Quantum and semi-classical transport in RTDs using NEMO 1-D

Gerhard Klimeck, Phillip Stout[$] and R. Chris Bowen
Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA 91109
[$]CFDRC, Huntsville, AL 35899
email: gekco@jpl.nasa.gov website: http://hpc.jpl.nasa.gov/PEP/gekco

NEMO 1-D has been developed primarily for the simulation of resonant tunneling diodes (RTDs), and quantitative and predictive agreements with experimental high performance, high current density devices have been achieved in the past. There are four key ingredients to the success of these simulations: 1) the treatment of the extended contacts including quasi bound states and empirical relaxation time approximation scattering with a surface Green function, 2) accurate description of bandstructure using empirical tight binding models, 3) quantum charge self-consistency including a Hartree and exchange potential, and 4) the proper numerical integration over the transverse momentum.

The treatment of the contacts assumes that the device is subdivided into three distinct regions: 1/2) a left/right reservoir in local equilibrium with the left/right contact with well established left/right quasi-Fermi levels, and 3) a central device region which is treated to be in non-equilibrium using the non-equilibrium Green function formalism (NEGF). The central device region is considered to be the current limiting element in the device. The left/right reservoirs are assumed to be in local equilibrium with a flat Fermi level and conductive enough to provide current without depletion of the reservoir. Despite the successful comparisons to experiments one question remained lingering in the treatment of the reservoirs: How good is the assumption of a local equilibrium? or How good is the assumption of a flat Fermi level? The expansion of the NEMO 1-D code to couple a drift-diffusion model in the reservoirs to the central non-equilibrium region addresses these questions.

It can be shown that the drift diffusion equation can be formulated such that the current density in a particular device region is $J \propto \mu_i n_i \nabla E_{F,i}$, where μ_i, n_i, and $E_{F,i}$ are the device site (i) dependent mobility, electron density and quasi Fermi level). The expression holds for an arbitrary density of states for arbitrary electron distributions. Continually assuming that the central quantum region dominates the current flow in the de[illegible] the spatially dependent quasi Fermi level in the left/right contact is compute[illegible] th a quantum mechanically computed electron density.

This model is tested on a standard I[illegible]EMO test matrix. Figure 1a shows potential profiles and corresp[illegible]as of 0.333V assuming two different constant contact mobilities: [illegible]A resistor-like drop in the potentials in the emitter is visible th[illegible], the overall effect in the device is more complicated than a sin[illegible]p, since the Fermi level, the quantum mechanical electron dens[illegible] treated self-consistently with the current that is drawn out of the [illegible]ticularly evident in the corresponding current-voltage characteristic in forwar[illegible]verse sweep are shown in Figure 2b. The peak current in the two curves (insert of 1b) differs between the two simulations, while a simple series resistance would simply shift the I-V curve. Also shown is the associated bi-stability, which increases with increasing contact resistence as expected. It is noted here that simulations using mobilities ranging from 20000 to 100cm^2/Vs show almost indistinguishable results. A mobility of less than 100cm^2/Vs, however, appears to be unreasonably low for these high performance devices and it can be concluded that a quasi Fermi level drop in the contacts appears to be negligible.

Call when cleared

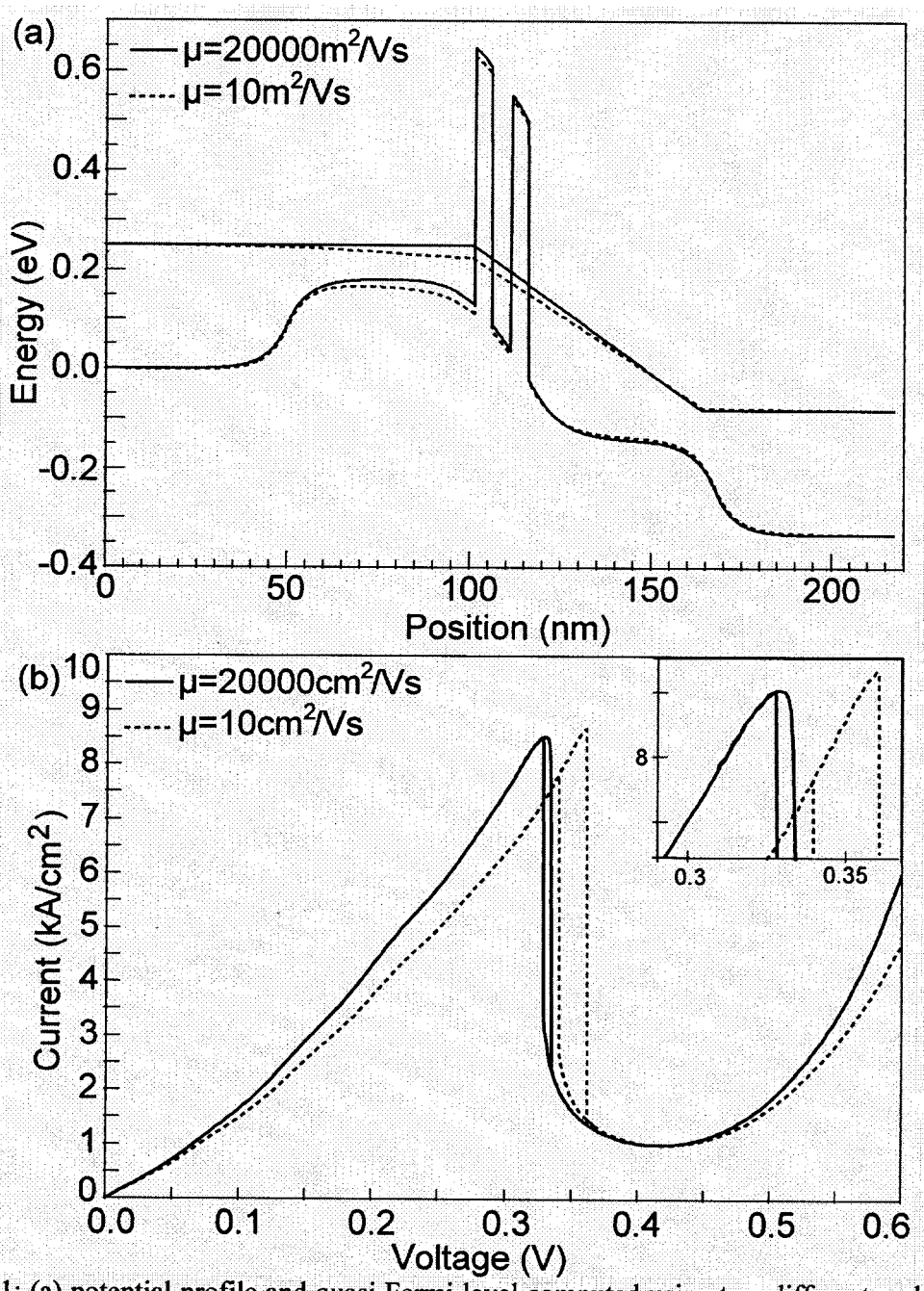


Figure 1: (a) potential profile and quasi Fermi level computed using two different mobilities at an applied bias of 0.333V. The low mobility profile shows a resistive potential drop in the emitter region. (b) Corresponding current-voltage characteristics in forward and reverse sweep. The inset shows the different peak amplitude due to the reduced contact mobility. The region of bi-stability is also increased with decreased mobility similar to a simple series resistance effect.

Quantum and semi-classical transport in RTDs using NEMO 1-D

(Overview)

Gerhard Klimeck
Jet Propulsion Laboratory, California Institute of Technology

gekco@jpl.nasa.gov
(818) 354 2182
http://hpc.jpl.nasa.gov/PEP/gekco

This research was carried out by at the Jet Propulsion Laboratory, California Institute of Technology under a contract with the National Aeronautics and Space Administration.

Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation

- **Motivation**
- **NEMO 1-D modeling**
  - Resonant Tunneling
  - Boundary conditions
  - Bandstructure
  - Scattering
  - Software development

NEMO 1-D:
Texas Instruments / Raytheon (1995-1997)
Roger Lake, R. Chris Bowen, Tim Boykin, Dan Blanks, Bill Frensley, C. Fernando, M. Leng
>50,000 person hours of R&D
250,000 lines of code in C, FORTRAN,F90

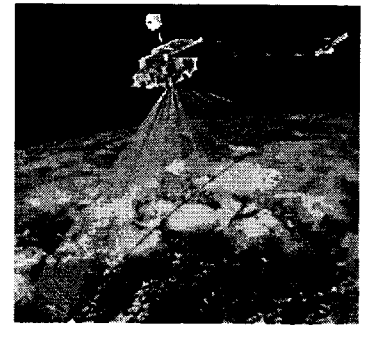
- **Design and Synthesis** **(Tom Cwik , Calos Salazar-Lazaro)**
  - GENES (Genetically Engineered Nanostructured Devices)
- **3D modeling** **(R. Chris Bowen, Tim Boykin, Fabiano Oyafuso)**
  - Massively parallel numerical developments
  - Quantum Dots
- **Future Efforts / Conclusions**

High Performance Computing at JPL

- JPL is the Lead Center for Robotic Space Exploratio
  - Deep Space Missions
  - Earth Observing Missions

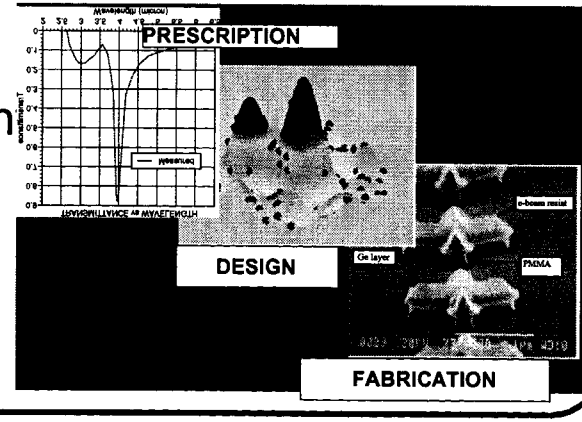
http://mars.jpl.nasa.gov

- JPL Builds Observational Systems for Remote Sensing
  - Imaging instruments across all wavelengths
  - Spectroscopic and in-situ instruments for planetary investigation
  - Fundamental technology development for new instruments

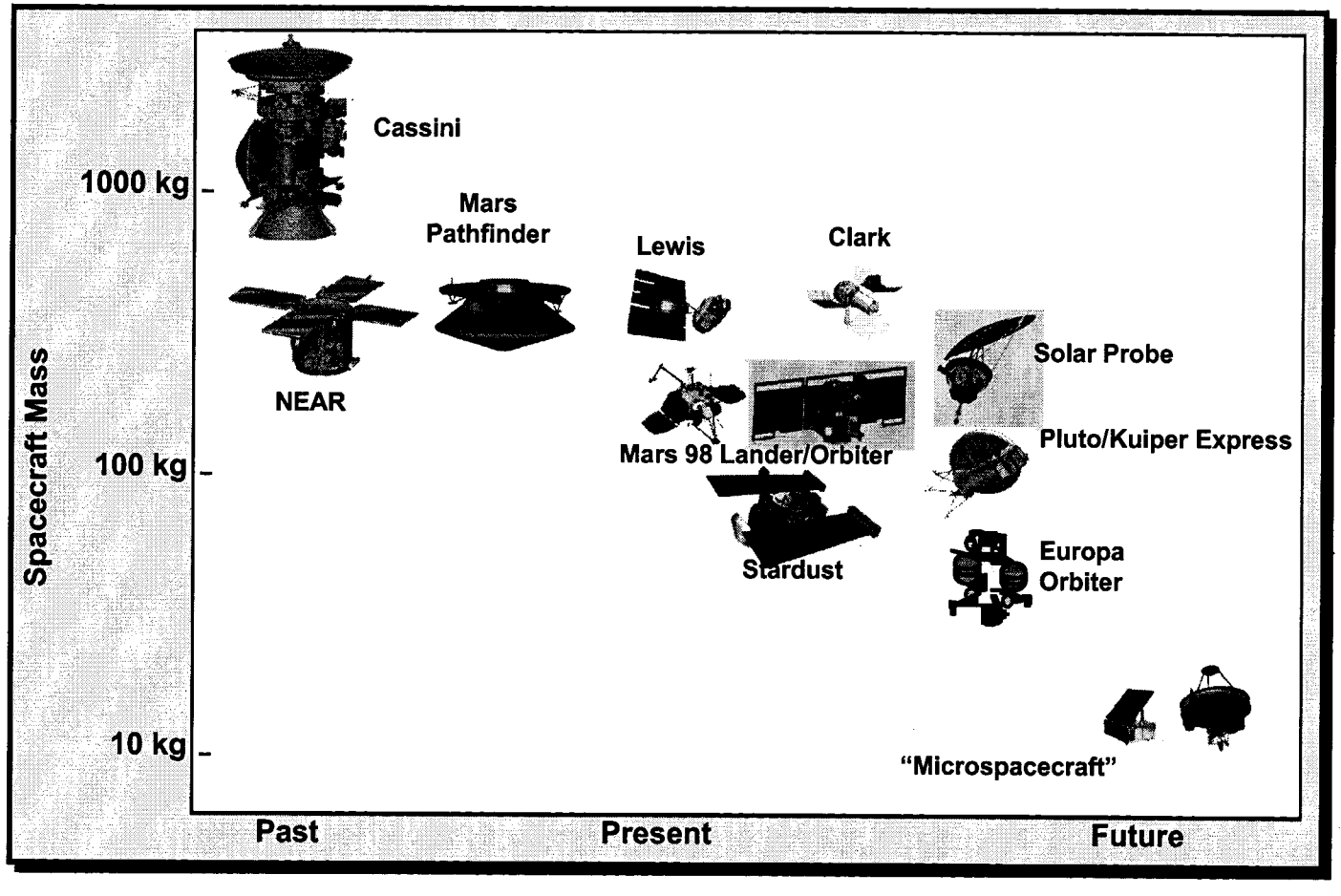


http://www-misr.jpl.nasa.gov

- JPL High Performance Computing is a Key Technology
  - Modeling and simulation of devices and instrumen
  - Rapid data reduction and analysis
  - Advanced software design, implementation and application
  - Integrated Design, Optimization and Synthesis

