy states in crystals. If the expectation value of an electron’s total energy is a constant $E$, the Schrödinger equation becomes

$$-\frac{i}{\hbar} \frac{\partial \psi}{\partial t} = E \psi$$

Using separation of variables the wave function can be expressed as

$$\psi(r, t) = \phi(r)e^{-iEt/\hbar}$$

space-dependent wave function  

time-varying phase factor
For zero potential solution is a plane wave

\[ V(\vec{r}, t) = 0 \quad \text{Volume} = \Omega \]

\[ \Psi(\vec{r}, t) = \frac{1}{\sqrt{\Omega}} e^{i\left(\vec{k} \cdot \vec{r} - \frac{E}{\hbar} t\right)} = \frac{1}{\sqrt{\Omega}} e^{i(\vec{k} \cdot \vec{r} - \omega t)} \]

\[ E = \hbar \omega = \frac{1}{2} m v^2 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \]

\[ \omega = \frac{\hbar k^2}{2m} \quad p = \hbar k \]
Time-independent Schrödinger equation

\[ i \hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \Psi + V(r)\Psi \]

\[ \psi(r, t) = \phi(r)e^{-iEt/\hbar} \]

\[ -\frac{i}{\hbar} \frac{\partial \psi}{\partial t} = E \psi \]

\[ -\left( \frac{\hbar^2}{2m} \right) \nabla^2 \phi(r) + V(r)\phi(r) = E\phi(r) \]

The time-independent equation is the basis to solve one-electron energy band structure and related problems in crystals.
Momentum Space representation

Fourier transform of potential and wave function

\[
\tilde{\psi}(\vec{k}) = \int \psi(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} d^3 r
\]

\[
\tilde{V}(\vec{k}) = \int V(\vec{r}) e^{-i\vec{k} \cdot \vec{r}} d^3 r
\]

Momentum-space of Schrödinger equation

\[
\frac{\hbar^2 k^2}{2m} \tilde{\psi}(\vec{k}) + \int \frac{d^3 k'}{(2\pi)^3} \tilde{V}(\vec{k} - \vec{k}') \tilde{\psi}(\vec{k}') = E \tilde{\psi}(\vec{k})
\]
Quantum wells are very important in optoelectronics

Infinite quantum well

Region I: $x \leq -\frac{L}{2}$
$\Psi(x) = Ae^{ikx} + Be^{-ikx}$

Region II: $-\frac{L}{2} \leq x \leq \frac{L}{2}$
$\Psi(x) = Ce^{ikx} + De^{-ikx}$

Region III: $x \geq \frac{L}{2}$
$\Psi(x) = Fe^{ikx} + Ge^{-ikx}$
Infinite quantum well – The solution in each region has the form of two counter-propagating plane waves

\[ \Psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{where} \quad k = \sqrt{\frac{2m^*}{\hbar^2}}(E - V) \]

The constants A and B are determined by applications of boundary conditions. In Region 1 and 3, \( k \) is purely imaginary (evanescent wave) and there is only a forward wave in region 3 and a backward wave in region 1. However, because the potential is infinite, there is no wave penetration and the wave function must be zero at the boundaries of the well.

Solution:

\[ k = \frac{n\pi}{L}, \quad E_n = \frac{n^2\pi^2\hbar^2}{2L^2m^*} \]
Combination of the two waves give a cosine standing wave for odd integer and a sine standing wave for even integer

\[ \Psi(x) = C \cos\left(\frac{\pi}{L} x\right) \]

\[ \int_{-\frac{L}{2}}^{\frac{L}{2}} C^2 \cos^2\left(\frac{\pi}{L} x\right) dx = 1, \quad C = \sqrt{\frac{2}{L}} \]

\[ \Psi(x) = \begin{cases} 
\sqrt{\frac{2}{L}} \cos\left(\frac{n\pi}{L} x\right), & n = 1, 3, 5, \ldots \\
\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right), & n = 2, 4, 6, \ldots 
\end{cases} \]
Example

$L = 10$ nm

$m = 0.066 \, m_o$
Finite square well

\[-\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} \Psi(x) + V(x) \Psi(x) = E_n \Psi(x)\]

\[V(x) = \begin{cases} V_0, & \text{for } |x| \leq \frac{L}{2} \\ 0, & \text{for } |x| > \frac{L}{2} \end{cases}\]

\[m^*_B = 0.092\]

\[m^*_w = 0.06\]

V = 0.25 eV

\[V = 0\]

Region I: \( x \leq -\frac{L}{2} \)

\[\Psi(x) = Ae^{ix} + Be^{-ix}\]

Region II: \( -\frac{L}{2} \leq x \leq \frac{L}{2} \)

\[\Psi(x) = Ce^{ix} + De^{-ix}\]

Region III: \( x \geq \frac{L}{2} \)

\[\Psi(x) = Fe^{ix} + Ge^{-ix}\]
Boundary conditions

(i) continuity of the wavefunction across the boundary.
(ii) continuity of the electric current across the boundary.

