Advanced Device Simulation at Agere Systems

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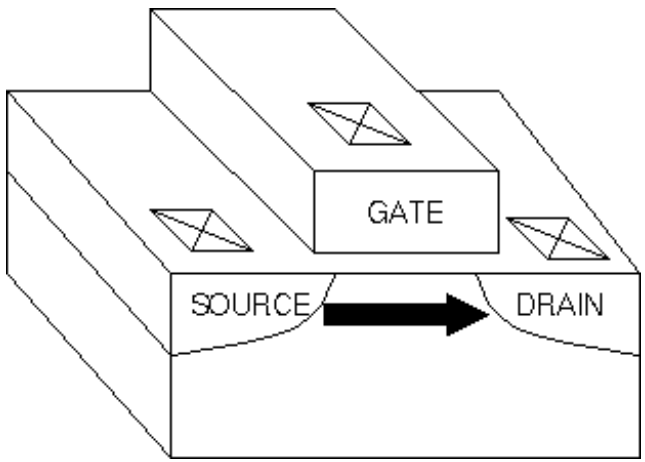
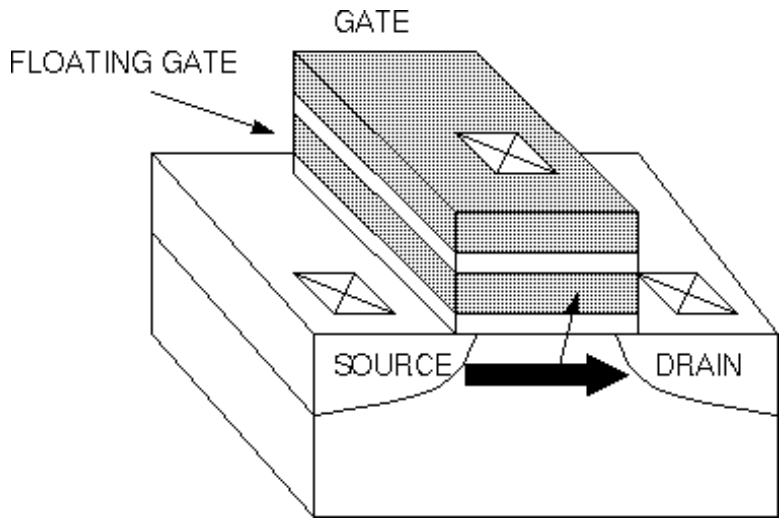
Overview

- Monte Carlo Device Simulation
  - Introduction
  - Problem formulation
  - Numerical methods
- Laser simulation
  - Optics
  - Electronics
  - Simulation

Device simulation - introduction

- Traditional drift-diffusion models describe the behavior of the mean-energy carriers
- Many important effects depend on high energy carriers
  - Ballistic transport
  - Damage from hot-carrier injection into dielectrics
  - Memory programming by injection of hot carriers into floating gates





BTE for device simulation

- Full problem is described by distribution of electrons in space and momentum
- 6-dimensional problem, 3 space dimensions, 3 momentum dimensions
- Boltzmann Transport Equation

$$\frac{\partial f}{\partial t} + \vec{v} \bullet \frac{\partial f}{\partial \vec{r}} + \vec{F} \bullet \frac{\partial f}{\partial \vec{k}} = \left(\frac{\partial f}{\partial t} \right)_{coll}$$

- Direct solution extremely challenging
  - Monte Carlo approach generally adopted

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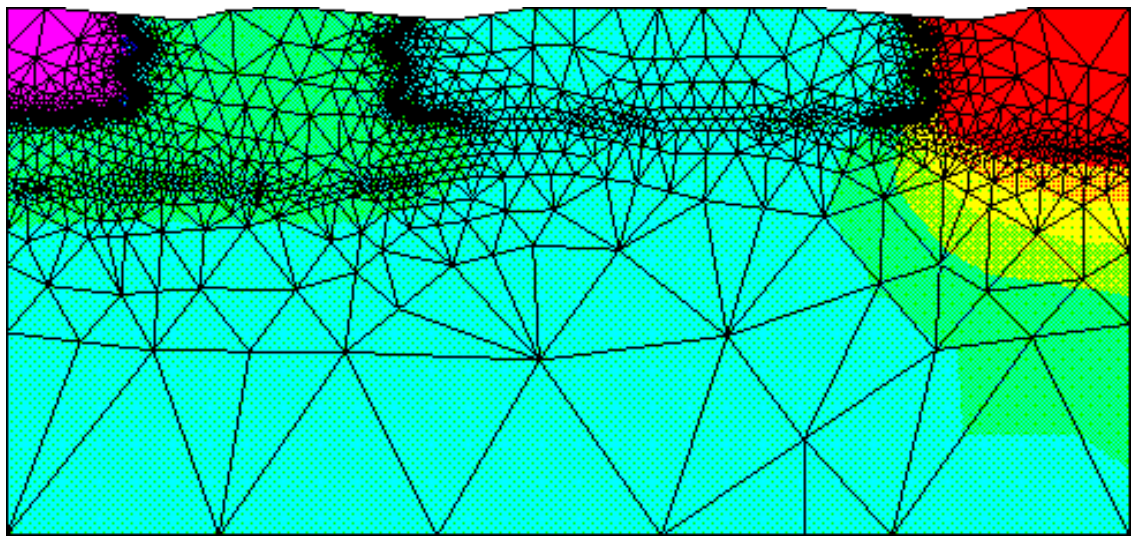
Monte Carlo device simulation

- Inject electrons and holes, one at a time, close to contacts, with momentum randomly distributed so that energy mean is at thermal equilibrium
- Integrate equations of motion, subject to random scattering events with lattice vibrations (phonons) and dopant atoms
- Follow until particle exits or comes to equilibrium
- Use statistical enhancement techniques to avoid following 'boring' particles
- Accumulate statistics over many particles

Monte Carlo simulation - discretization

- Represent phase space by a Cartesian product of a space (x) grid and a momentum (k) grid
  - X-grid is typical transistor grid with simplices of dimension 1-100nm
  - K-grid is a tetrahedral decomposition of unit momentum cell
    - Main focus of this presentation



Equations of motion

$$\frac{d\vec{r}}{dt} = \frac{1}{\hbar}\nabla_{\vec{k}} E_n(\vec{k})$$

$$\frac{d\vec{k}}{dt} = \frac{e}{\hbar}\nabla_{\vec{x}} V(x)$$

E – energy

V - electrostatic potential

$\vec{r}, \vec{k}$ - position, momentum

- Applied during free-flight time
  - Time-step inversely proportional to scattering rate
  - Time-step also limited by time to reach cell edge
- Inside a Tx-Tk cell, energy and potential are linear, gradients are constant, equations can be integrated exactly
- Much better than numerical integration, no gain/loss of energy

Scattering rates

$$S_{k\to k'} = \sum_{mechanisms} \int d^3k' D(E_{k'})(1-f(k'))\mathbf{M}(k,k')\delta(E_k - E_{k'} - \Delta E_{mech})$$

$$\text{elastic: } \Delta E = 0$$

$$\text{acoustic: small } \Delta E$$

$$\text{optical: large } \Delta E$$

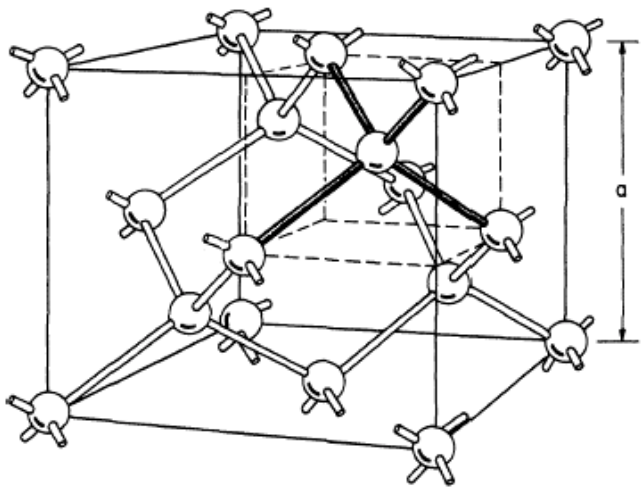
- Scatter from a state with momentum k to a state with a different momentum k' with or without change in energy
- Requires selection of final state *with specific energy*
- Requires knowledge of density of states $D(E_{k'})$ ~ area of energy isosurface with energy $E_{k'}$