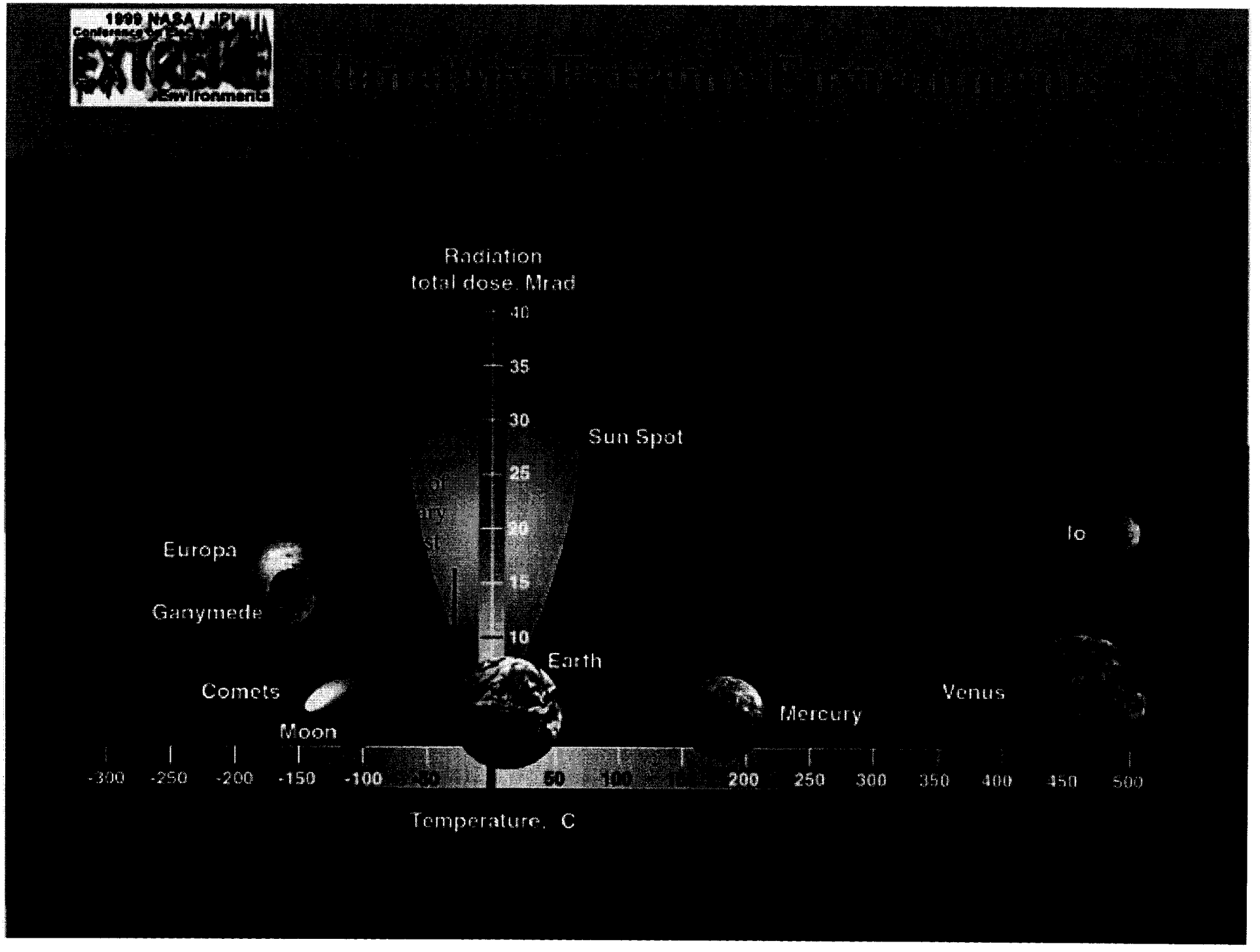


Progressive Spacecraft Miniaturization

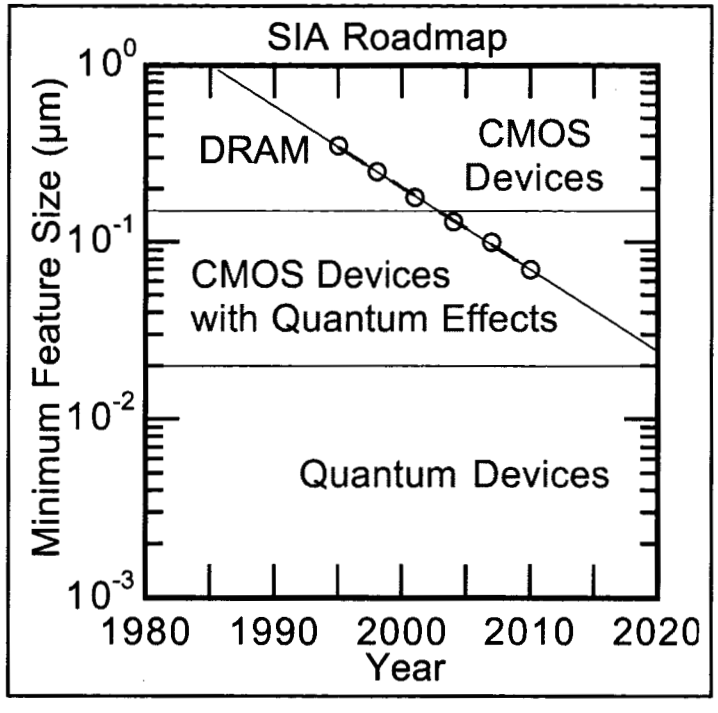


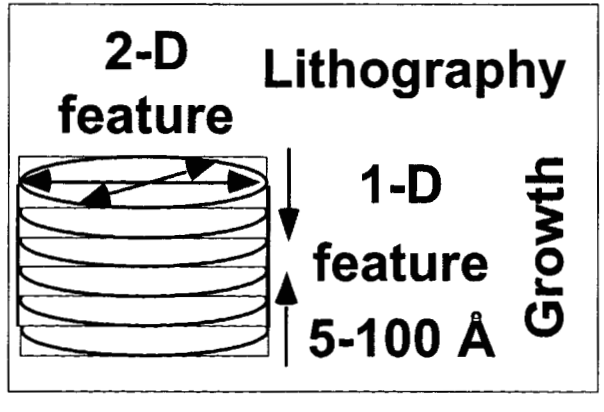
Low weight, low power and high efficiency

Have a special meaning to NASA


1999 NASA / JPL
Conference on Extreme Environments
Radiation
total dose, Mrad
40
35
30
25
20
15
10
Sun Spot
Europa
Ganymede
Io
Earth
Comets
Moon
Mercury
Venus
-300
-250
-200
-150
-100
50
100
200
250
300
350
400
450
500
Temperature, C

Microdevices Head for Atomic Dimensions



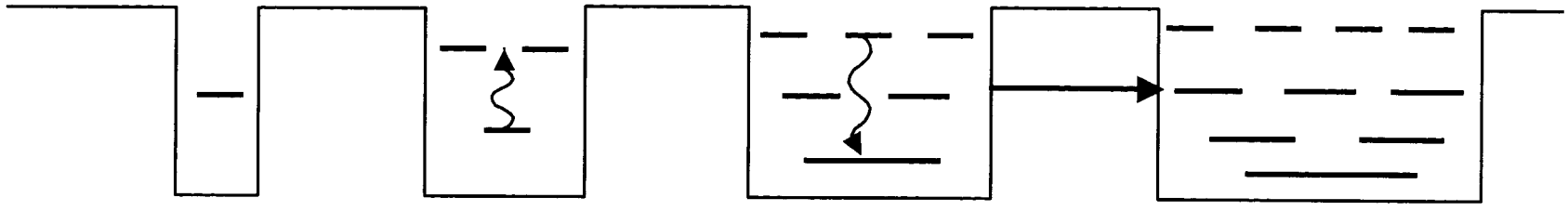


- Moore's Law shows quantum devices in the far future.
- Lithography data alone is deceiving: Layer thicknesses are already on the atomic length scale!
- Commercial devices see quantum limitations:
  - direct tunneling
  - state quantization
- Advanced devices utilize the quantum mechanical behavior:
  - Resonators (RTDs)
  - Active and passive sensors tunable by design - not by material system choice (QWIP).

-> 1D quantum device modeling

-> NEMO

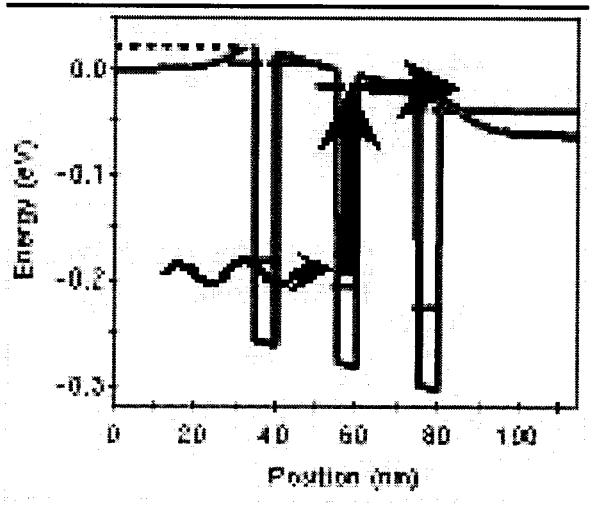
Transitions / Transport Controlled by Design



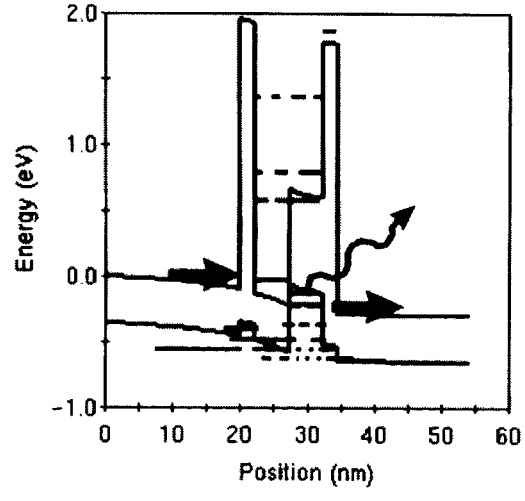
Photon Absorption → Detectors

Photon Emission → Lasers

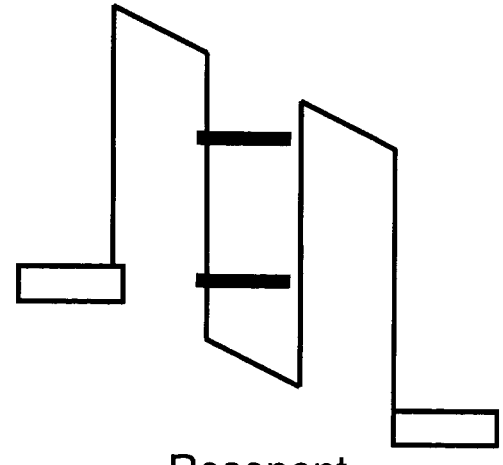
Tunneling → Logic / Memory



Quantum Well Infrared Detector

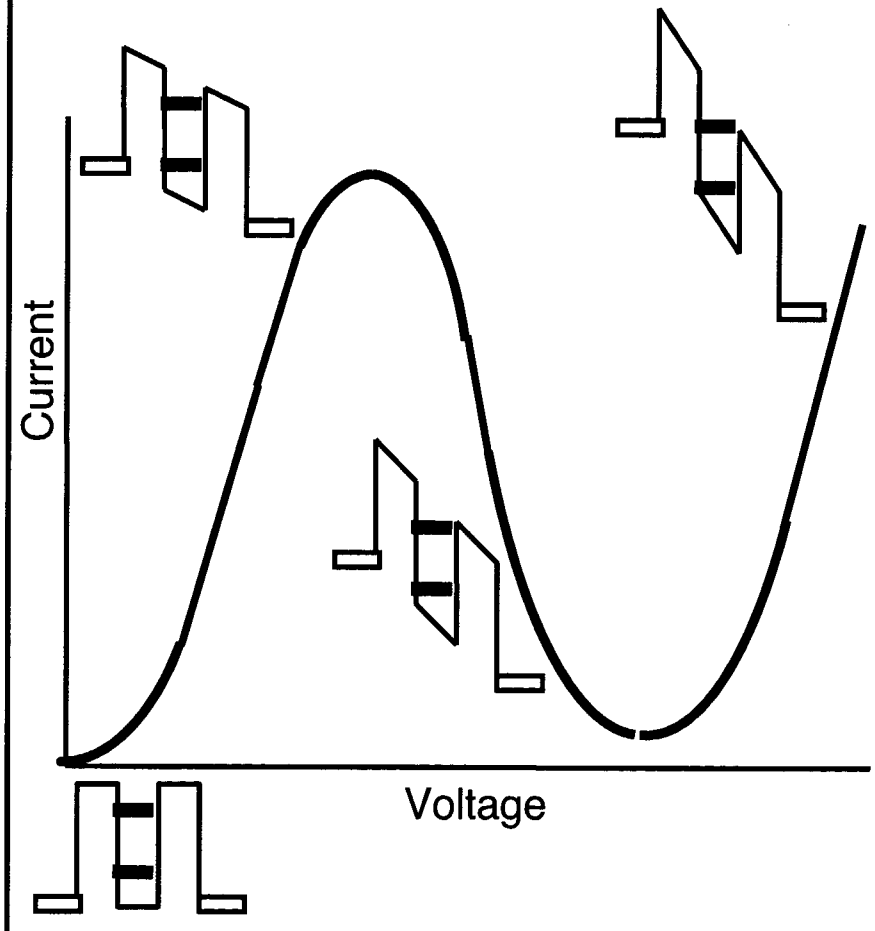


Quantum Cascade Laser

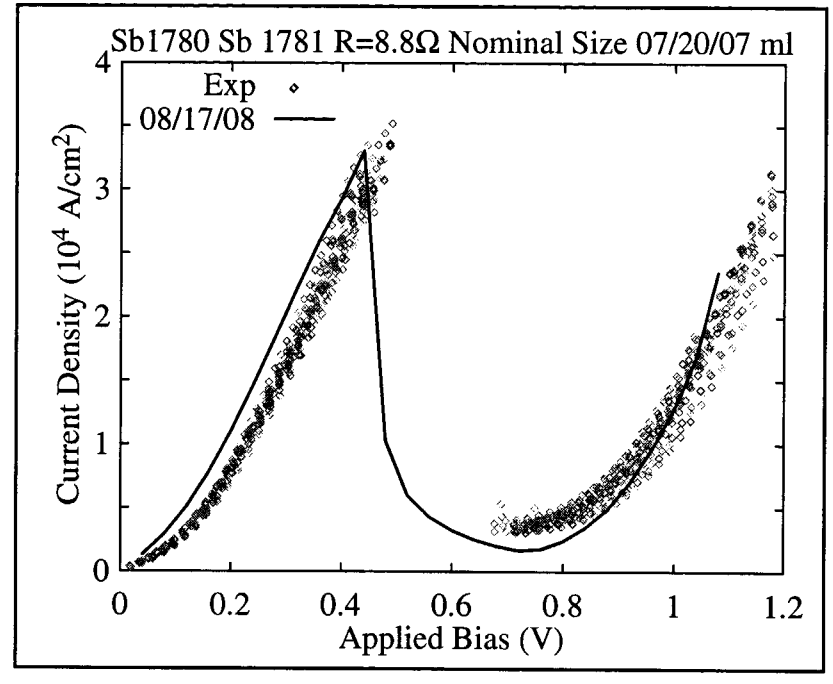


Resonant Tunneling Diode

Resonant Tunneling Diode



Conduction band diagrams for different voltages and the resulting current flow.

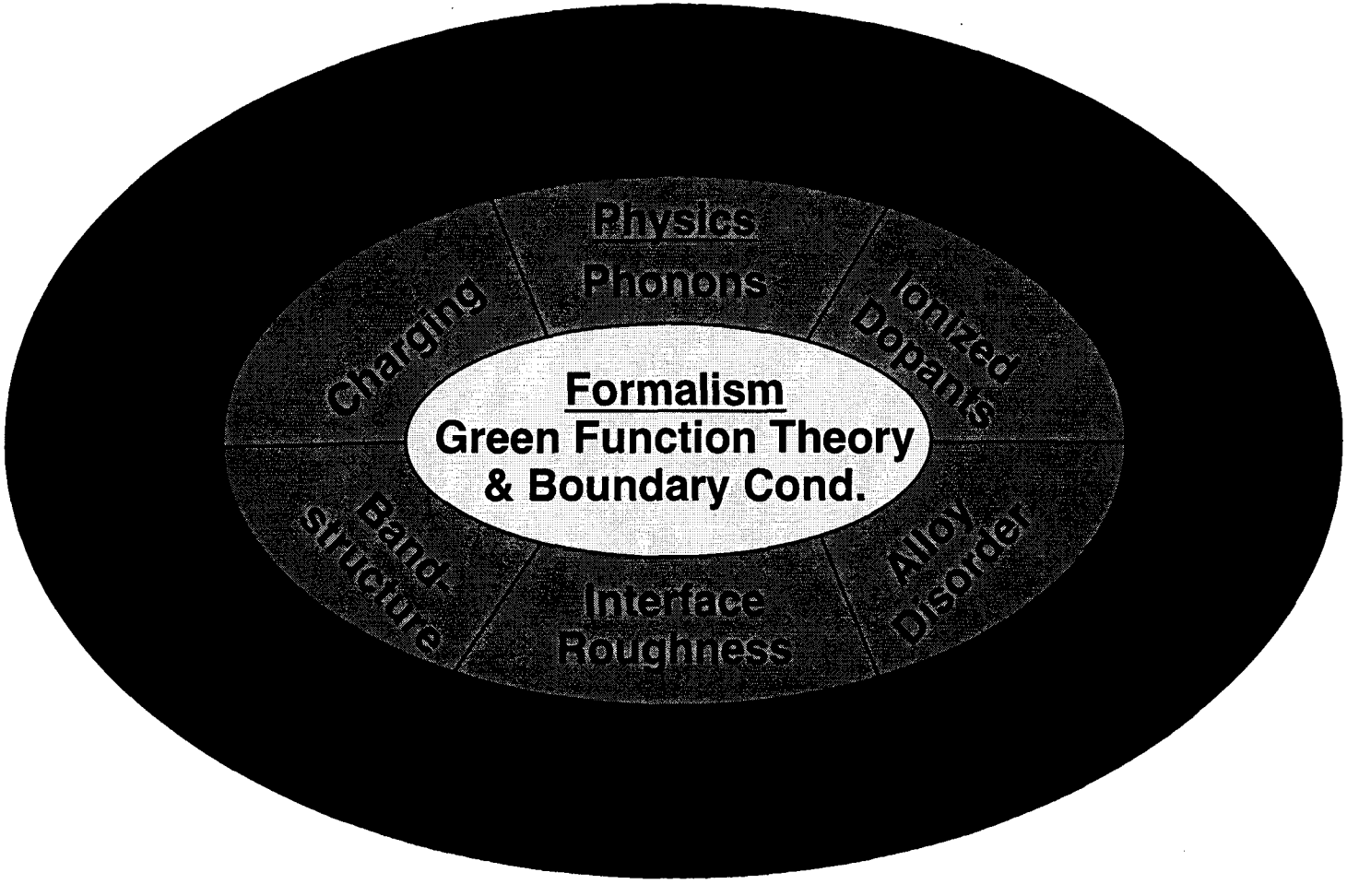


12 different I-V curves: 2 wafers, 3 mesa sizes, 2 bias directions

50nm	1e18	InGaAs
7 ml	nid	InGaAs
7 ml	nid	AlAs
20 ml	nid	InGaAs
7 ml	nid	AlAs
7 ml	nid	InGaAs
50 nm	1e18	InGaAs

NEMO: A User-friendly Quantum Device Design Tool

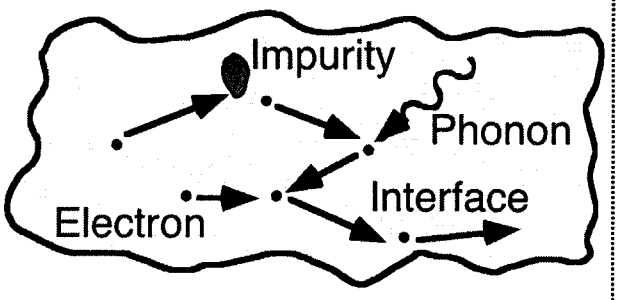
Formalism, Physics, and Technology



Approximately 250,000 lines of code

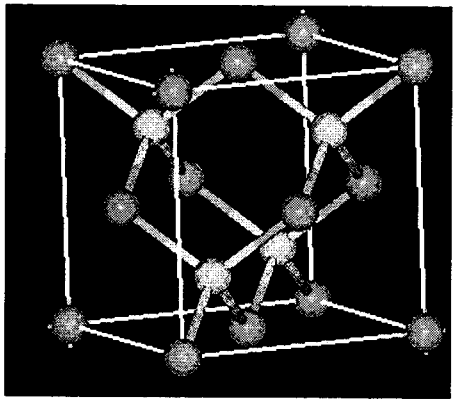
Where is NEMO compared to other models?