Current carried by one electron

\[ I = -qv = -q \frac{m^* v}{m^*} = -q \frac{\hbar k}{m^*} = iq \frac{\hbar}{m^*} \frac{d}{dx} \Psi(x) \]

Boundary condition conserving electric current

\[ \frac{1}{m^*_W} \frac{d}{dx} \Psi_{\text{region II}}(x) \bigg|_{x=\frac{L}{2}} = \frac{1}{m^*_B} \frac{d}{dx} \Psi_{\text{region III}}(x) \bigg|_{x=\frac{L}{2}} \]
Application of Boundary conditions

Using the same procedure

\[
x = \frac{L}{2}
\]

\[
Ce^{ik\frac{L}{2}} + De^{-ik\frac{L}{2}} = Fe^{-\kappa\frac{L}{2}}
\]

\[
\frac{ik}{m^*_W} \left( Ce^{ik\frac{L}{2}} - De^{-ik\frac{L}{2}} \right) = -\frac{\kappa}{m^*_B} Fe^{-\kappa\frac{L}{2}}.
\]

\[
\frac{ik}{m^*_W} \left( Ce^{ikL} - D \right) = -\frac{\kappa}{m^*_B} \left( Ce^{ikL} + D \right)
\]

\[
Ce^{ikL} \left( \kappa m^*_W + ikm^*_B \right) + D \left( \kappa m^*_W - ikm^*_B \right) = 0
\]

Using the same procedure

\[
x = -\frac{L}{2}
\]

\[
Ce^{-ikL} \left( \kappa m^*_W - ikm^*_B \right) + D \left( \kappa m^*_W + ikm^*_B \right) = 0
\]
The equation gives the energy of the quantized states in the well. It can be solved by numerical iteration to a desired accuracy. It can also be solved graphically.
\[ L = 10 \text{ nm} \]

\[ \cot(kL) \]

\[ \frac{\left(\frac{k m_B^*}{2}\right)^2 - \left(\frac{k m_W^*}{2}\right)^2}{2 k m_B^* k m_W^*} \]
Comparison between wells

\[ L = 10 \text{ nm} \]

<table>
<thead>
<tr>
<th></th>
<th>( V_0 )</th>
<th>( m^*_B )</th>
<th>( m^*_W )</th>
<th>( E_1 ) (eV)</th>
<th>( E_2 ) (eV)</th>
<th>( E_3 ) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Infinite well</td>
<td>( \infty )</td>
<td>–</td>
<td>0.066</td>
<td>0.056</td>
<td>0.223</td>
<td>0.502</td>
</tr>
<tr>
<td>Finite well</td>
<td>0.25 eV</td>
<td>0.092</td>
<td>0.066</td>
<td>0.03</td>
<td>0.121</td>
<td>0.245</td>
</tr>
</tbody>
</table>

In many practical situations relevant for optoelectronics, quantum wells have only several energy levels.
In realistic conditions, there is a field across quantum well, due to applied potentials, differences in electron affinity between the heterostructure materials which define the well, and to the charge distribution associated with the wave functions and with ionized impurities, as well as.

The time-independent Schrödinger equation should be solved simultaneously with the Poisson equation for a self-consistent solution.

In addition, there may be onset of quantum Stark effect which tends to separate energy levels in confined spaces when an electric field is applied. The energy shift can be calculated by perturbation theory.
Example: Voltage drop of 0.1 V across the 10 nm well examined earlier, cause an electric field of $10^5$ V cm$^{-1}$.

The estimate for shift in energy caused by Stark effect is about 2 meV
Transmission coefficient – analytical result for rectangular well

\[ T = \frac{1}{\cosh^2(\kappa L) + \left(\frac{1}{4}\right) \left(\frac{\kappa m_1^*}{\kappa m_2^*} - \frac{\kappa m_2^*}{\kappa m_1^*}\right)^2 \sinh^2(\kappa L)} \]
Tunneling

Case I \( m_1^* = m_2^* = 9 \times 10^{-31} \text{ kg} \)

the barrier width is 10 nm and the barrier height is 0.25 eV
Tunneling

Case I $m_1^* = m_2^* = 9 \times 10^{-31}$ kg
the barrier width is 10 nm and the barrier height is 0.25 eV
Tunneling

Case II $m_1^* \neq m_2^*$

$m_1^* = 9 \times 10^{-31}$ kg. $m_2^* = 0.066 m_1^*$.