Band structure (1)

- Electrons in free space: momentum and energy are simply related by

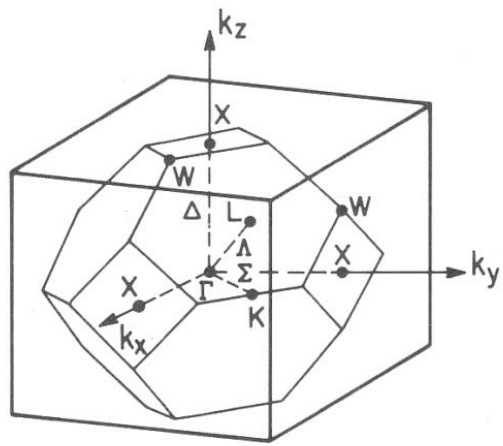
$$E = \frac{1}{2}\frac{\vec{k} \bullet \vec{k}}{m}$$

- Electrons in a periodic crystal: momentum is characterized by a band index and a momentum which varies over a minimum periodic cell in reciprocal space



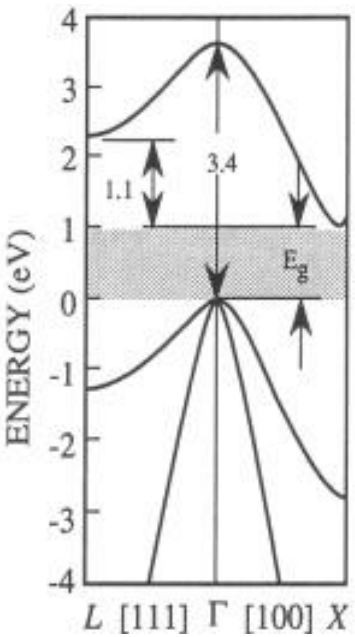
Brillouin Zone

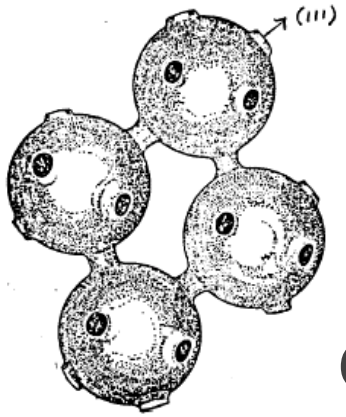
(k-space)



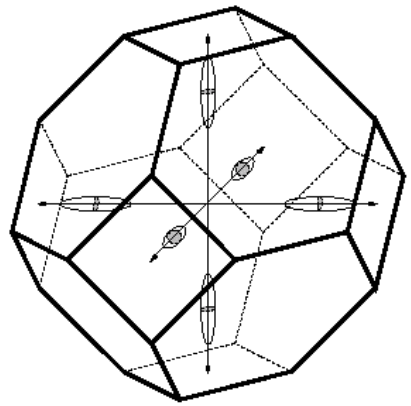
Band structure (2)

- Surfaces of constant energy no longer spherical





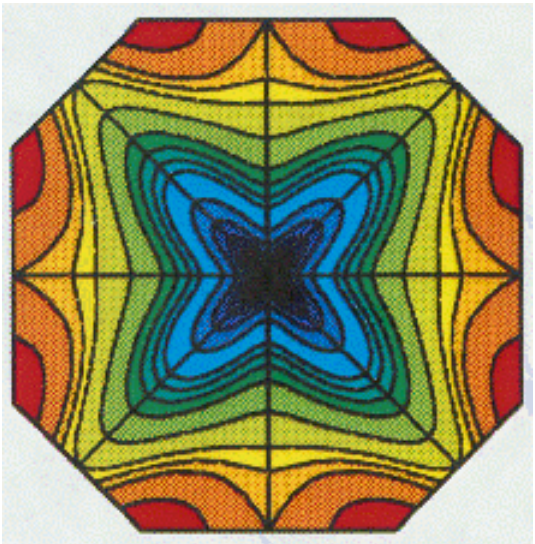
Cu



Si

- For low energy electrons or holes, parabolic ok
- For higher energies, analytic bands *maybe* ok
- For hot carriers, must take full band shape into account
  - Difficult to identify states with particularly energy
  - Difficult to calculate area of iso-energy surface
  - But must be accurate since $\vec{v} \propto \nabla_{\vec{k}} E_n(\vec{k})$

Hole bands

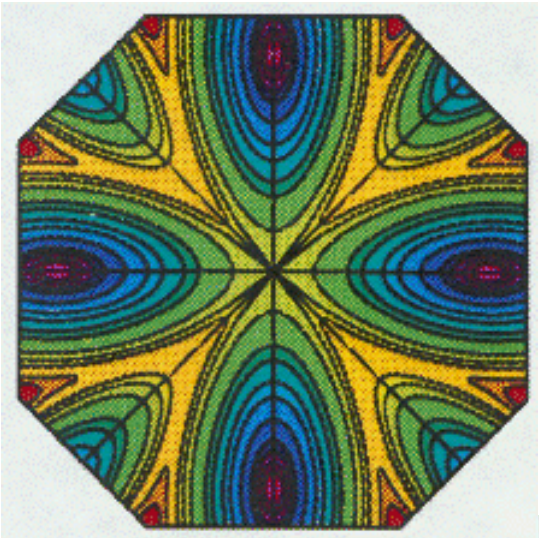


B2

B3

- Cross section of k-space at $k_z = 0$
- Energy contours

Electron bands



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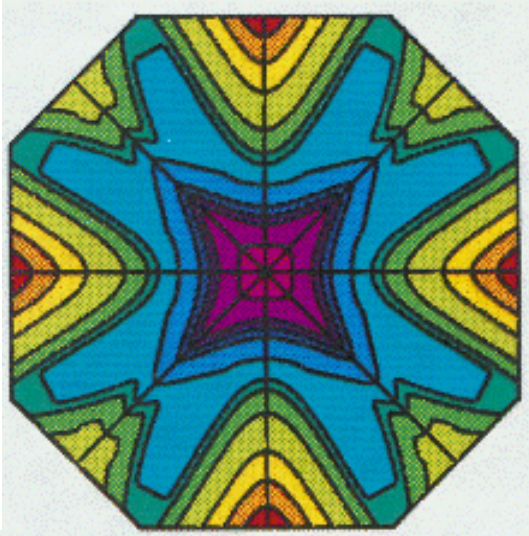

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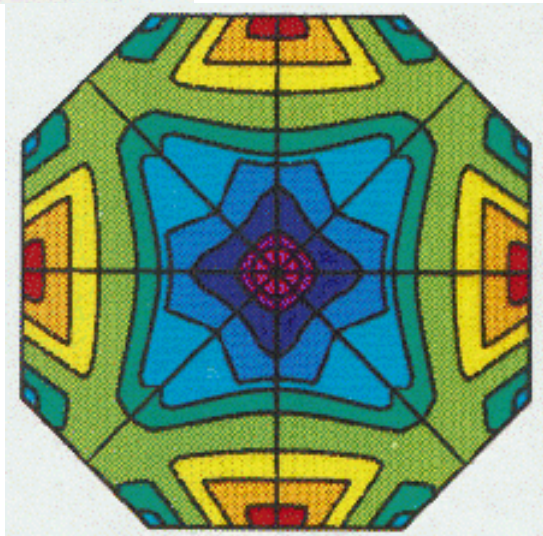
B5



B7

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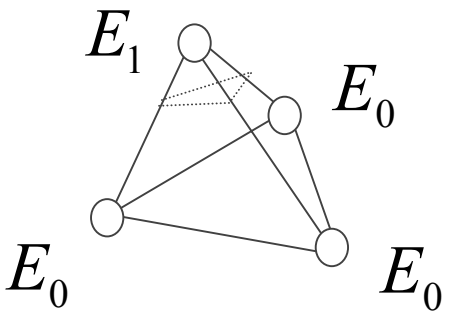
Full band representation