What is Needed for Quantum Electron Transport?



NEMO

Charging
Bandstructure
Scattering
Interference



Drift-Diffusion Boltzmann Eq.

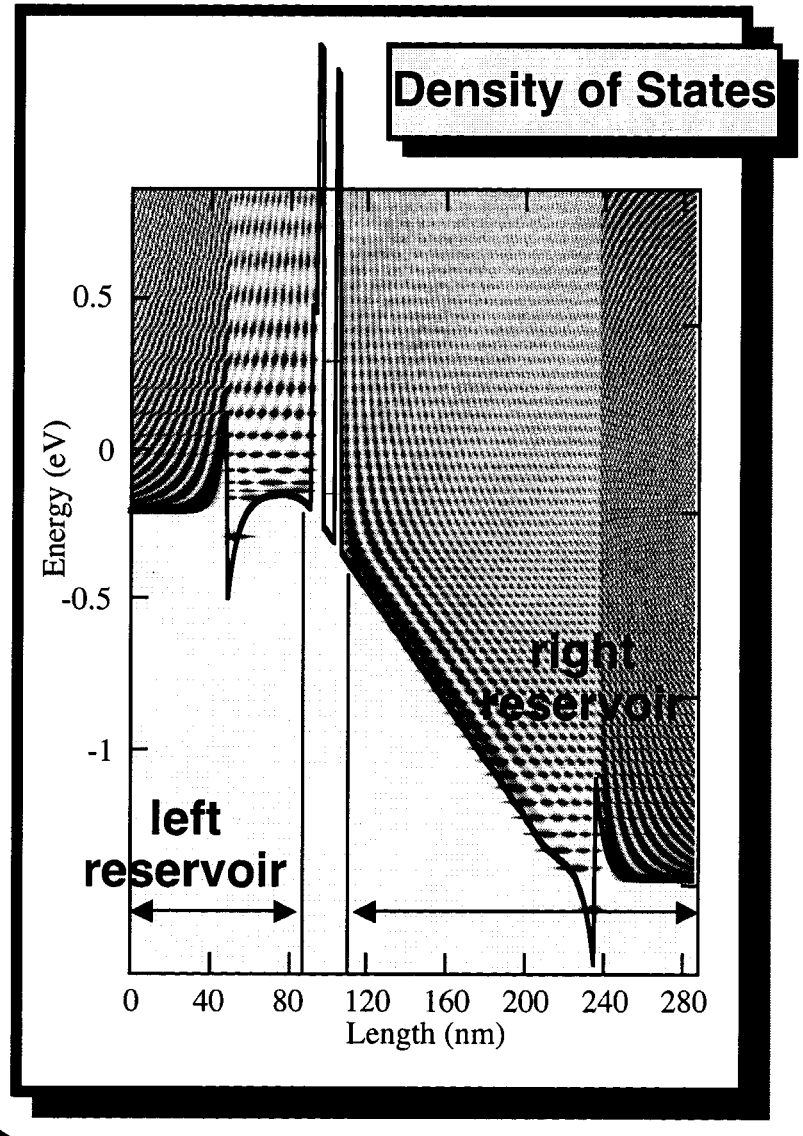
Non-Equilibrium Green Functions

Schrödinger Equation

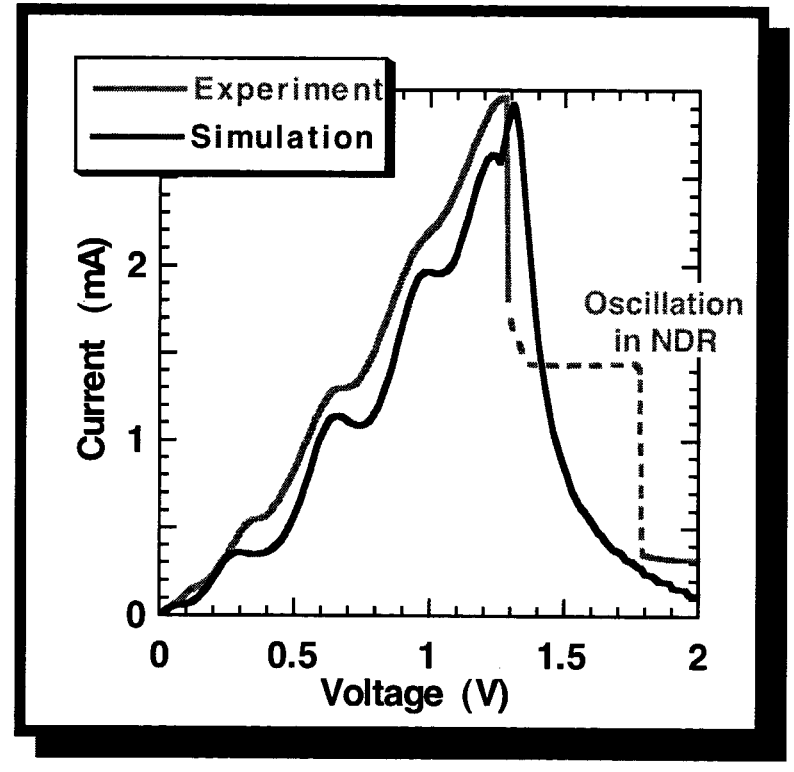
Transport with particle interaction

Quantum Mechanics

Realistic Devices Have a Large Extent!!!



Quantum Optical Switch



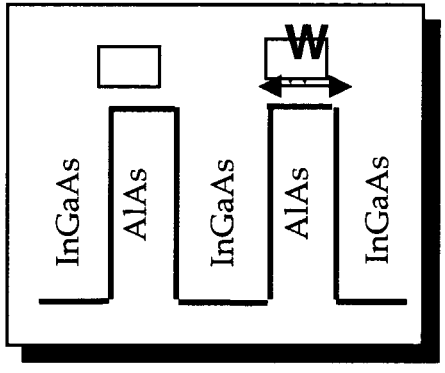
Calculate charge self-consistently in

- **the left and right reservoir**
- **central device region**

Testmatrix-Based Verification (room temperature)

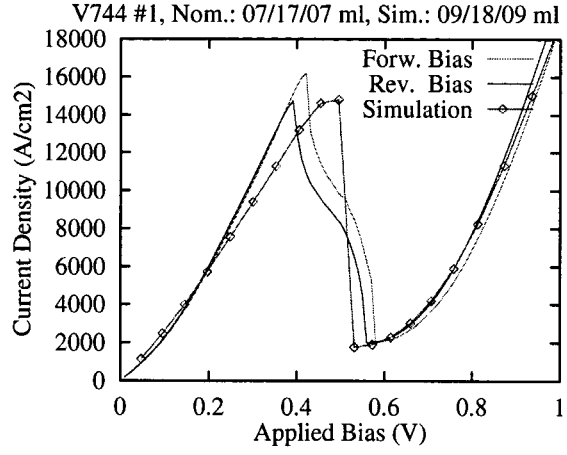
Strained InGaAs/AlAs 4 Stack RTD with Asymmetric Barrier Variation

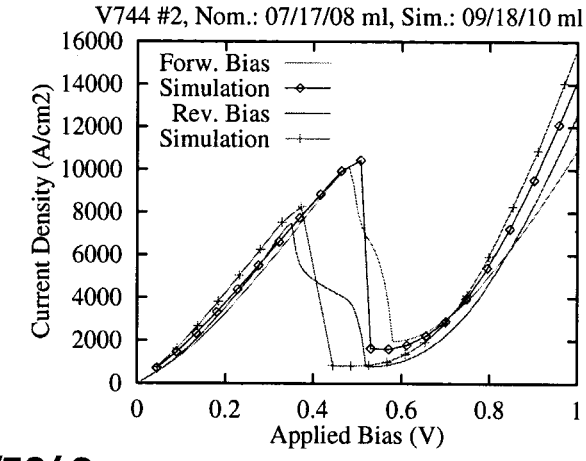
Vary One Barrier Thickness



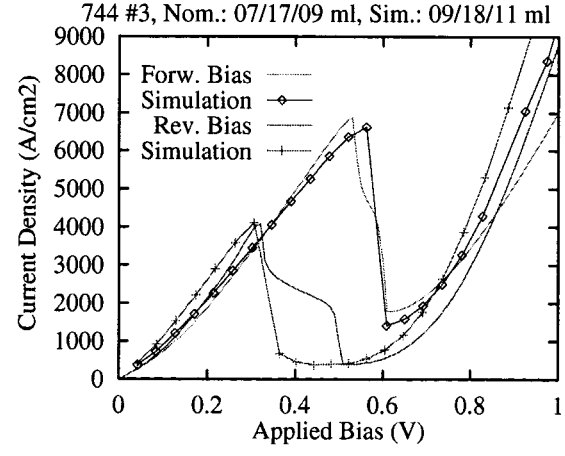
Four increasingly asymmetric devices:

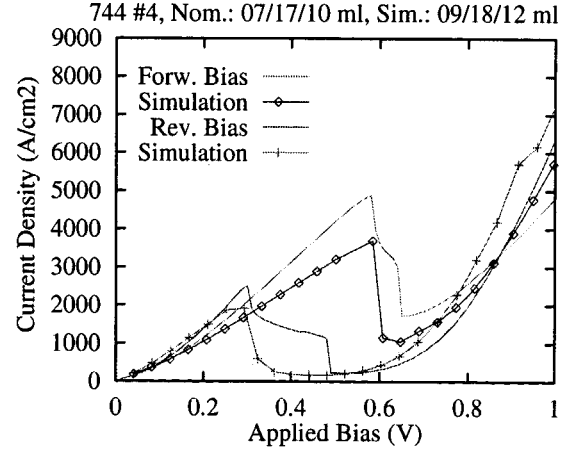
20/50/20 Angstrom
20/50/23 Angstrom
20/50/25 Angstrom
20/50/27 Angstrom