The barrier width is 10 nm and the barrier height is 0.25 eV.
Tunneling

Case II \( m_1^* \neq m_2^* \)

\[ m_1^* = 9 \times 10^{-31} \text{ kg. } m_2^* = 0.066m_1^*. \]

the barrier width is 10 nm and the barrier height is 0.25 eV.
Tunneling in reverse biased p-n junctions
Simple model for tunneling current (GaAs)

\[ J_{\text{Tunn}} = n q \nu_{\text{sat}} \]

\[ n = N_V T \]

\[ \nu_{\text{sat}} = 1.2 \times 10^7 \text{ cm s}^{-1} \]

\[ N_V = 4 \text{ valence electrons/atom} \times 8 \text{ atoms/unit-cell/unit-cell volume} \]

\[ = 1.7 \times 10^{23} \text{ cm}^{-3} \]

Transmission coefficient

\[ T = \frac{1}{\cosh^2(\kappa L) + \left( \frac{1}{4} \left( \frac{\kappa m_1^*}{\kappa m_2^*} - \frac{\kappa m_2^*}{\kappa m_1^*} \right) \right)^2 \sinh^2(\kappa L)} \]

(Approximation: this is for a rectangular well. Well is actually triangular)
Simple model (GaAs)

electrons at the valence band edge have thermal energy

barrier height \[ V_0 = E_g = 1.43 \text{ eV} \]

approximate average wave vector in the forbidden gap

\[ \kappa = \frac{1}{\hbar} \sqrt{2m^* (E_g - k_B T)} \quad \text{and} \quad |\kappa| = 1.4 \times 10^9 \text{ m}^{-1} \gg |k| \]

width of the barrier

\[ \mathcal{E} = \frac{E_g/q}{L} = \sqrt{\frac{2qN_D V}{\epsilon \varepsilon_0}}, \quad \text{where} \quad V = V_{\text{Applied}} + \phi_{\text{built-in}} \]

(Assume one sided junction with \( N_D = 10^{16} \text{ cm}^{-3} \) and reverse bias \( V = -1 \text{ V} \))

\[ L = \frac{E_g}{\sqrt{\frac{2qN_D V}{\epsilon \varepsilon_0}}} = 2.7 \times 10^{-7} \text{ m} \]

Note: \( \kappa L \gg 1 \)
Simple model (GaAs)

set effective masses \( m_1^* = m_2^* = m^* \)

approximate transmission coefficient since \( \kappa L \gg 1 \)

\[
T = \frac{1}{\cosh^2(\kappa L) + \left( \frac{1}{4} \right) \left( \frac{k m_1^*}{k m_2^*} - \frac{k m_2^*}{k m_1^*} \right)^2 \sinh^2(\kappa L)} \approx 16 e^{-2\kappa L} \left( \frac{k \kappa}{k^2 + \kappa^2} \right)^2 \approx 16 \left[ \frac{k}{\kappa} \right]^2 e^{-2\kappa L}
\]

also

\[
\kappa L = \frac{E_G}{\hbar} \sqrt{\frac{2m^* E_G \varepsilon \varepsilon_0}{2qN_D V}} = C_0 V^{-\frac{1}{2}} \quad \left( \frac{k}{\kappa} \right)^2 \approx \frac{3k_B T}{2E_g}, \text{ where } T \text{ is the temperature}
\]

finally

\[
T \approx 16 \left( \frac{3k_B T}{2E_g} \right) e^{-2C_0 V^{-\frac{1}{2}}}
\]

\[
J_{tunneling} \approx 16N_v q v_{sat} \left( \frac{3k_B T}{2E_g} \right) e^{-2C_0 V^{-\frac{1}{2}}} \text{ amps} \cdot \text{cm}^{-2}
\]
Result from a simple tunneling model
Density of States

\[ g(E) \propto (E - E_0)^{d/2-1} \]

\[ d = 1, 2, \text{ or } 3 \]
2D Density of States

\[ g(k)\,dk = \frac{2\pi k\,dk}{4\pi^2} = \frac{k\,dk}{2\pi} \]

\[ k = \frac{\sqrt{2m^*E}}{\hbar} \quad \text{and} \quad dk = \frac{\sqrt{2m^*}}{\hbar} \frac{dE}{2\sqrt{E}} \]

\[ \frac{k\,dk}{2\pi} = \frac{1}{2\pi} \frac{\sqrt{2m^*E}}{\hbar} \frac{\sqrt{2m^*}}{2\sqrt{E}} \frac{dE}{\hbar} \]

\[ = \frac{m^*}{2\pi \hbar^2} \frac{dE}{\hbar} = g(E)\,dE \]

\[ g(E) = 2 \frac{m^*}{\text{spin}} \frac{1}{2\pi \hbar^2} = \frac{m^*}{\pi \hbar^2} \]

(area of annular region)

(# allowed k-states per unit area)
1D Density of States

\[ k = \frac{\sqrt{2m^*E}}{\hbar} \]

\[ dk = \frac{\sqrt{2m^*}}{\hbar} \frac{dE}{2\sqrt{E}} \]

\[ g(k)dk = \frac{2dk}{2\pi} = \frac{dk}{\pi} \]

\[ \frac{2dk}{2\pi} = \frac{1}{\pi} \frac{\sqrt{2m^*}}{\hbar} \frac{dE}{2\sqrt{E}} = g(E)dE \]

\[ g(E) = \frac{2}{\text{spin}} \cdot \frac{1}{\pi} \frac{\sqrt{2m^*}}{\hbar} \frac{1}{2\sqrt{E}} = \frac{\sqrt{2m^*}}{\pi \hbar} \frac{1}{\sqrt{E}} \]
Reading Assignments

Chapter 3 of the book by Chuang.