- Decompose Brillouin zone into 48 wedges, all of which are related to the first by symmetry (8 axis inversion, 3 cyclic permutation, 2 axis switching)
- Discretize irreducible wedge into tetrahedral mesh in k-space
- Linear shape function in tet –> constant E surface easy
- Further important simplification if tet is energy aligned so that nodes are on constant energy surfaces
  - Simplifies choice of k' with specific energy
  - Greatly simplifies iso-energy surface area calculation

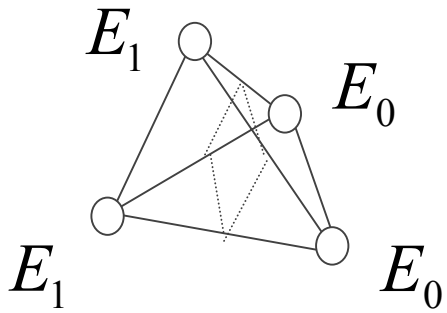
Interpolation

Type A



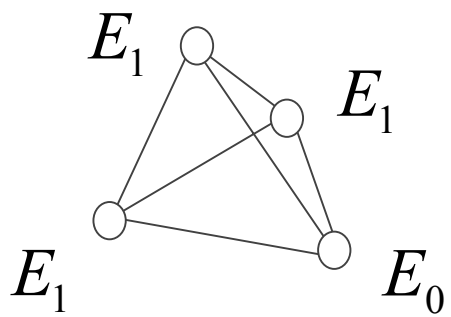
$$D^A(E) = D_T^A(1-\varphi)^2$$

Type B



$$D^B(E) = D_T^B(1-\varphi)\varphi$$

Type C



$$D^C(E) = D_T^C\varphi^2$$

define $\varphi = \dfrac{E - E_0}{E_1 - E_0}$

$$E_0 < E < E_1$$

The three quantities

$$D_T^A, D_T^B, D_T^C$$

are functions of the tet geometry only and can be precomputed

Total DOS of a constant energy surface

$$D(E) = D^A(1-\varphi)^2 + D^B(1-\varphi)\varphi + \mathrm{D}^C\varphi^2$$

The integrated DOS are pre-computed for each contour level of the mesh

$$D^A(E_0) = \sum_{T \in T^A(E_0)} D_T^A$$

$$D^B(E_0, E_1) = \sum_{T \in T^B(E_0)} D_T^B$$

$$D^C(E_0) = \sum_{T \in T^C(E_0)} D_T^C = D^A(E_1)$$

A complete DOS calculation requires under a dozen arithmetic operations

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Final state selection

- Given a desired final state energy $E_{k'}$, choosing a new momentum state k' after scattering is also easy
  - Identify tets with $E_i < E_{k'} < E_{i+1}$
  - Select tetrahedron type randomly among A,B,C
  - $E_{k'}$ defines isosurface inside tet
  - Choose two random variables distributed randomly over a right triangle (type A or C) or a square (type B)
  - Treat as barycentric coordinates to choose k' on isosurface

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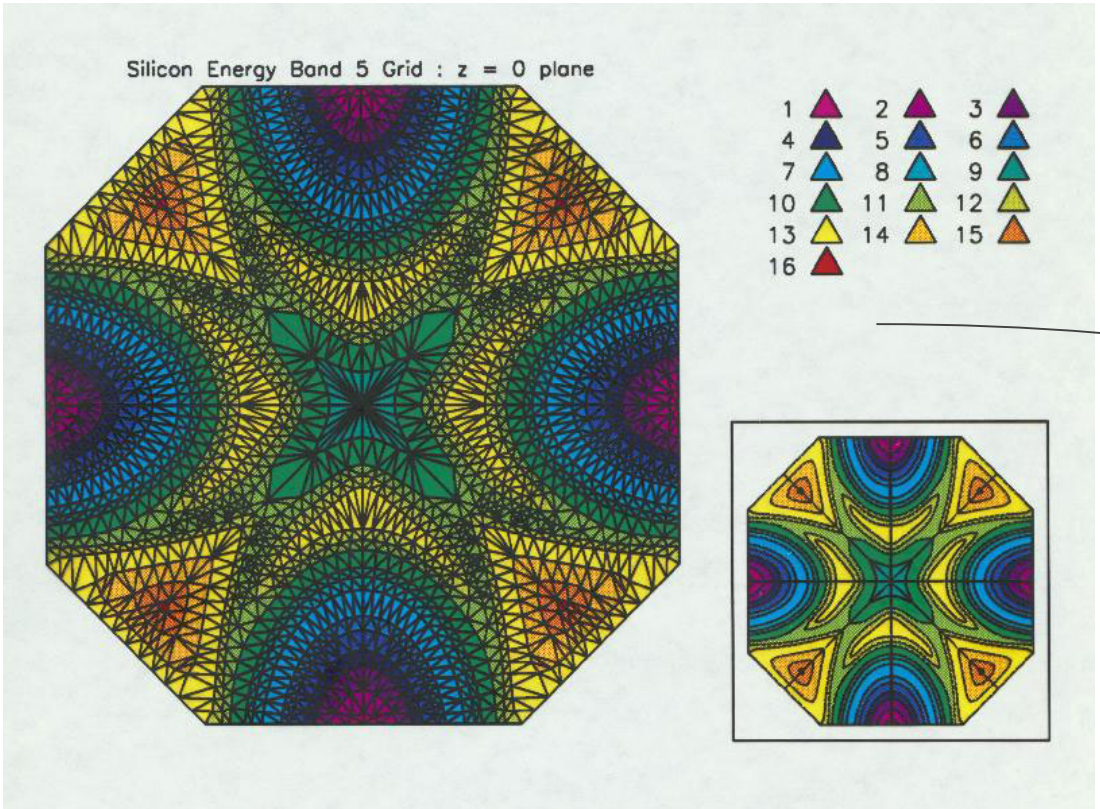
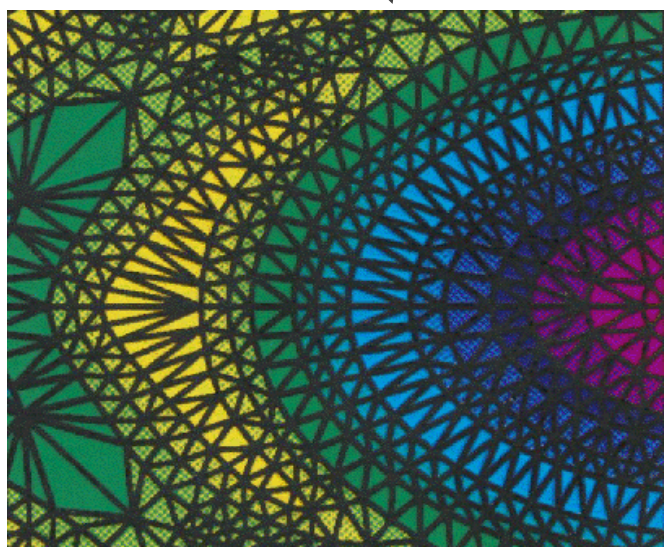
Mesh generation

- Special purpose mesh-generation carried out once for each material (silicon, GaAs, InP, …)
- Calculate fine 3d mesh of E(k) using band-structure code
  - Build skeleton from critical points $\nabla_k E = 0$ and ridge lines
  - Use ridge lines to divide into regions
  - Within each region, generate vertices along contours
    - Adhere to ridge lines
    - Adhere to wedge boundaries
    - Piecewise linear approximation to region boundaries
  - Contour-aligned grid produced by refining grid edges
    - Edges crossing more than one countour subdivided
  - Curvature used to monitor discretization error