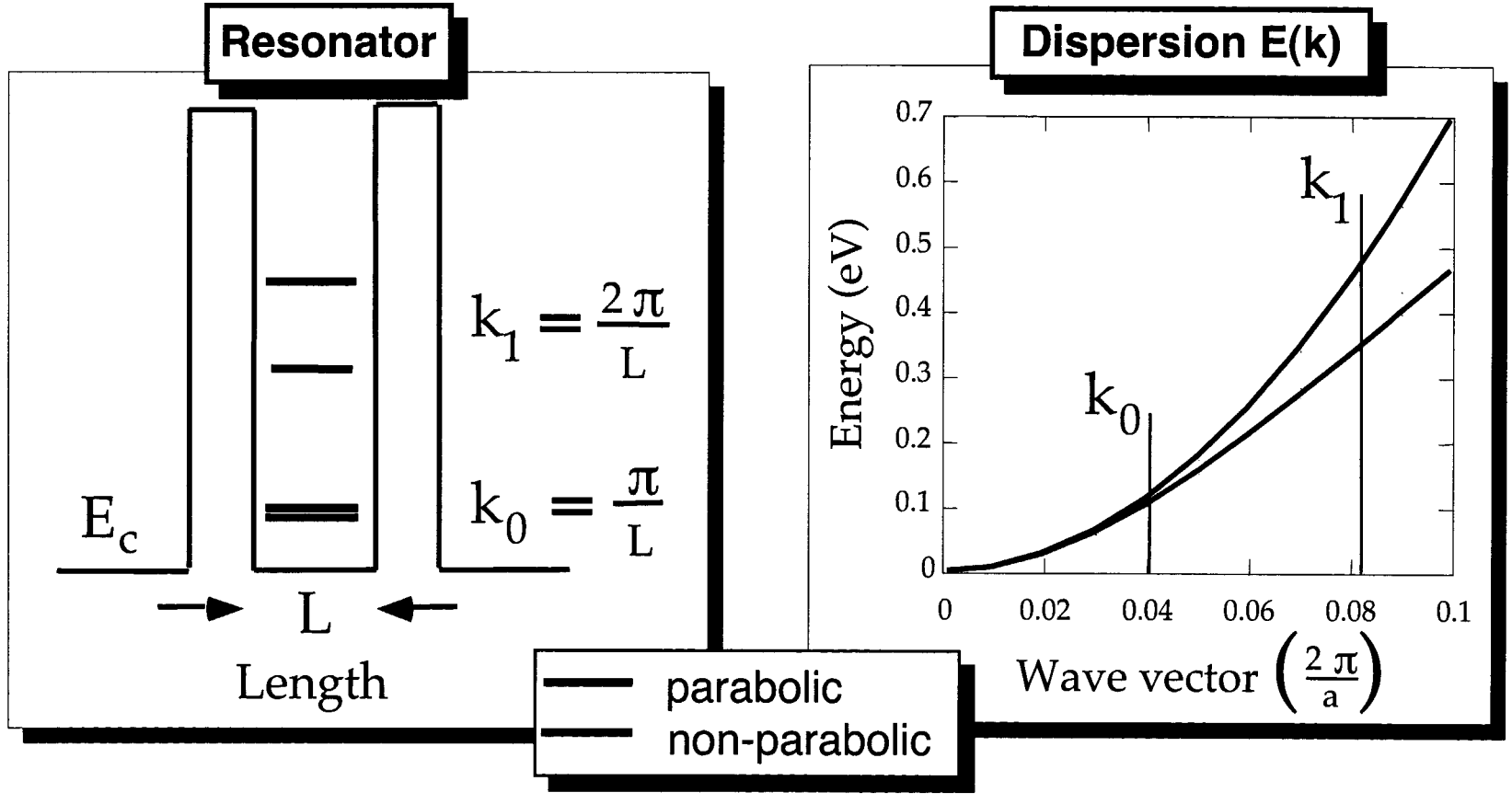
20/50/ 2





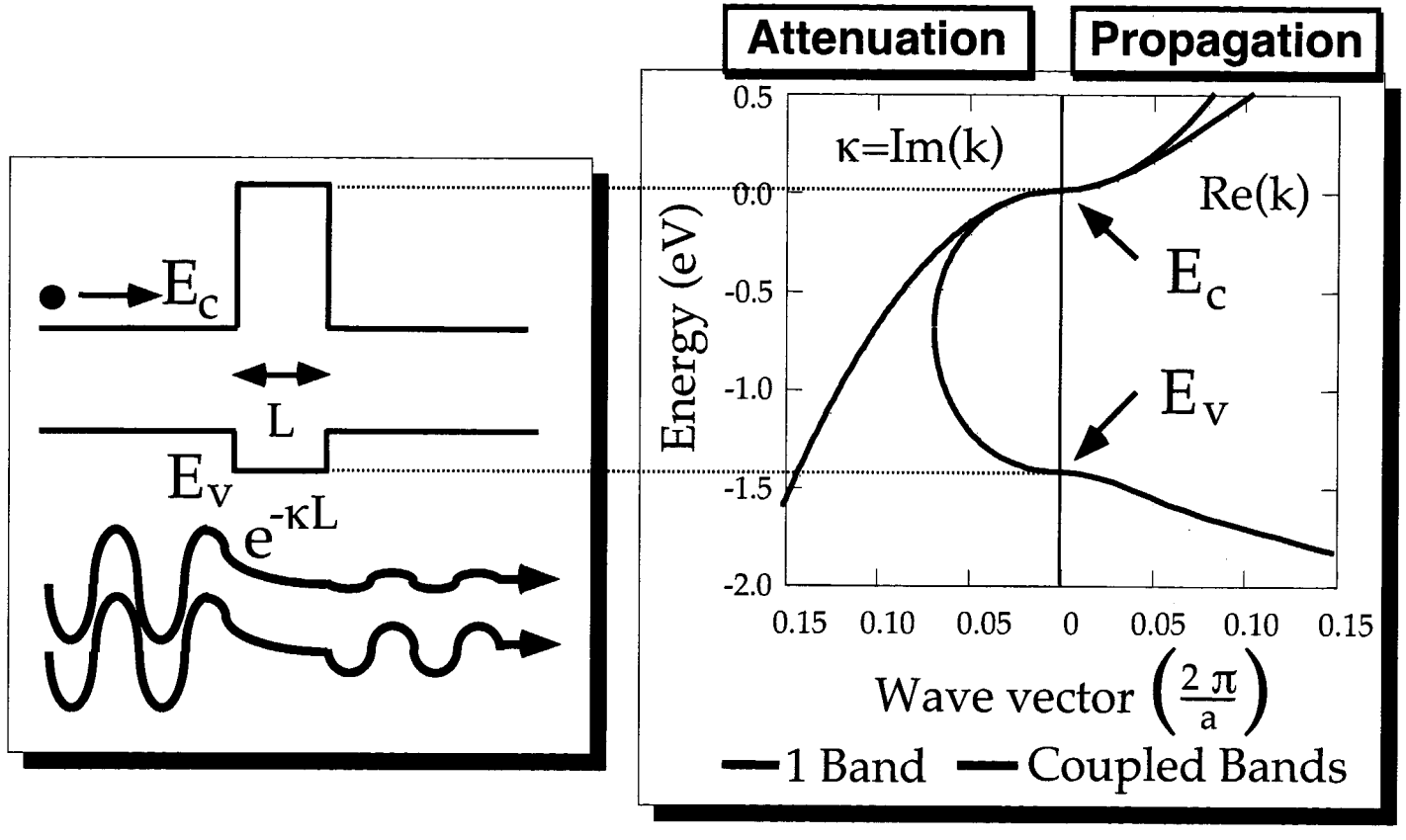
Presented at IEEE DRC 1997, work performed at Texas Instrument, Dallas

Resonance State Lowering due to Band Non-Parabolicity



Second diode turn-on at lower voltages.

Wave Attenuation in Barriers



- Attenuation is smaller with coupled bands
- Tunneling probability increases
- Current increases

Transport via Transmission Coefficients

$$I \propto \int dk_x \int dk_y \int dE T\left(E, k_x, k_y\right)\left(f_L(E) - f_R(E)\right)$$

$\downarrow$ **Cylindrical Coordinates**

$$I \propto \int d\varphi \int k dk \int dE T\left(E, k, \varphi\right)\left(f_L(E) - f_R(E)\right)$$

$\downarrow$ **Throw out angular dependence**

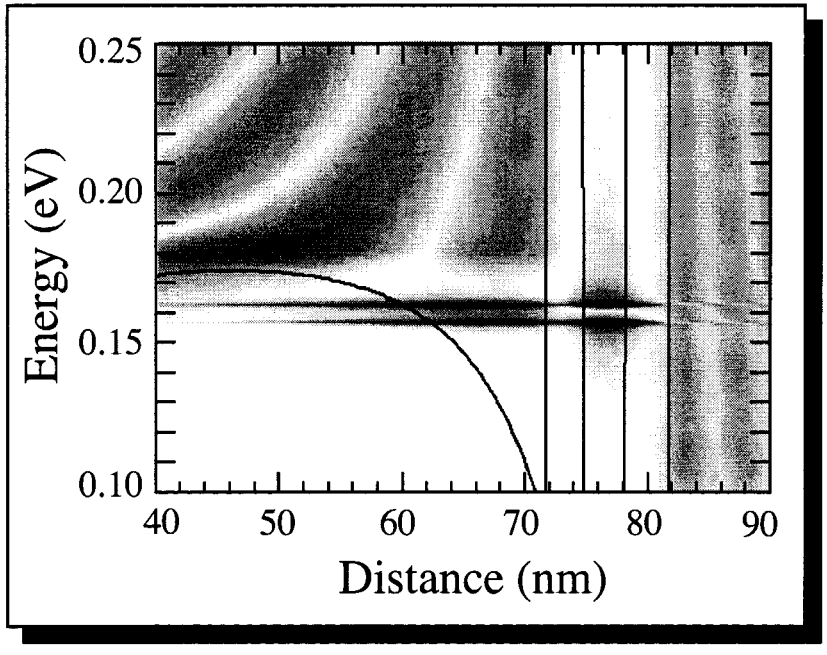
$$I \propto 2\pi \int k dk \int dE T\left(E, k\right)\left(f_L(E) - f_R(E)\right)$$

$\downarrow$ **Parabolic transverse subbands**

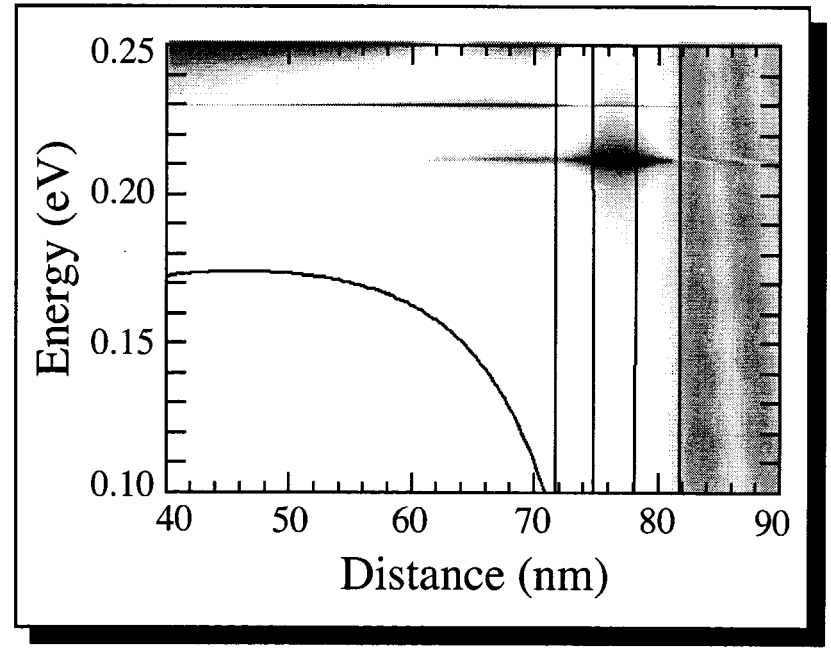
$$I \propto \rho_{2D} \int T(E)\left(f_L(E) - f_R(E)\right)$$

Resonance Coupling vs. Transverse Momentum

Density of States (k_x=0.00)

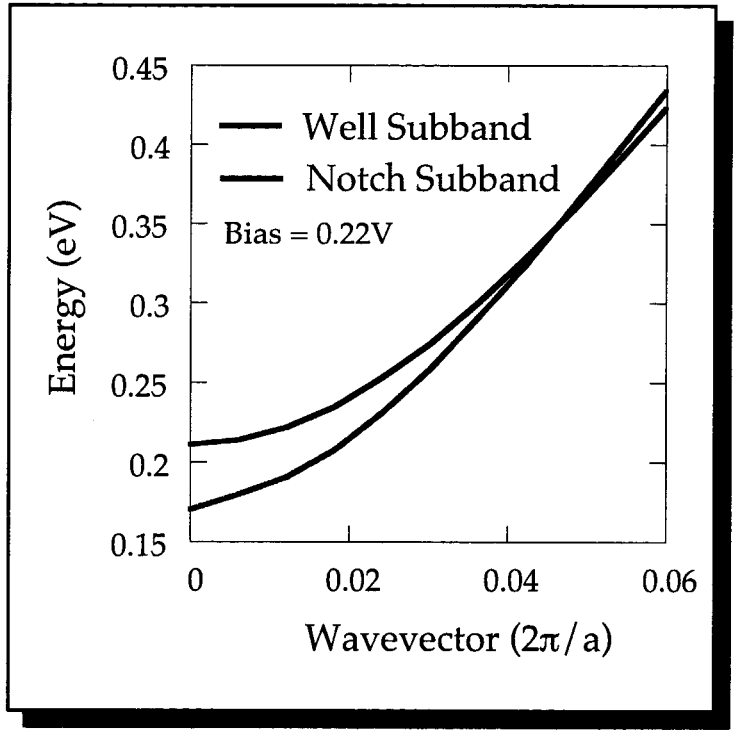


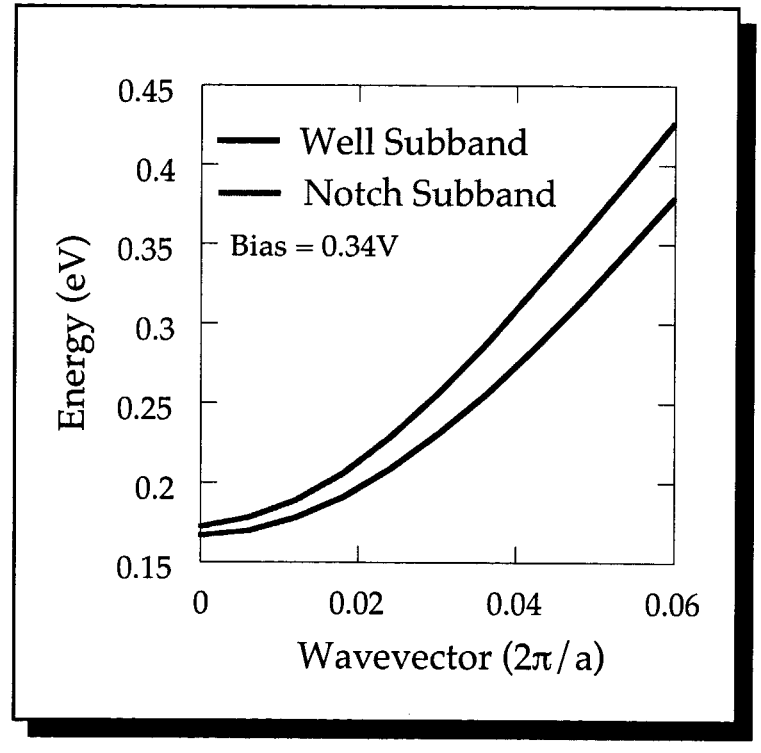
Density of States (k_x=0.03)



Resonance coupling depends on the transverse momentum

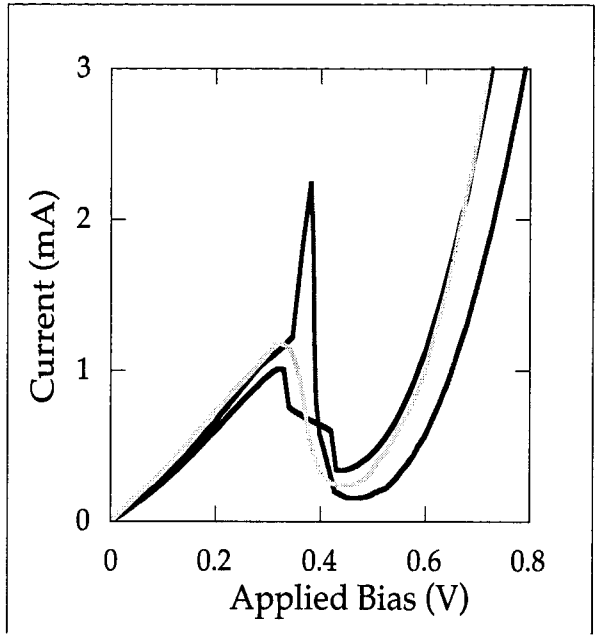
Quantum Well and Notch Subbands

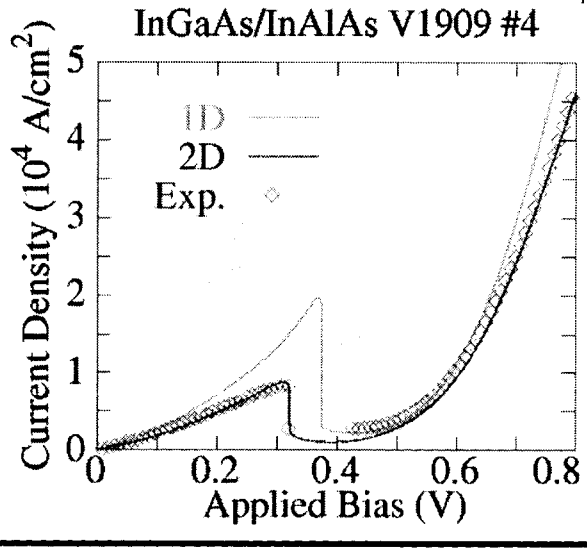




- The dispersions are non-parabolic
- There is no "perfect" overlap of the subbands

Full Band Simulation of Electron Transport

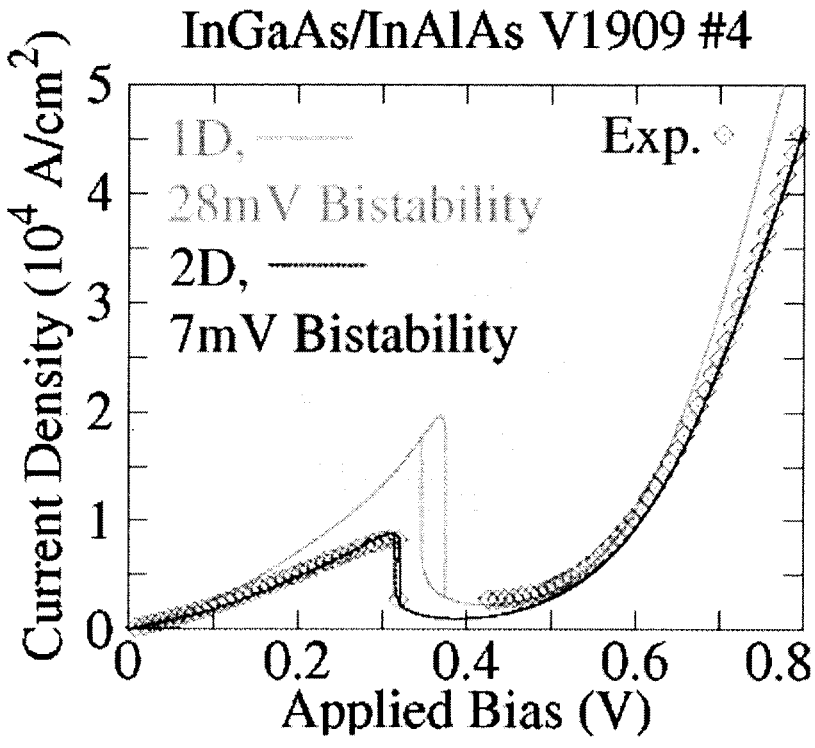


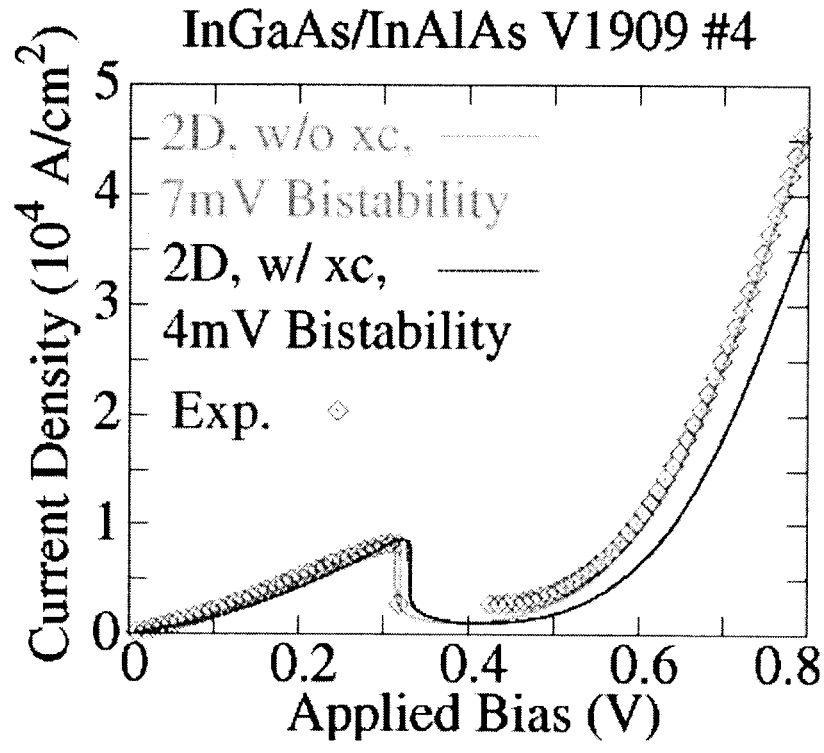


- 1D integration assuming parabolic subbands can lead to unphysical current overshoots.
- 2 Examples on InGaAs/InAlAs simulations:
  - Sp3s* simulation with partial charge self-consistency -> sharp spike at turn-off
  - Parameterized single band simulation which incorporates the band-non-parabolicity -> overall current overshoot.
- -> 2D integration fixes these unphysical results.