Mesh generation





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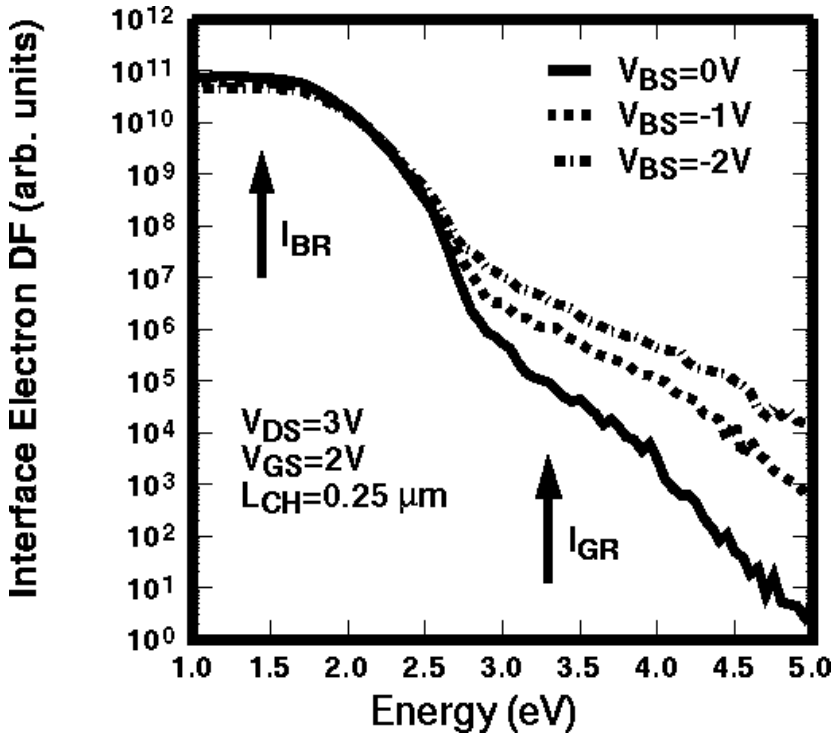
Mesh generation statistics

Band	Vertices	Tetrahedra	Contours	Quality
1(h)	349	1198	24	0.567
2(h)	530	2268	19	0.611
3(h)	414	1617	18	0.590
4(e)	1343	6143	16	0.529
5(e)	1658	8077	17	0.564
6(e)	613	2431	13	0.456
7(e)	419	1542	11	0.421

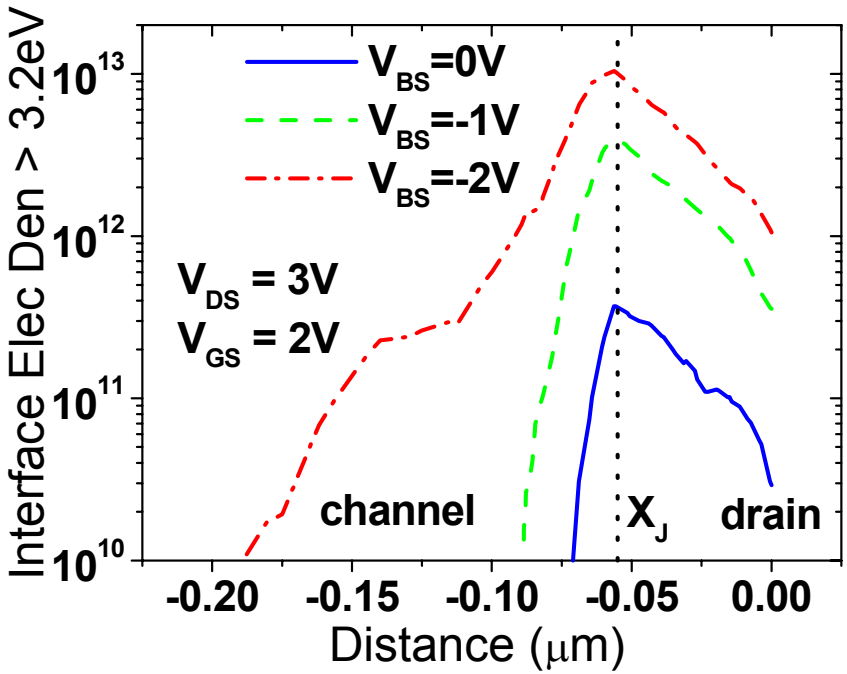
Error tolerance of 0.02eV, and 0.002eV near minima

Results

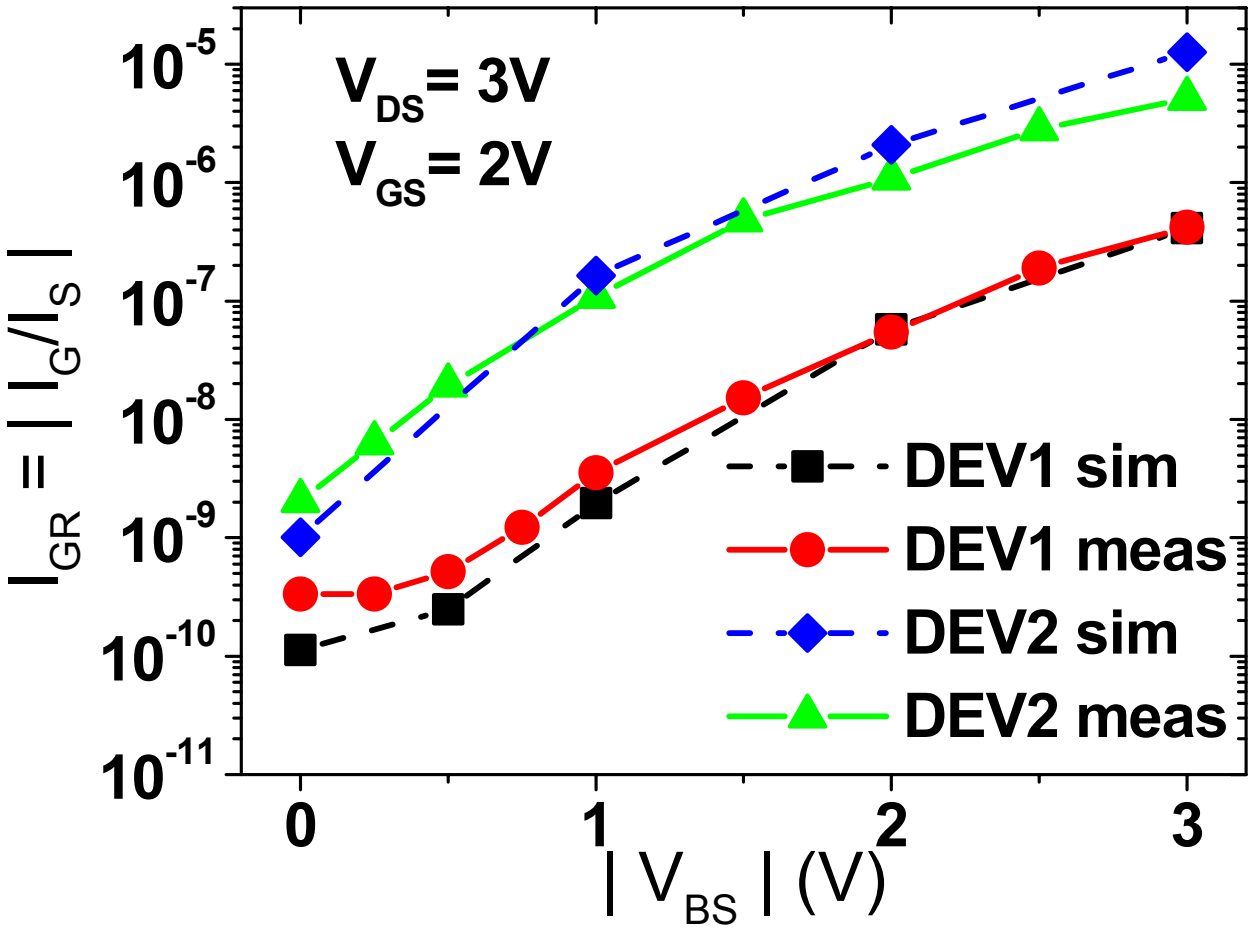
- Simulation times in hours, not weeks
- Huge dynamic range in carrier distribution functions
- Smooth variation of output with input (low statistical noise)
- Availability of new simulation methods has led to the development of new types of flash memory using physical mechanisms not previously understood



Good spatial resolution available - essential for accurate damage modeling

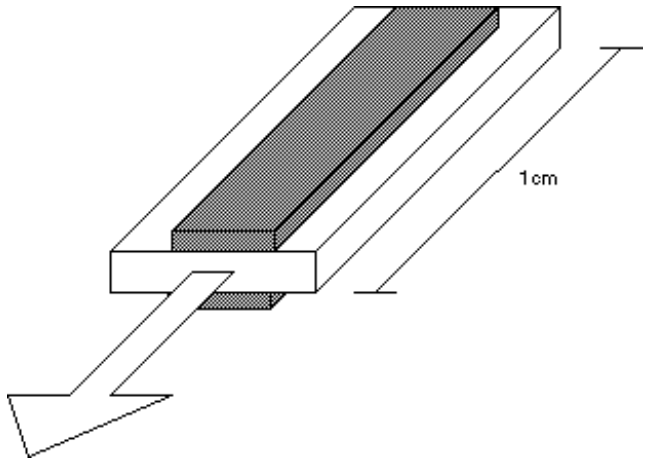


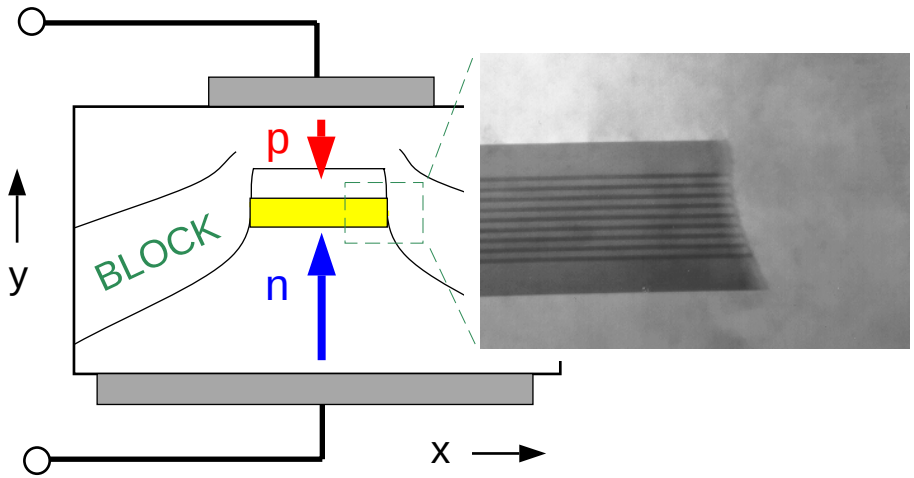
Simulation Versus Measurement – Resolution of High Energy Tail Essential to Match Experiment

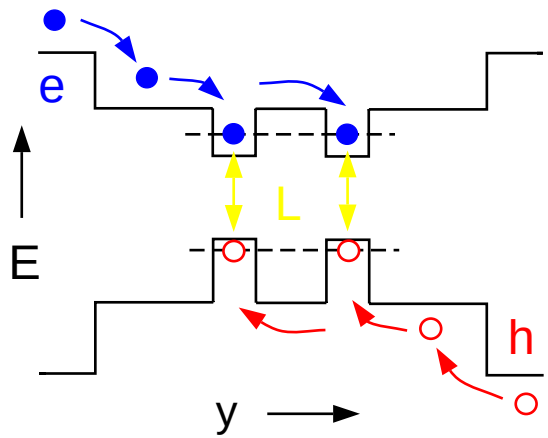


Microscopic Laser Simulation

- Fundamental Processes
  - Quantum optics
  - Carrier transport
  - Carrier recombination
  - Quantum well capture
  - Quantum well gain
  - Length scales (10Å - 10μm)

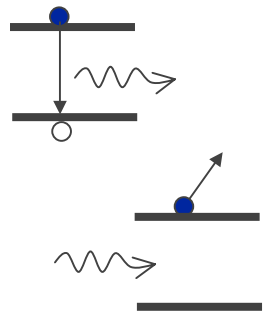




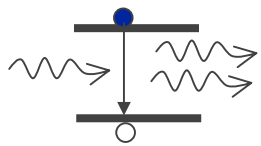


Optical processes

- Photons generated when electrons meet holes (spontaneous emission)



- Photons absorbed by free carriers
- Photons lost at mirror ends of device (absorbed or escaped)
- Photons stimulate emission of photons (basis of laser action - stimulated emission)



$$\frac{dS}{dt} = -\alpha_{mirr} - \alpha_{FCA} + G.S + R_{sp}$$

- In steady state

$$S = \frac{R_{sp}}{\alpha_{mirr} + \alpha_{FCA} - G}$$

Optical modes

- Shape of mode is determined by scalar wave equation

$$(\nabla^2 + \omega^2 \varepsilon / c^2)\Theta = \kappa^2 \Theta$$

- Lateral length scale much smaller than longitudinal, write

$$\Theta = \Theta_T e^{ik_z z}$$

- Solve for lateral mode (eigenvalue problem)

$$(\nabla_T^2 + \omega^2 \varepsilon / c^2)\Theta_T = (\kappa^2 + k_z^2)\Theta_T$$

- Generally only one lateral mode active, determines center energy (~1eV), with a number of longitudinal modes separated by ~1meV energy
- Laser is designed so center energy (determined by device geometry) corresponds to energy emitted when e-h pair recombines
- Product $S\Theta$ determines local optical power at each point in space

Free carriers

- Drift-diffusion equation for free carriers (aka 3d carriers)
  - Charge balance

$$\varepsilon \nabla^2 V = q(p_{3d} + p_{2d} + N_D - n_{3d} - n_{2d} - N_A)$$

  - Electron transport

$$\nabla \bullet (-D_n \nabla n_{3d} - \mu_n n_{3d} \nabla V) = (R_{3d} + C_n)$$

  - Hole transport

$$\nabla \bullet (-D_p \nabla p_{3d} + \mu_p p_{3d} \nabla V) = (R_{3d} + C_p)$$

- p_{3d}, n_{3d}, V discretized as scalar variables, one per mesh point
- Recombination R_{3d} algebraic function
- Capture of electrons into wells C_n a (messy, but local) function of electron density, electrostatic potential and captured electron density
- Exponential upwinding used (Scharfetter-Gummel)

Bound carriers - modes

- Bound-carrier space distribution is determined by eigenvalue problem (Schrödinger equation)

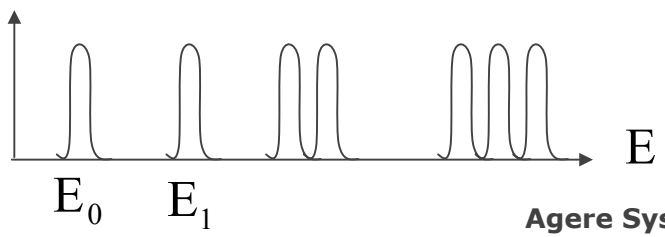
$$(\mathbf{H}+V)\varphi = \mathrm{E}\varphi$$

E.g. parabolic bands: $\mathbf{H} = \frac{\hbar^2\nabla^2}{2m}$
(if life were easy, in fact **H** is much more complex)

- Solutions

$$E_0, \varphi_0$$
$$E_1, \varphi_1$$
$$E_2, \varphi_2$$
$$\ldots$$

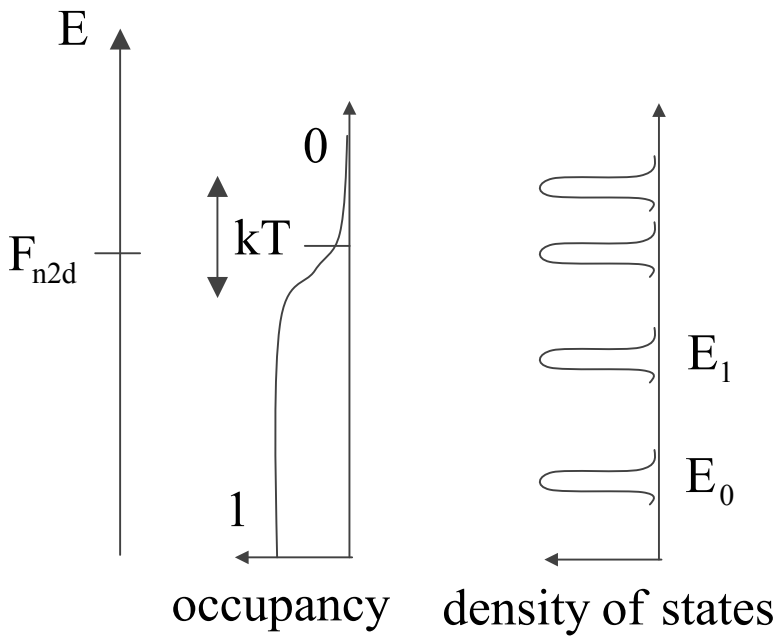
- Various scattering processes broaden sharp levels, accounted for empirically
  - Density of states ~ $A(E) = \frac{\Gamma}{(E-E_i)^2+\Gamma^2}$