More Physics -> Better results

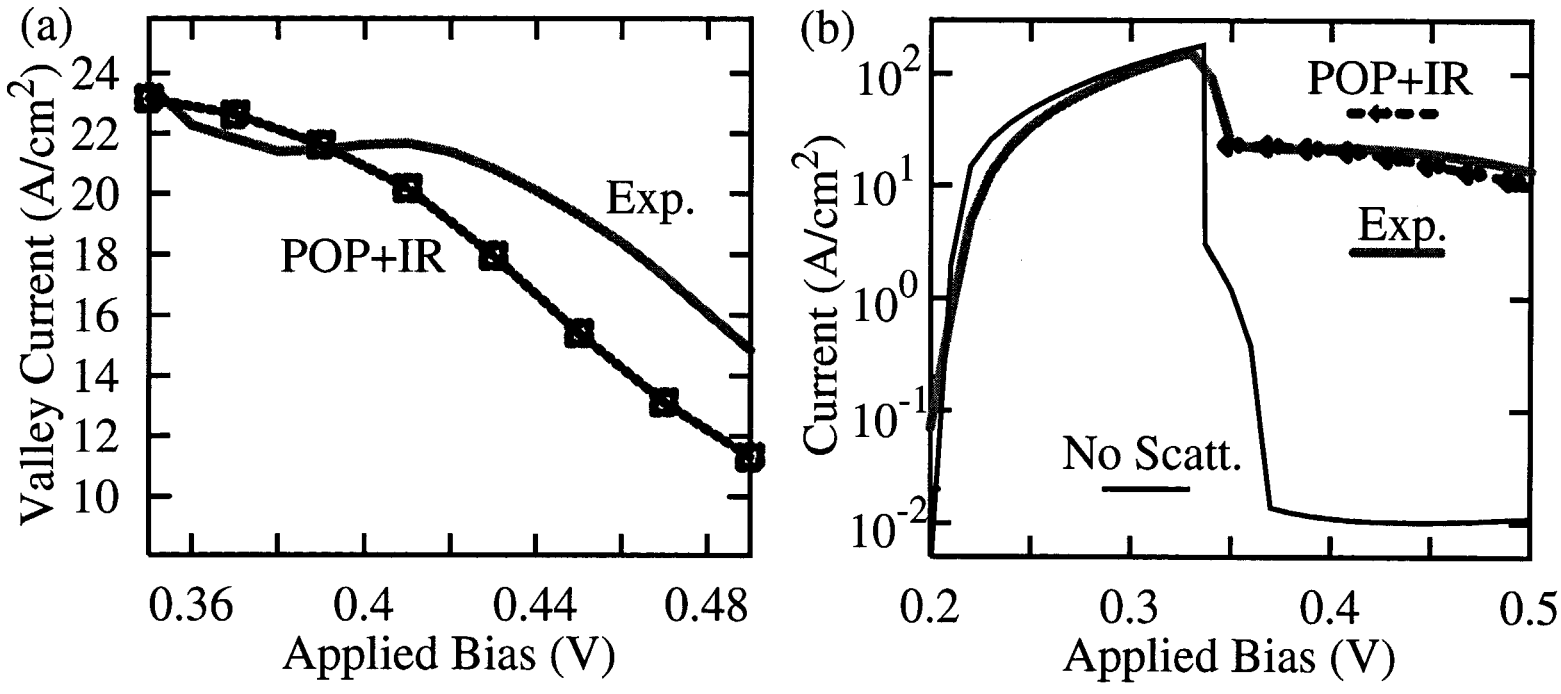
Full band integration + Exchange&Correlation





- Calculate the exchange and correlation potential in the local density approximation.
- Exchange and correlation energy does not eliminate (in general) the bistability, it does reduce it however.
- Inclusion of scattering in the simulation reduces the bistability region as well.

Tow Temperature: Polar Optical Phonon and Interface Roughness Scattering



scattering raises valley current by several orders of magnitude

Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation

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  - Boundary conditions
  - Bandstructure
  - Scattering
  - Software development
- **Design and Synthesis**
  - GENES (Genetically Engineered Nanostructured Devices)
- **3D modeling**
  - Massively parallel numerical developments
  - Quantum Dots
- **Future Efforts / Conclusions**

Novel Interactive Documentation Tool

- Pseudocode is a step by step description of a program in a natural language (high level and low level)
- Maintain pseudocode and code in **one** document -> easy to keep it up-to-date
- Generated automatically from comments in the code
- Cross references to
  - theory description
  - further pseudocode
  - the actual code

*

Calculate the bare Green function $g^R = G_0^R$, Eq. (2.30), for all sites and all energies E_z. g^R is only a function of energy E_z not E_{tot}.
function: `MakeGbare` (see pseudocode on pg. ❑)
Go to code

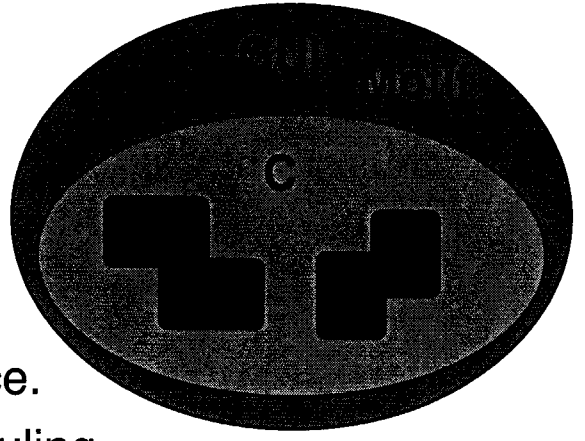
*

Fill in the ir structure (combinations of physical constants useful for calculating the interface roughness self energies).
function: `Fill_ir` (see pseudocode on pg. ❑) **Go to code**

*

Calculate $\sigma_{ac}^R(E)$ due to acoustic phonons, Eqs. (2.31) and (2.36). This self-energy is only a function of total energy, E, and does not have to be in the loop over longitudinal energies, E_z.
function: `Make_sr_ac` (see pseudocode on pg. ❑)
Go to code

Software Structure : Hybrid C, FORTRAN, and FORTRAN 90

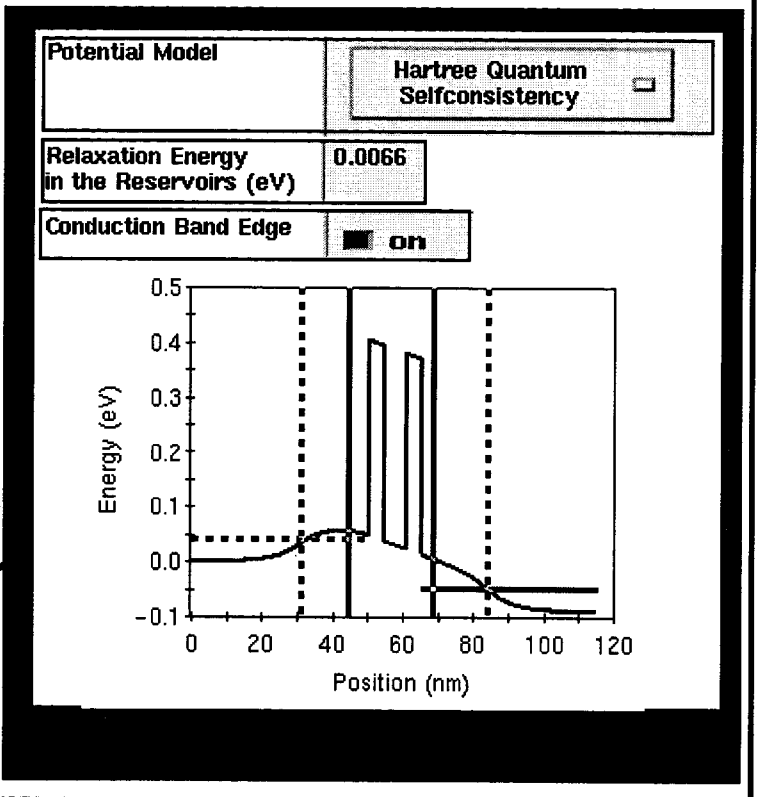


- Advantages of C:
  - flexible data design, fast prototyping.
  - simple hook-up of the graphical user interface.
  - close to the UNIX system level for job scheduling.
- Advantages of FORTRAN
  - speed for floating point arithmetic.
  - 4x speed-up for the same algorithm comparing C and F77 on HP.
- Advantages FORTRAN90 = FORTRAN + ...
  - standardized vector and matrix arithmetic.
  - data structures.

Generic Data Structure I/O

Dynamic GUI Design.
- data structure
- member descriptor

-> I/O for GUI or files



Data Structure

```
PotType potential
real hbarovertau
Boolean Ec
RangeStruct NonEq
```

Theorist

Translator

Software Engineer

Create

Read

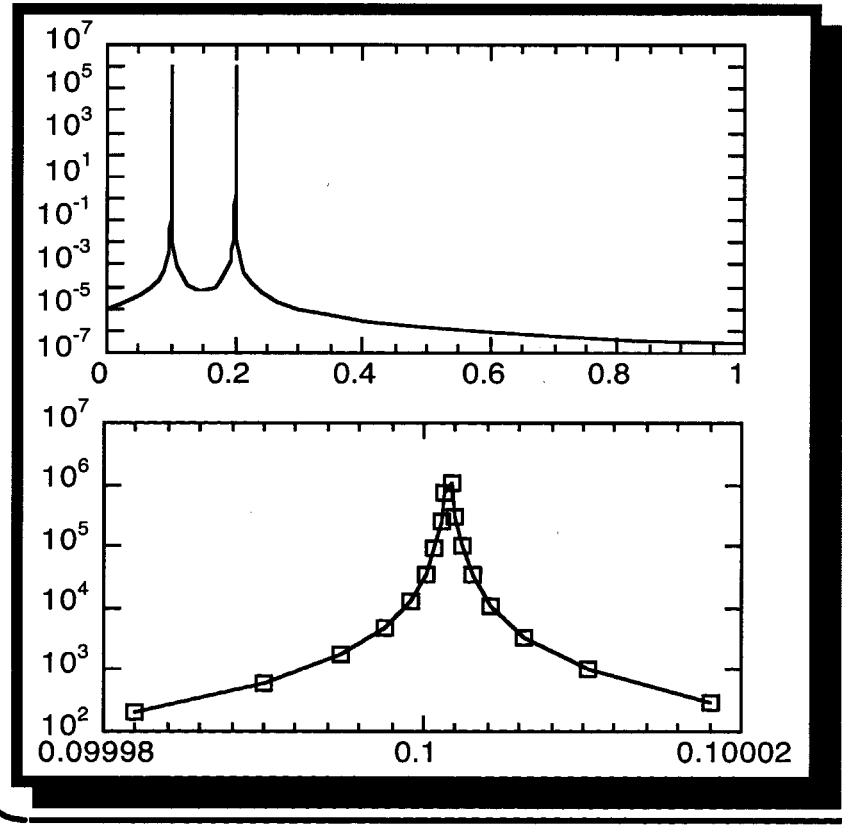
Read

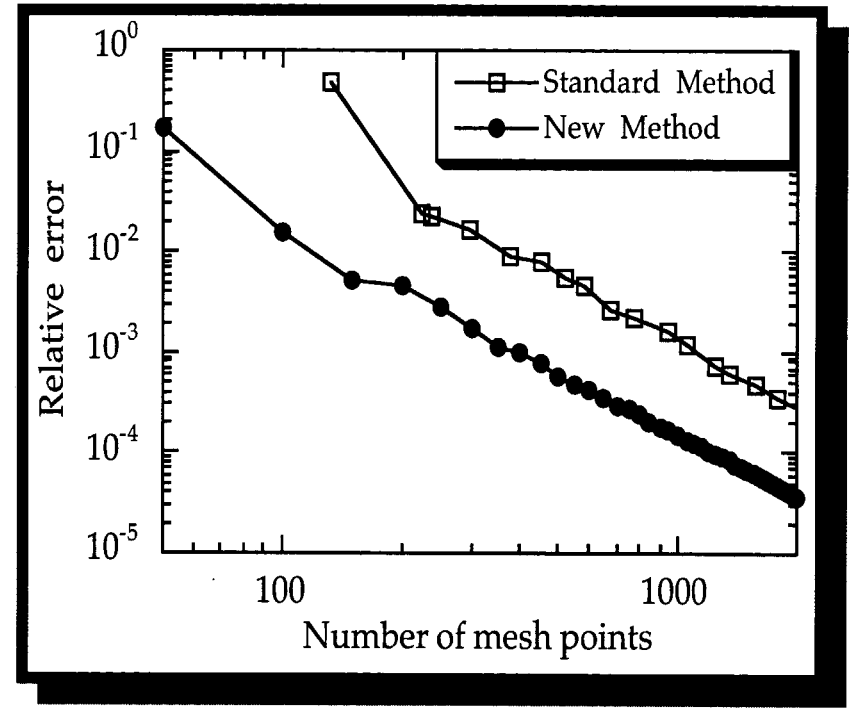
Create

```
potential=Hartree
hbarovertau=0.0066
Ec=FALSE
< start=45, end=69 >
```

Novel Energy Grid Generator

- **Problem: need to integrate over typically very sharp spectral features**
- **Assume we know where the resonances are -> toy problem**





Reduction of mesh points here: 4x

=> Speedup: 4x-16x

=> Memory Savings: 4x, 16x, 64x

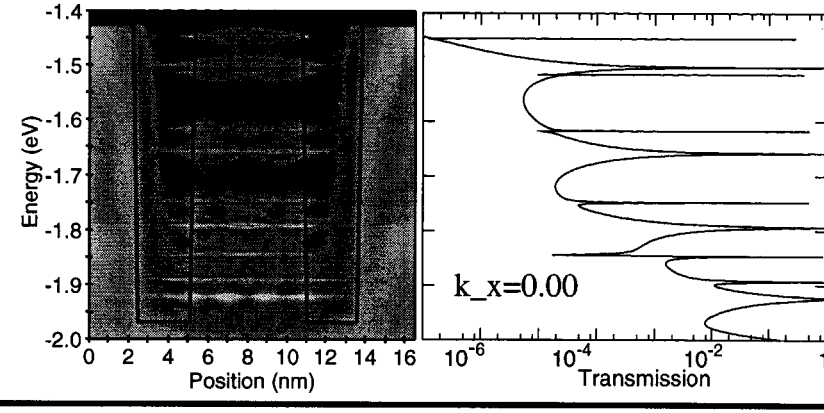
No Time to Talk About:

Hole Transport in Heterostructures:
- **Resonant Tunneling Diodes**
- **Cascade Lasers**

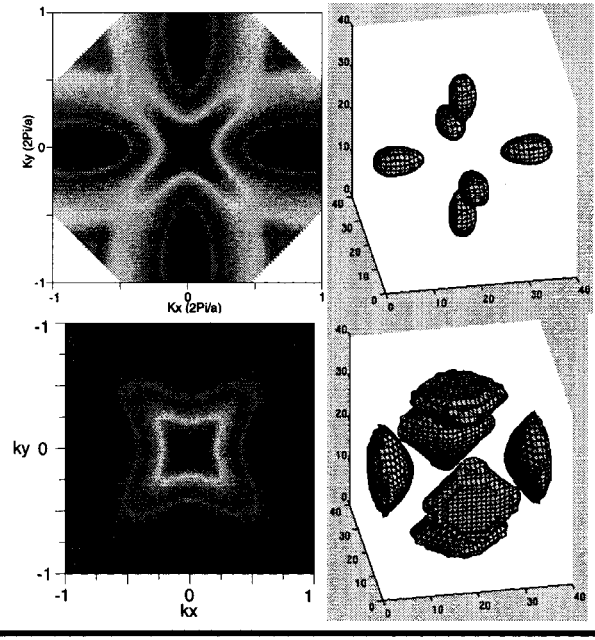
THz response in Heterostructures:
- **Resonant Tunneling Diode**

Limitations of Bandstructure Models.