Bound carriers - density

- Total number of bound (2d) carriers is determined by position of levels relative to bound carrier fermi-level

$$n_{2d} = \sum_{levels} \int dE \frac{1}{1 + e^{E - F_{n2d}/kT}} A(E - E_{level})$$

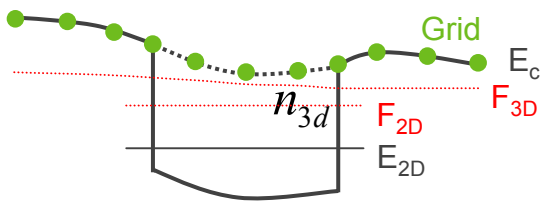


Bound carriers - interaction with free carriers

- Number of bound carriers is determined by balance of capture, recombination and emission processes

$$C_n(F_{n2d}, F_{p2d}, n_{3d}, p_{3d}, n_{3d}) - G(F_{n2d}, F_{p2d})S - R_{sp} = 0$$

- Either F_{n2d} or n_{2d} serves to characterize bound carrier population
- Convenient to keep both variables as solution variables and add the relationship between them as an extra equation
  - $C_n(n_{3D},Fn_{2D},V)$ appears in n_{3D} equations near quantum well
  - But F_{2D} (V) non-locally through the quantum well region
  - Solution: introduce F_{2D} as an auxiliary solution variable



Capture and gain expressions

- Convolution integrals involving the fermi function and its integrals

$$f(x) = \frac{1}{1+e^{x}} \qquad f_p(x) = \int_0^\infty \frac{x'^p}{1+e^{x'-x}} dx'$$

- Capture rate

$$C_n = \left[\frac{f_{3/2}(F_{n3d} - E_c/kT)}{f_{1/2}(F_{n3d} - E_c/kT)} - \frac{f_{3/2}(F_{n2d} - E_c/kT)}{f_{1/2}(F_{n2d} - E_c/kT)} \right] \frac{n_{3d}}{\tau}$$

  - $F_{n3d} = V + kT/q \ln(n_{3d}/n_i)$ analagous to F_{n2d}

- Gain $G \sim \sum_{levels} |p_{level}|^2 \int dE dE' \left(f_v(E) - f_c(E')\right) \times$

$$\times A_{vk}(E) A_{ck}(E') \delta\left(\hbar\omega - \left(E' - E\right)\right)$$

Gain: Qualitative Physics

- Carrier scattering: broadening
- Probability of emission

  Integrate:

  $A_h(E_h) f_h(E_h) A_e(E_e) f_e(E_e)$

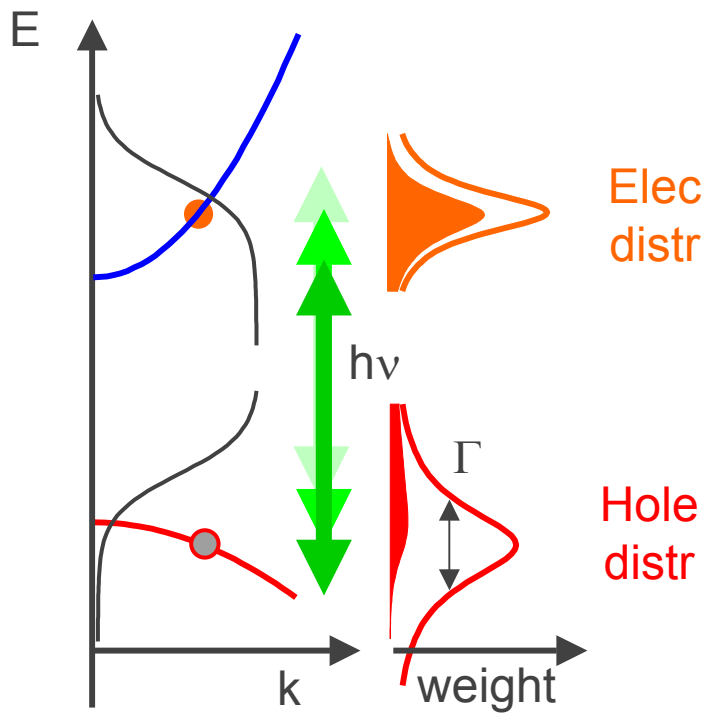
  for $h\nu = E_e - E_h$

- Key point
  - Usually simplify: $\Gamma << k_B T$

    common Lorentzian approximation:

    $f_h(E_{hk})\, f_e(E_{ek}) L(h\nu - (E_{ek} - E_{hk}))$

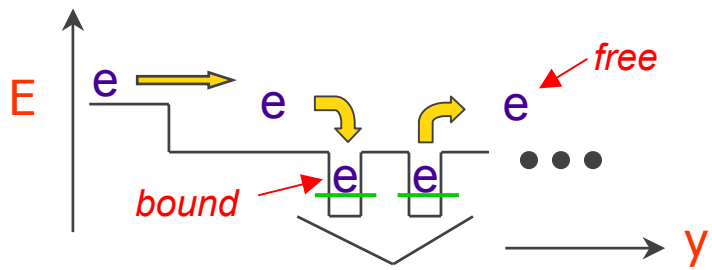
  - But for lasers: $\Gamma \sim k_B T$
    - ❑ full convolution required



Assemble all the pieces: Fully Coupled Device Equations

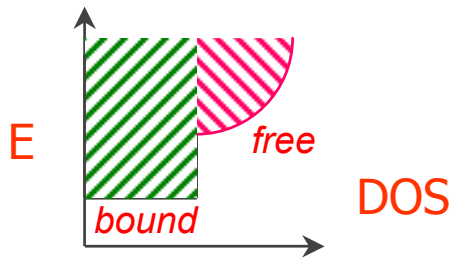
- Free Carriers (3D)

$$\nabla\cdot(\varepsilon\nabla V)=q(p_{3D}-n_{3D}+p_{2D}-n_{2D}+N_D-N_A)$$
$$\nabla\cdot J_n(n_{3D},V)=q(R_{3D}+C_n)$$
$$\nabla\cdot J_p(p_{3D},V)=q(R_{3D}+C_p)$$



- Bound Carriers (2D)

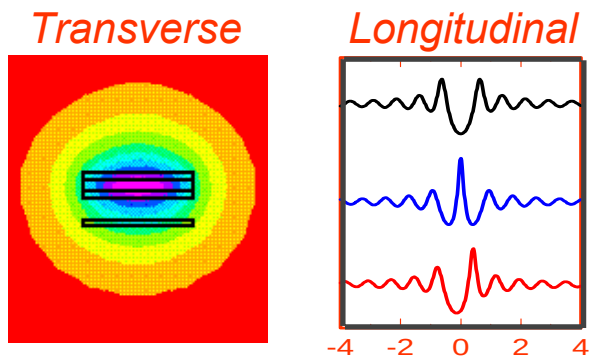
$$(H+V)\psi=E\psi$$
$$C_n-G(F_{n_{2D}},n_{3d})S-R_{2D}=0$$
$$C_p-G(F_{p_{2D}},p_{3d})S-R_{2D}=0$$



- Photon Modes

$$\left(\nabla^2+\omega^2\,\varepsilon(n,p)/c^2\right)\phi=\kappa^2\phi$$

$$S=\frac{\beta R_{sp}}{\alpha_{mirror}+\alpha_{FCA}(n,p)-G(n_{2D},p_{2D},\omega)}$$