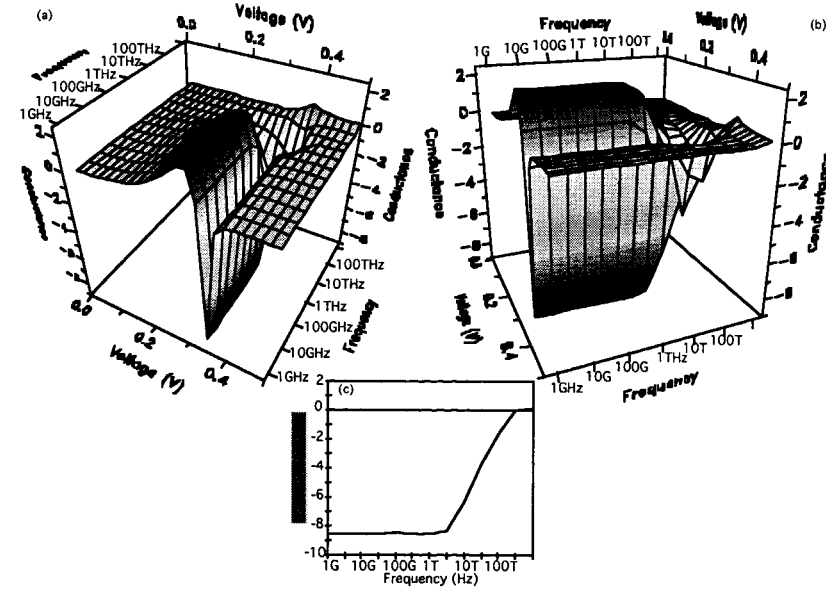
Hole Transport



Bandstructure Model Limitations



THz Response of a RTD



Gerhard Klimeck

Applied Cluster Computing Technologies Group

Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation

- **Motivation**
- **NEMO 1-D modeling**
  - Resonant Tunneling
  - Boundary conditions
  - Bandstructure
  - Scattering
  - Software development
- **Design and Synthesis**
  - GENES (Genetically Engineered Nanostructured Devices)
- **3D modeling**
  - Massively parallel numerical developments
  - Quantum Dots
- **Future Efforts / Conclusions**

Genetically Engineered Nanoelectronic Structures (GENES)

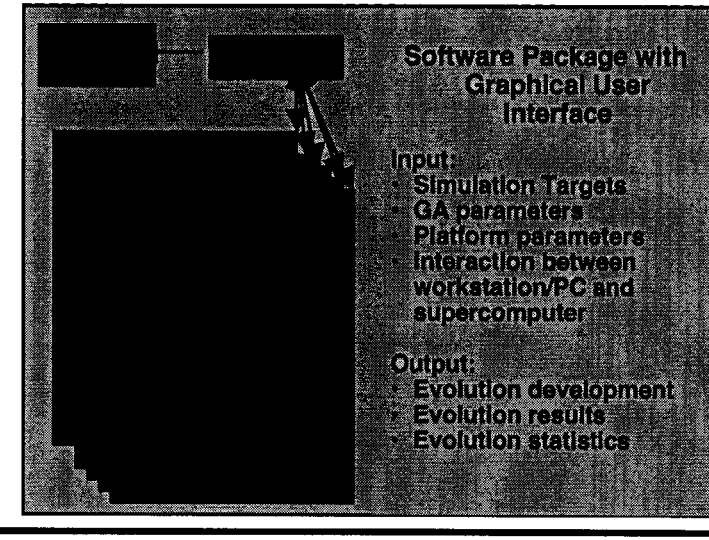
Objectives:

- Automate nanoelectronic device synthesis, analysis, and optimization using genetic algorithms (GA).

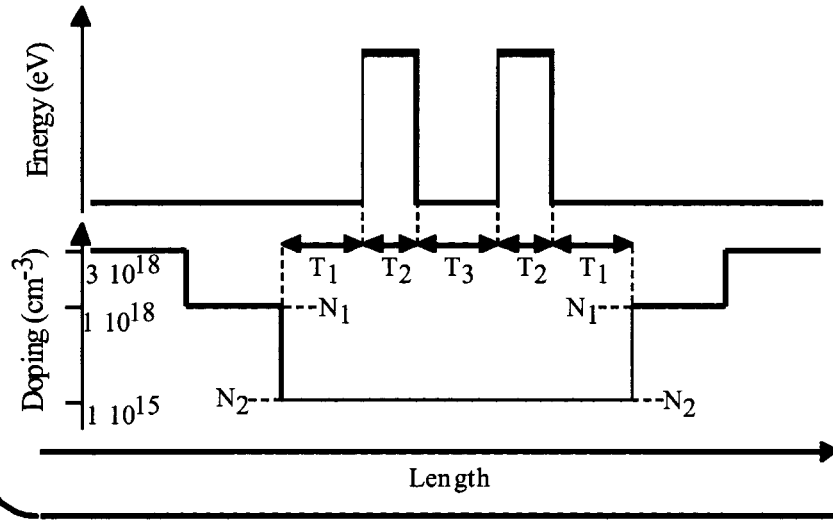
Approach:

- Augment parallel genetic algorithm (PGApack).
- Combine PGApack with NEMO.
- Develop graphical user interface for GA.

Architecture

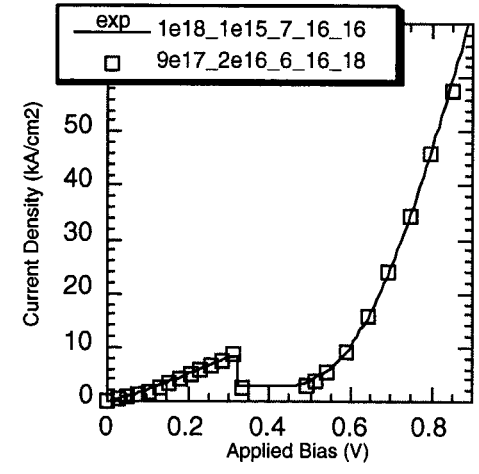


How do you know what you have built?



Results:

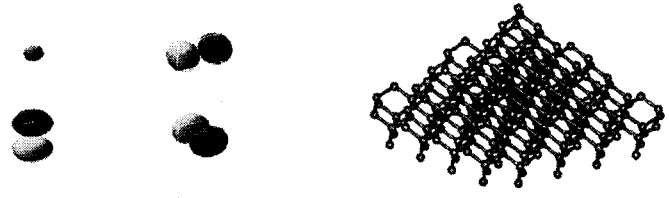
Nanoelectronic Device Structural analysis



GA analyzed atomic monolayer structure and doping profile of RTD device

Black: structure specs, Blue: Best fit

Mapping of Orbitals to Bulk Bandstructure



Atomic Orbitals
size: 0.2nm

+

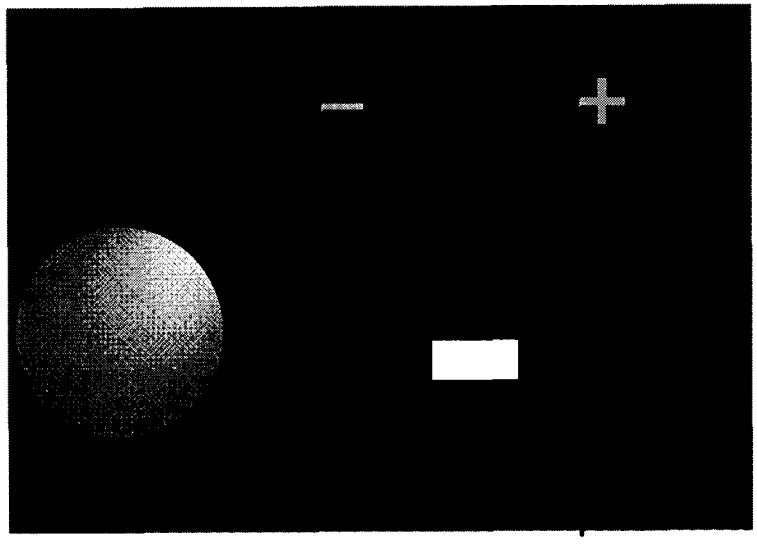
Structure

Bulk Semiconductors are described by:

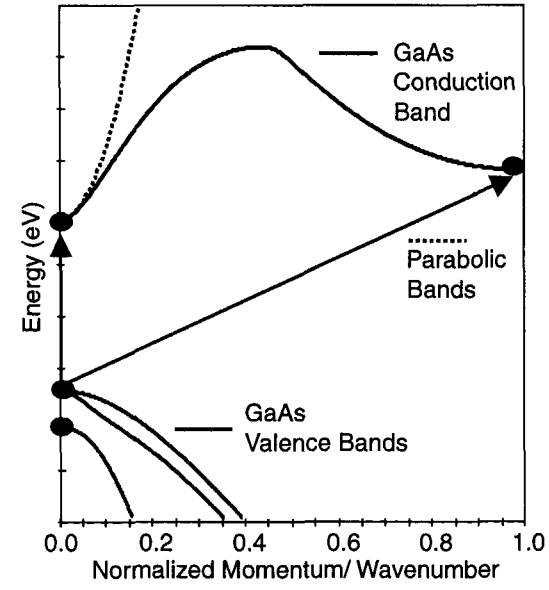
- Conduction and valence bands, bandgaps (direct, indirect), effective masses
- 10-30 physically measurable quantities

Tight Binding Models are described by:

- Orbital interaction energies.
- 15-30 theoretical parameters

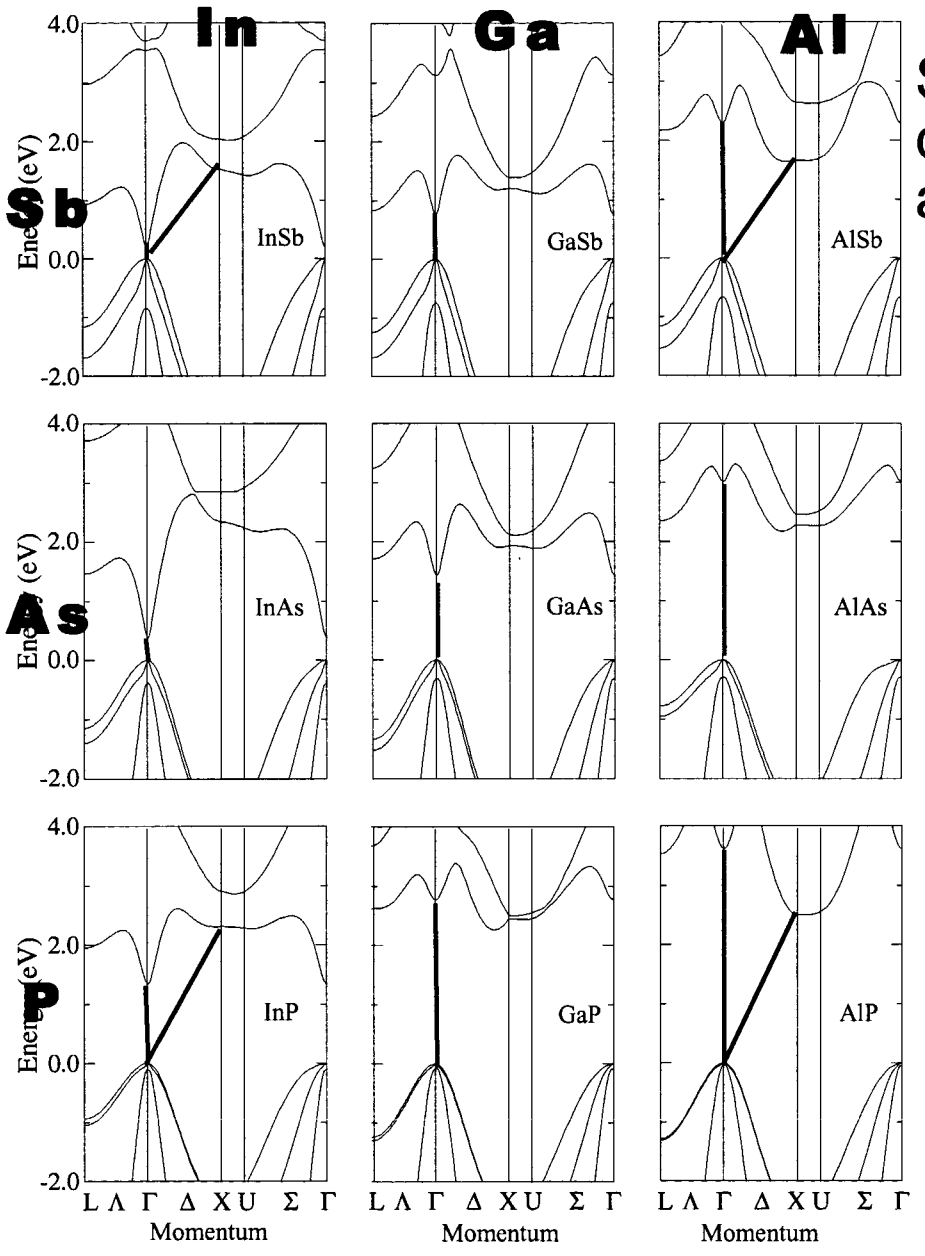


High Dimensional Fitting Problem



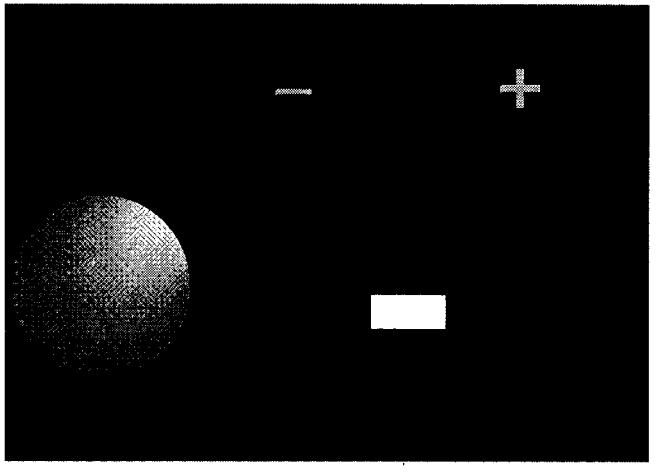
15-30 theoretical interaction energies

10-30 data points of bands and masses



Semiconductor Compounds:
cation: In, Ga, Al
anion: Sb, As, P

- Match experimental data in various electron transport areas of the Brillouin zone:
  - Effective masses of electrons at Γ, X and L
  - Effective masses of holes at Γ
  - Bandedges at Γ, X and L
- Each individual material poses a 15 dimensional fitting problem.



Nanoelectronic Modeling (NEMO): Moving from commercial grade 1-D simulation to prototype 3-D simulation

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  - Boundary conditions
  - Bandstructure
  - Scattering
  - Software development
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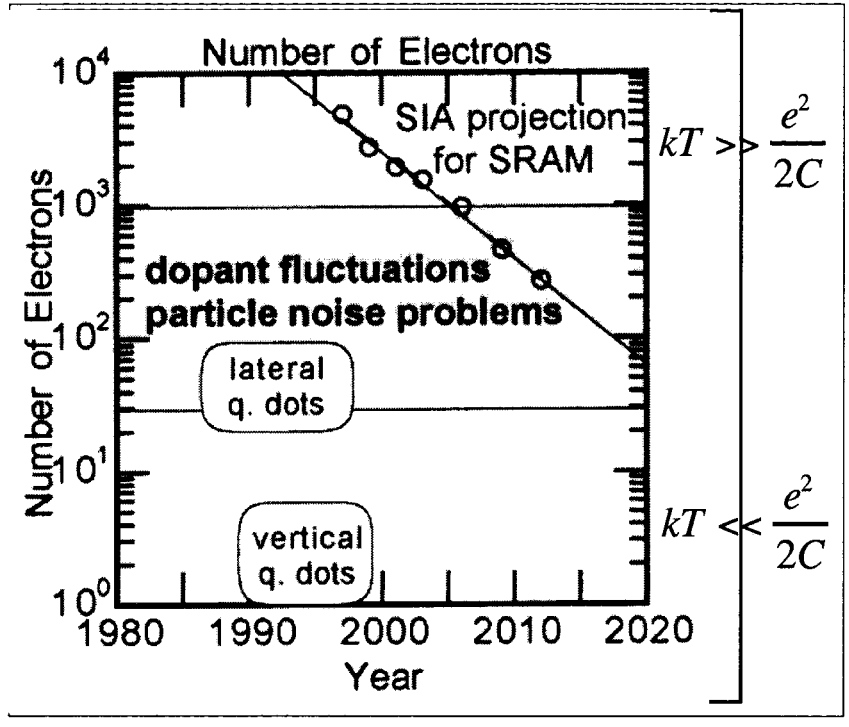
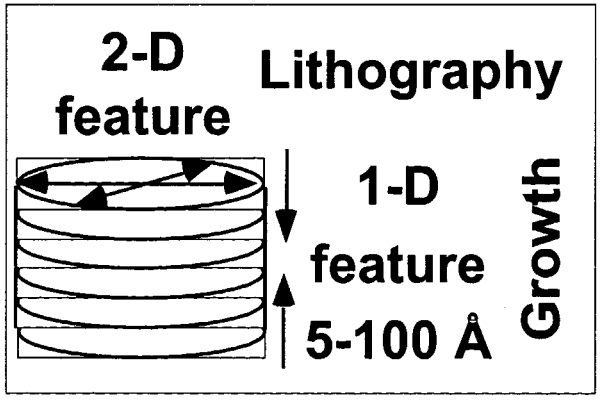
  - GENES (Genetically Engineered Nanostructured Devices)
- **3D modeling**
  - Massively parallel numerical developments
  - Quantum Dots
- **Future Efforts / Conclusions**

Microdevices Head for Single-Electronics





Reduction of Device Size

↓

Reduction of electron #
Reduction of Capacitance

↓

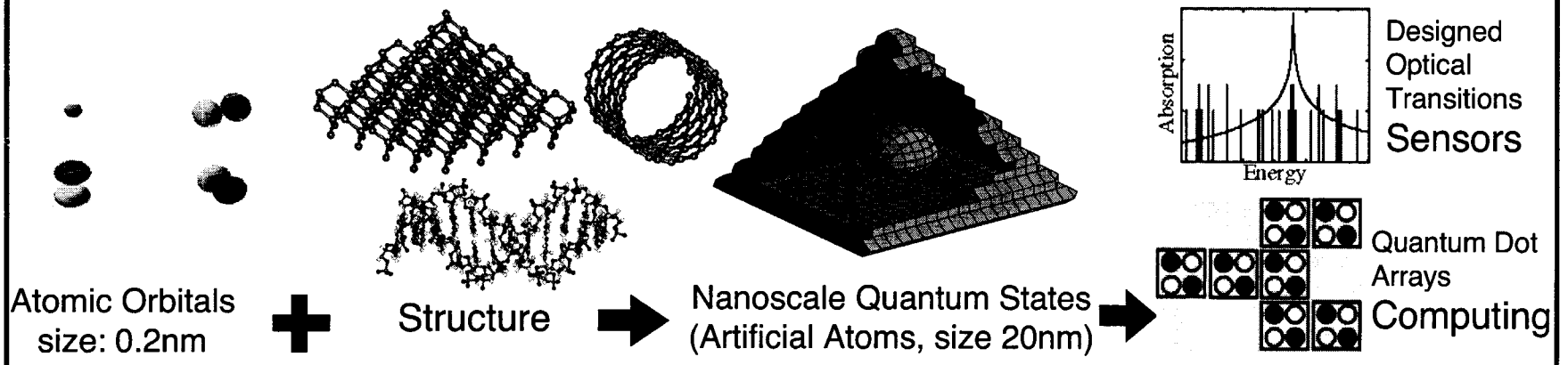
Problem:
Increase in thermal particle noise for tens and hundreds of particles

Solution:
Quantum Dots
Artificial Atoms/Molecules
Single Electronics

↓

System is stable against thermal particle noise

Quantum Dot Simulation for Revolutionary Computing and Sensing



Problem:

Nanoscale device simulation requirements:

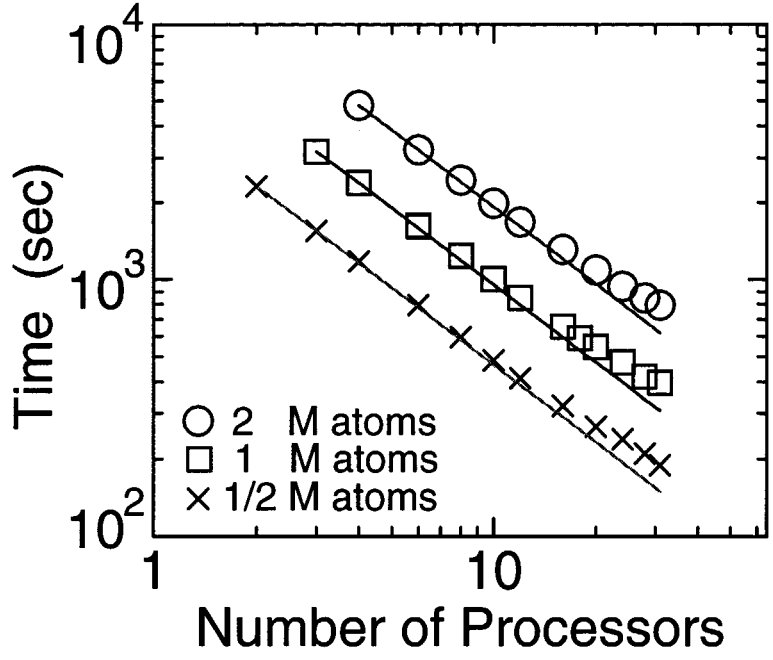
- Cannot use bulk / jellium descriptions, need description of the material atom by atom
  => use pseudo-potential or local orbitals
- Consider finite extent/transport, not infinitely periodic
  => local orbital approach
- Need to include about one million atoms.
  => need massively parallel computers
- The design space is huge: choice of materials, compositions, doping, size, shape. => need a design tool

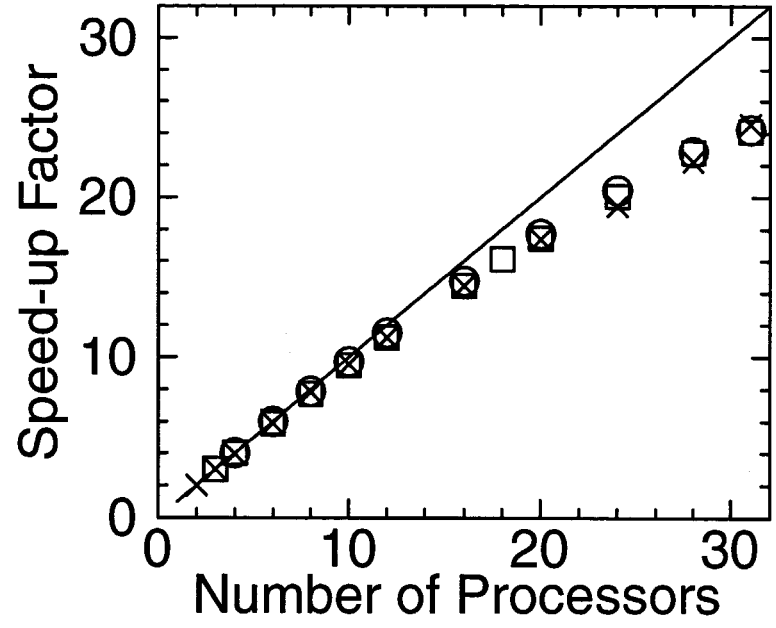
Approach:

- Use local orbital description for individual atoms in arbitrary crystal / bonding configuration
  - Use s, p, and d orbitals
    Use genetic algorithm to determine material parameter fitting
- Compute mechanical strain in the system.
- Develop efficient parallel algorithms to generate eigenvalues/vectors of very large matrices (N=40million for a 2 million atom system).
- Develop prototype GUI for (NEMO-3D)

Parallel Eigenvalue Solver on a Beowulf

(32 CPU Pentium III, 450MHz, Linux)





- Eigenvalue Computation for 1/2 , 1, and 2 Million atoms
  - Problems are too big for a single CPU (memory requirements)
  - sp3d5s* basis set
  - Matrix sizes 10^6x10^6, 2 10^6x2 10^6, and 4 10^6x4 10^6
  - Measure time for 20 Lanczos iterations
  - Full problem requires several thousand iterations
- Distributed Beowulf cluster scales very favorably to 32 nodes

Atomistic strain calculation followed by sp3s*d5 tight binding eigenvalue solution

Structure

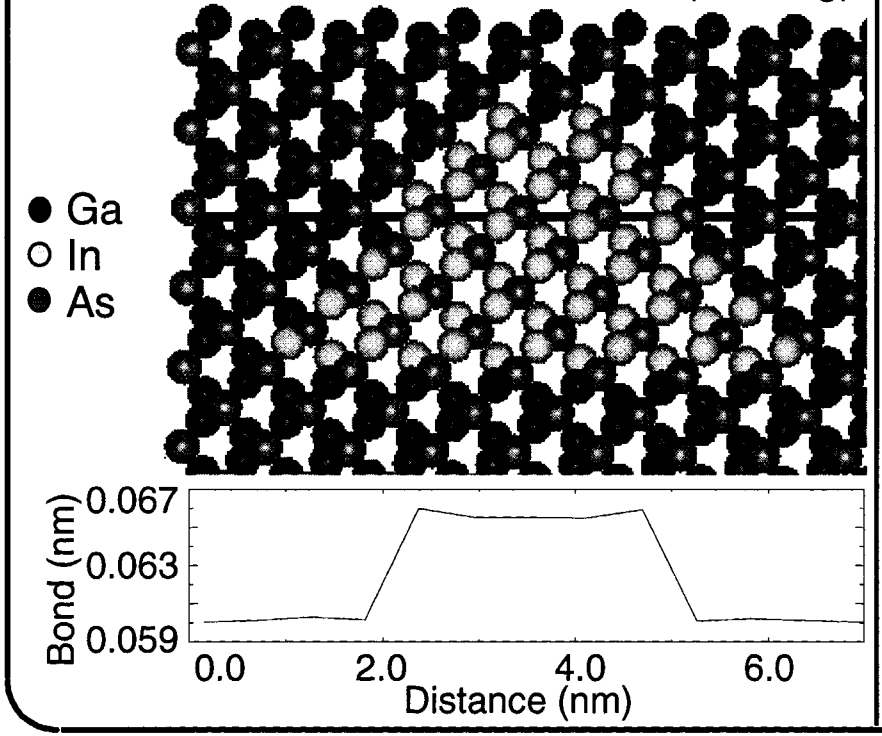
Dot Formation Due to Strain:

- Self-Assembly induced by strain in GaAs/InAs and Si/Ge material systems.
- Bond length and orientation distortion

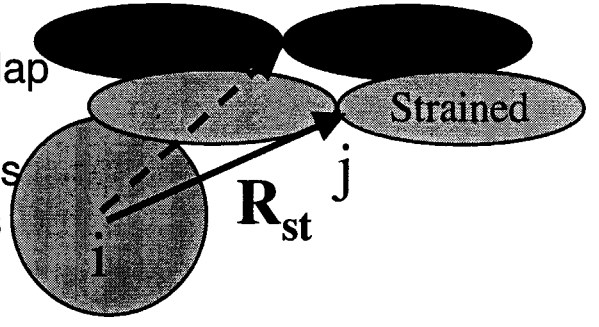
Strain affects Electronic Structure:

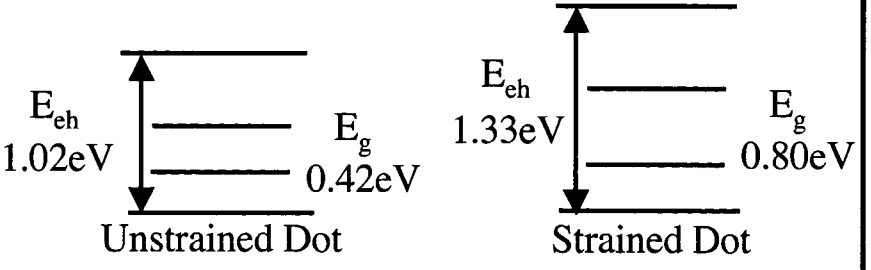
- Tight binding models can predict this!

Mechanics:Minimize elastic strain (Keating)



Electronics:
Orbital overlap changes
=> bandgaps and masses





Pyramidal InAs Dot Simulation
Base: 7nmx7nm Height: 3nm Embedded in GaAs

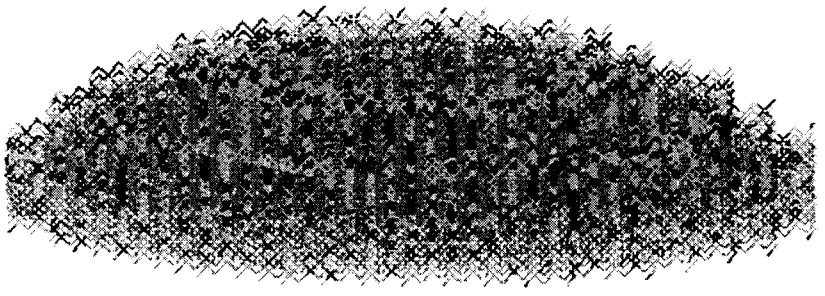
Alloy Disorder in Quantum Dots

Problem:
- Cations are randomly distributed in alloy dots.
- Does alloy disorder limit electronic structure uniformity for dot ensembles?

Approach:
- Simulate a statistical ensemble of alloyed dots.
- Requires atomistic simulation tool.

Results:
- Simulated 50 dots with random cation distributions.
- Inhomogeneous broadening factor of 9.4meV due to alloy disorder.

Impact:
- Fundamental uniformity limit for ensemble of alloy-based quantum dots.

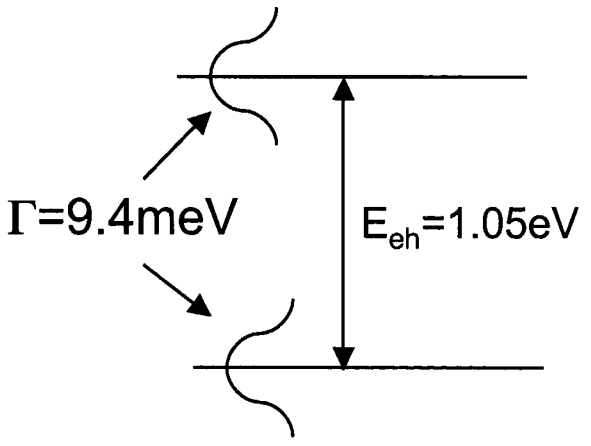


$In_{0.6}Ga_{0.4}As$ Lense Shaped Dot

Diameter=25nm,Height=5nm, GaAs embedded
382,024 Atom Simulation, sp3s* basis

In and Ga atoms are randomly distributed
Inhomegenious Broadening?