Key Numerical Issue - Laser Threshold

- Threshold for photon intensity
  - Pole as gain approaches loss
  - I ~ exp(V/kT)
  - 2X in current happens over 0.04V at V~0.8V
  - Solution: introduce slack variable to avoid negative photon number

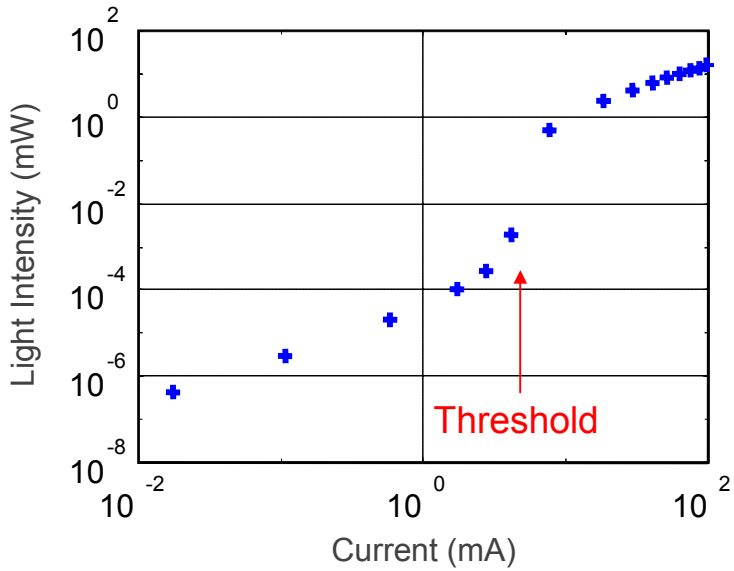
$$S = \frac{\beta R_{sp}}{\alpha_{mirror} + \alpha_{FCA} - G(n_{2D}, p_{2D})}$$

$$S = \beta R_{sp} \tau_m / \lambda^2$$

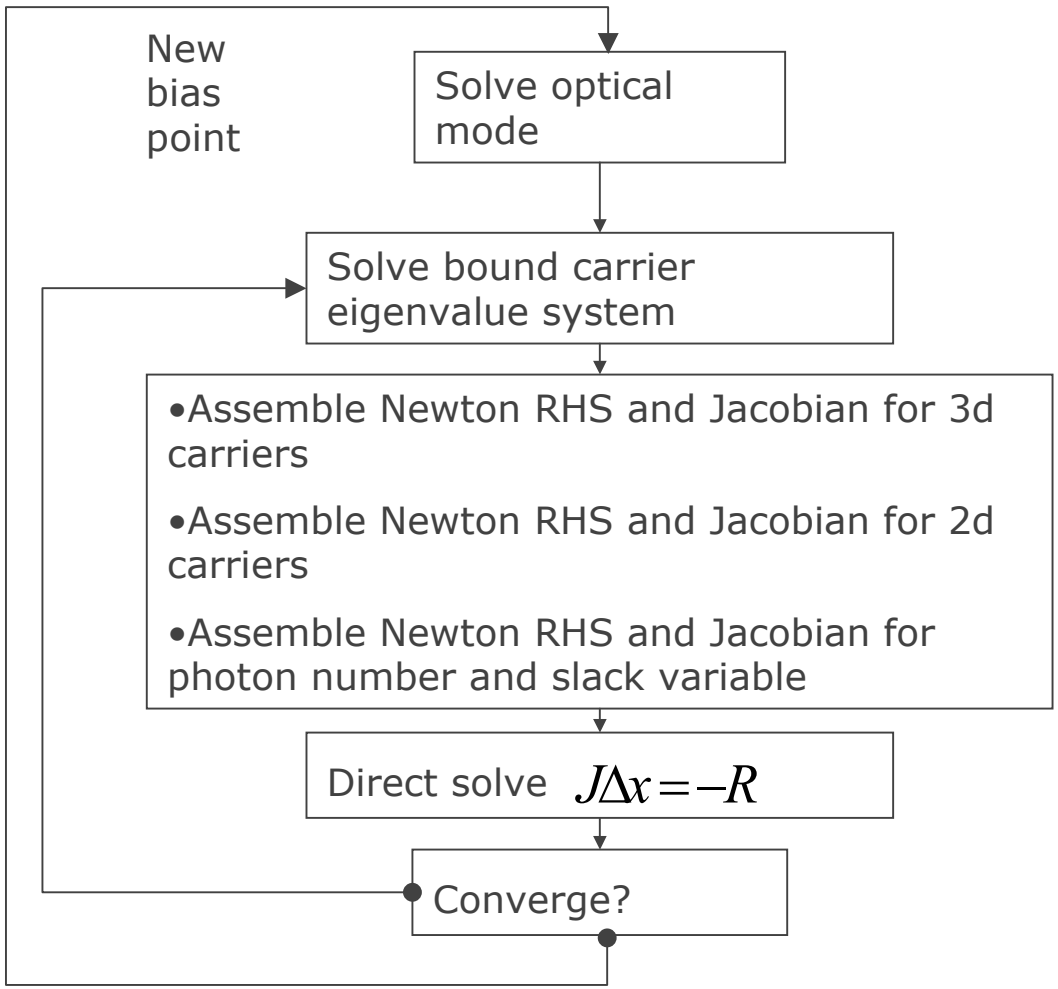
$$\lambda^2 = 1 + (\alpha_{FCA} - G(n_{2D}, p_{2D}, \omega))\tau_m$$

$$1/\tau_m = \alpha_{mirror}$$

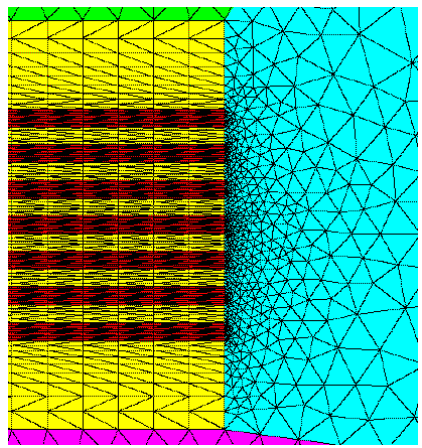
Light-Current Response



Solution Flowchart

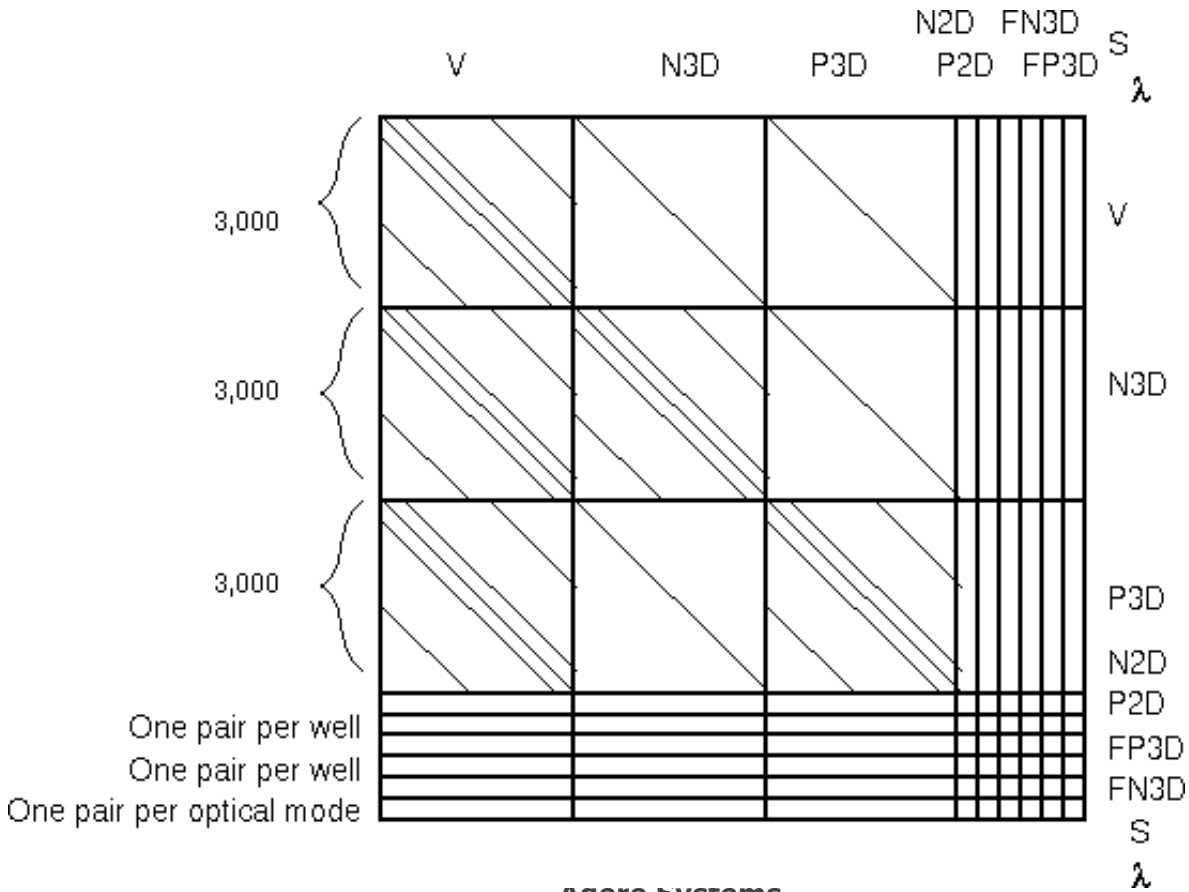


- **Electrical and optical PDEs discretized on same grid**
- **Fully self-consistent solution of bound and free electrons**
- **Slack variable for photon number**

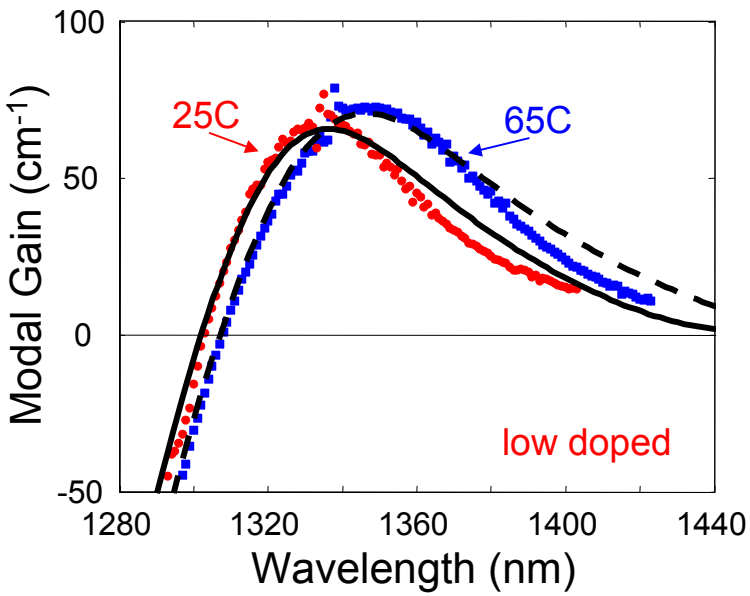


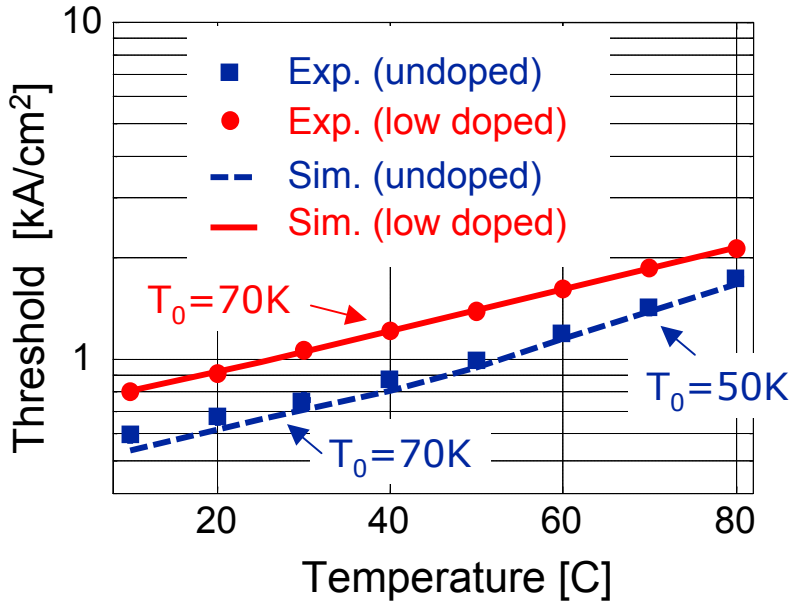
System Jacobian

- All derivatives evaluated
- Derivatives of eigenvalues wrt parameters of eigenvalue problem expanded using first-order perturbation theory



Steady State Results: Simulation vs Experiment

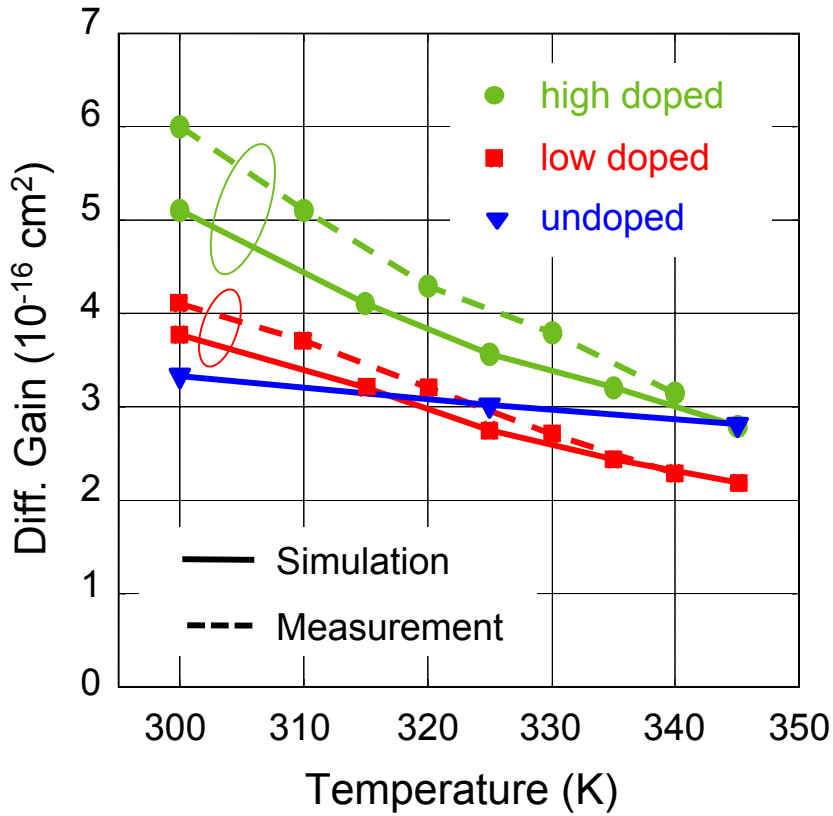




- Gain spectra near threshold
  - Spectral shape
  - Temperature dependence
  - Direct verification of key QW model
- Threshold current density
  - Change with doping
  - Temperature dependence
    - $J_{th} \propto exp(T/T_0)$
    - *Break in T_0 near 50 C*

Effective Differential Gain: Simulation vs Experiment

- Modulation efficiency increases with active layer doping
- But … Temperature sensitivity also increases !
- Simulation accounts for both the doping and the temperature dependence
  - ***No*** parameter is adjusted for the modulation efficiency



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Conclusion

- Demonstrate efficient, integrated *LASER* simulator
  - Fully self-consistent calculation of electron and photon processes
  - Solved using full Newton method
  - Slack variables solve threshold problem
- Excellent agreement with steady state and dynamic performance data for 1.3μm MQW lasers
  - Explain temperature dependent threshold (T_0)
  - Explain temperature & density dependent modulation efficiency
  - Explains diminishing returns of extra quantum wells