Simulation of Alloy Dot Ensemble



Measured Γ=34.6 meV (R. Leon, PRB, **58**, R4262)

9.4meV Represents Theoretical Lower Limit

Conclusion / Future Vision

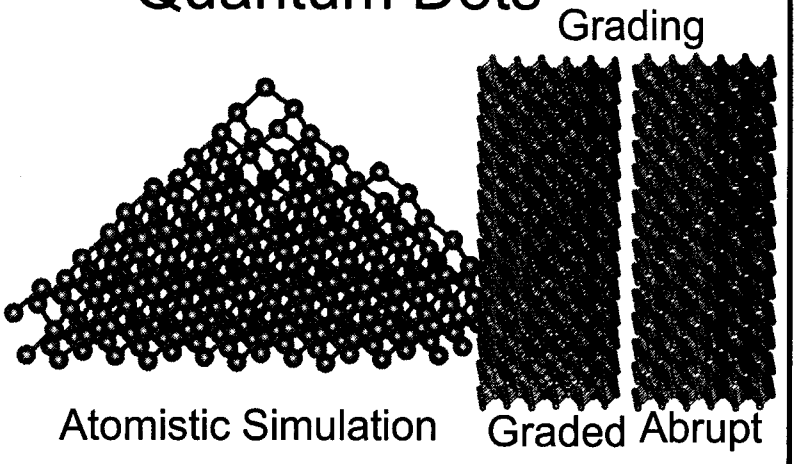
NEMO 1-D:
- Versatile heterostructure design tool
- IT'S FREE!!!

http://hpc.jpl.nasa.gov/PEP/gekco

NEMO 3-D:
- Heavily leveraged against 1-D
- Purely at research stage

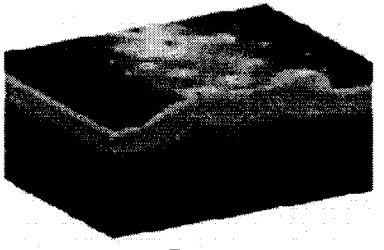
Lot's of nanoelectronics left to tackle

Quantum Dots

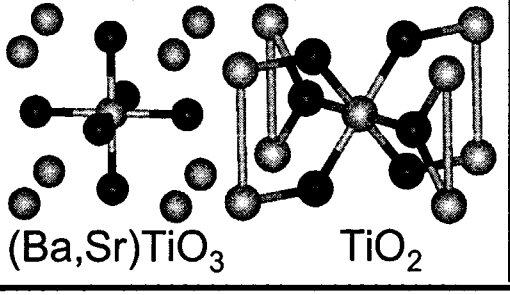


End of SIA Roadmap

Dopant Fluctuations in Ultra-scaled CMOS

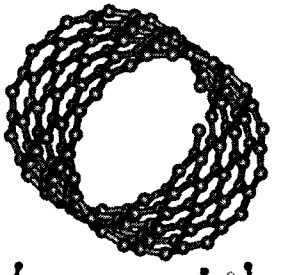


Electron Transport in Exotic Dielectrics

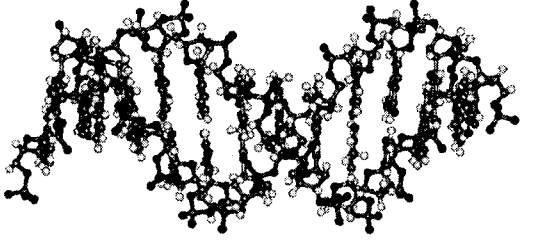


Transport in Molecules

Carbon Nanotubes



DNA



Acknowledgements

- NEMO was developed under a government contract to Texas Instruments and Raytheon from 1993-1997
  - Theory
    - Roger Lake, Chris Bowen, Gerhard Klimeck, Tim Boykin (UAH)
  - Graphical User Interface
    - Dan Blanks, Gerhard Klimeck
  - Programming Approach, Philosophy, and Prototypes
    - Bill Frensley (UTD), Gerhard Klimeck, Chris Bowen
  - Coding Help
    - Manhua Leng (UTD), Chenjing Fernando, Paul Sotirelis, Dejan Jovanovic, Mukund Swaminathan (UTA)
  - Experiments for verification
    - Ted Moise, Alan Seabaugh, Tom Broekaert, Berinder Brar, Yung-Chung Kao

- NEMO 3-D is being developed (1998-...) at JPL by Chris Bowen, Fabiano Oyafuso, Tom Cwik and Gerhard Klimeck.

Optical/E&M Analogies to Quantum Mech.

$$\nabla^2 \vec{E} = -\omega^2 \mu \varepsilon \vec{E}$$

$$k^2 = \omega^2 \mu \varepsilon$$

$$\nabla^2 \Psi = -\frac{2m}{\hbar}(E-U)\Psi$$

$$k^2 = \frac{2m}{\hbar}(E-U)$$

Physics are similar:

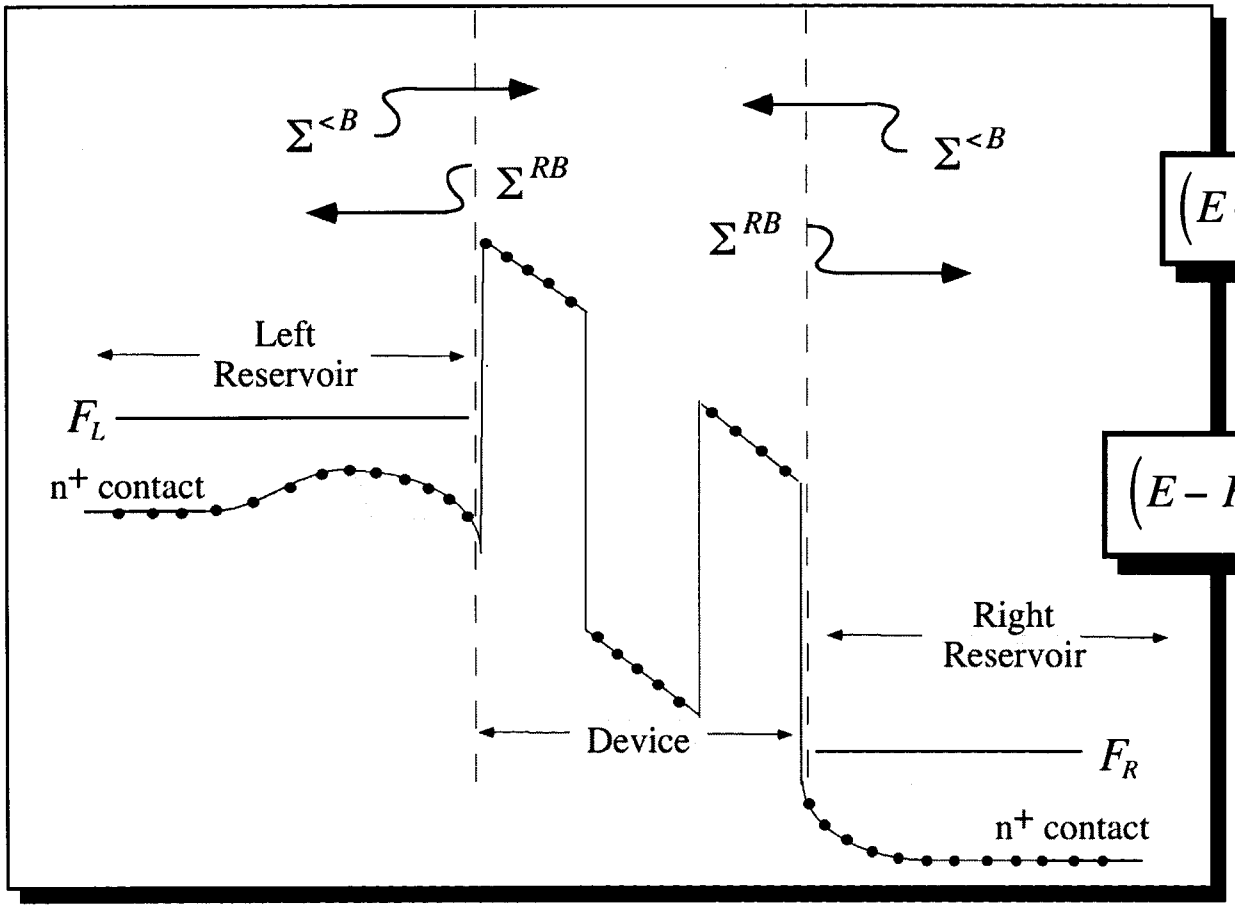
- Propagation as a wave phenomenon:
  - Antennas
  - Waveguides
- Propagation as a scattering problem:
  - Diffraction gratings
  - Radar cross-sections
- Green functions as propagators
- Finite difference, finite elements

But:

- Scattering is coherent & elastic rather than incoherent & inelastic
- Photons do not interact with themselves:
  - Calculate the propagation
  - Do not calculate the occupation
  - Exception is a laser!
- Electron and Laser Simulation need: Dynamics & Kinetics - States & Bean-counting

Generalized Boundary Conditions: Boundaries as a Scatterong Problem

- Left and right regions are treated as reservoirs.
- Quantum structure of reservoirs is included exactly.



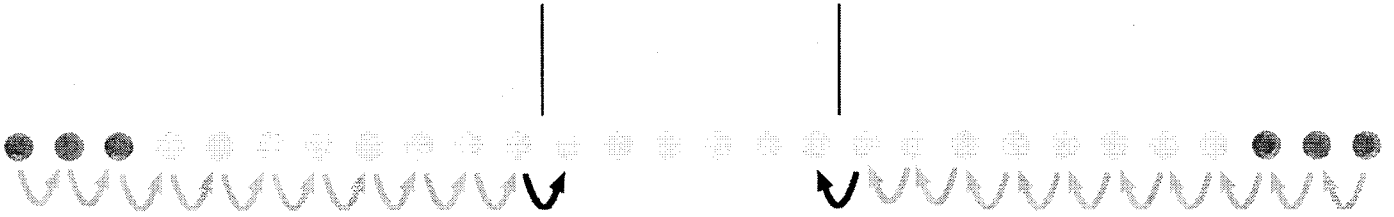
Dynamics

$$\left(E - H_0 - \Sigma^{RB}\right)G^R = 1$$

$$\left(E - H_0 - \Sigma^{RB}\right)G^< = \Sigma^{<B}G^A$$

Kinetics

Dyson Equation Treatment of the Leads



$$\Sigma_{0,0}^{RB} = g_{-1,-1}^{R} \left| t_{-1,0} \right|^2$$

$$\Sigma_{N-1,N-1}^{RB} = g_{N,N}^{R} \left| t_{N,N-1} \right|^2$$

$$\Sigma_{0,0}^{<B} = -2 \text{ IM} \left\{ \Sigma_{0,0}^{RB} \right\} f_L$$

$$\Sigma_{N-1,N-1}^{<B} = -2 \text{ IM} \left\{ \Sigma_{N-1,N-1}^{RB} \right\} f_R$$

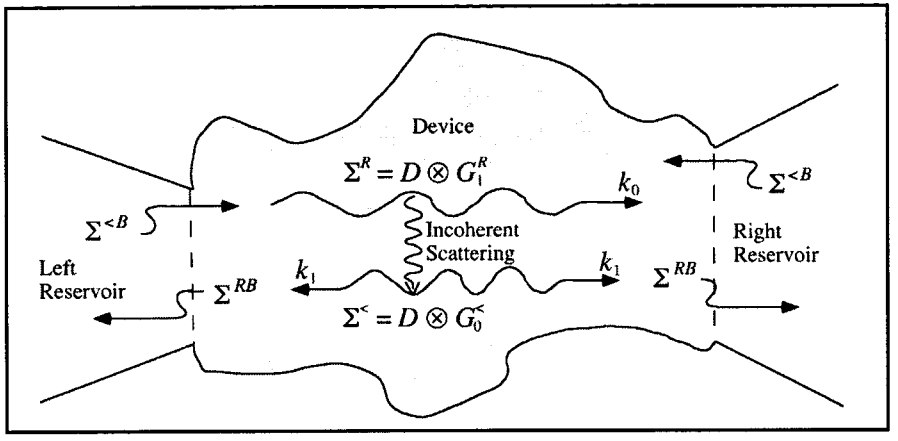
$$\left[G^R \right]^{-1} = \begin{bmatrix} E - \varepsilon_0 - \Sigma_{0,0}^{R} & t_{0,1} & & \\ t_{1,0} & E - \varepsilon_1 & \ddots & \\ & \ddots & \ddots & \\ & & & E - \varepsilon_{N-1} - \Sigma_{N-1,N-1}^{R} \end{bmatrix}^{-1}$$

$$\left(E - H_0 - \Sigma^{RB} \right) G^R = 1$$

Dynamics $\longrightarrow$ **Kinetics**

$$\left(E - H_0 - \Sigma^{RB} \right) G^{<} = \Sigma^{<B} G^A$$

Treatment of a single Incoherent Scattering Event



- **Scattering:**
  - **couples different propagation channels (k and E).**
  - **modifies the quantum mechanical spectrum of states (damped oscillator has a different eigen frequency)**
- **Incoherent Scattering:**
  - **Destroys phase memory**

$$(E - H_o^D - \Sigma^{RB})G_1^R = 1$$

$$\Sigma_0^R = D \otimes G_1^R$$

$$(E - H_o^D - \Sigma^{RB} - \Sigma_0^R)G_0^R = 1$$

$$G_0^{<} = G_0^R \Sigma^{<B} G_0^A$$

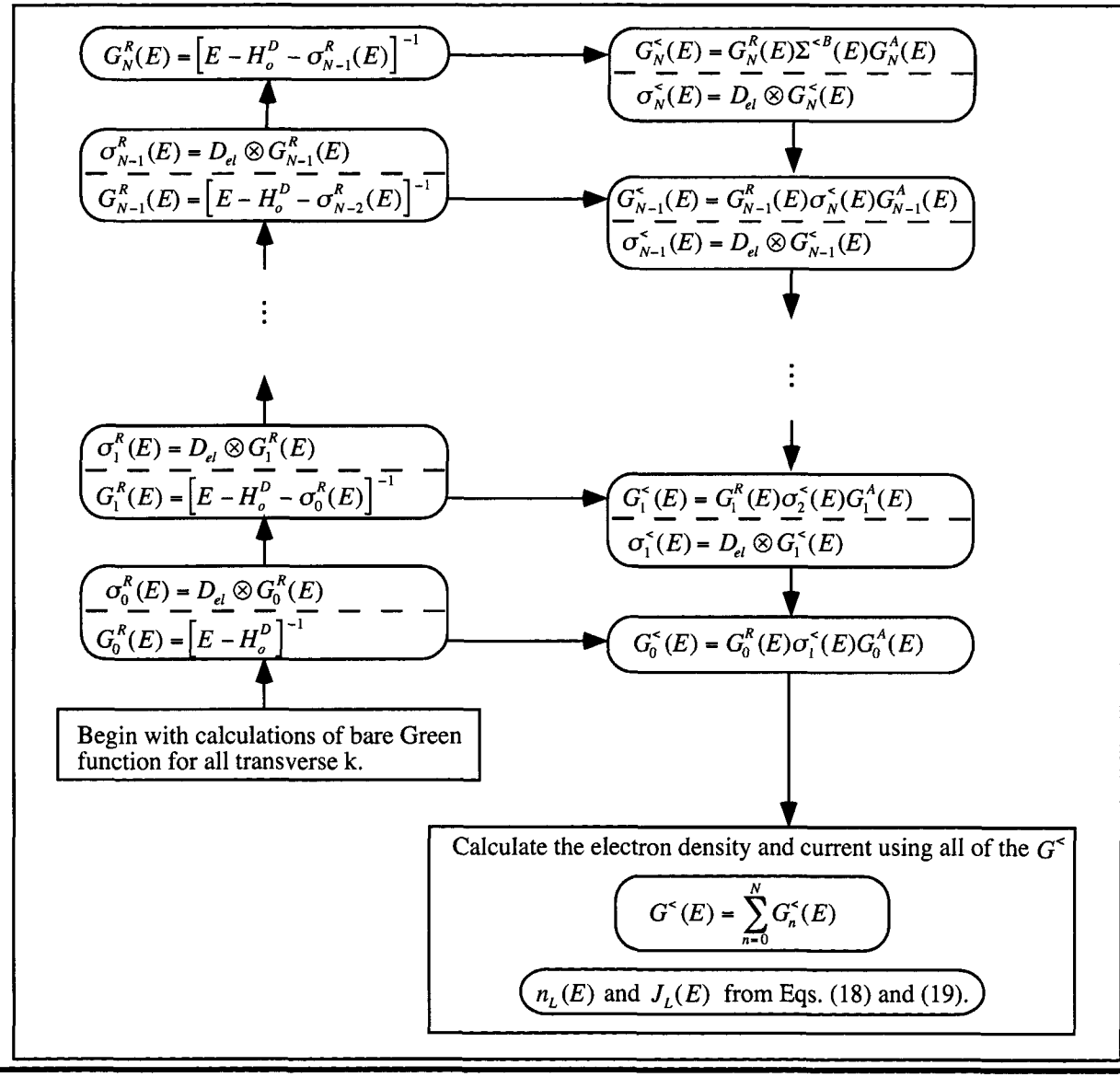
$$\Sigma_0^{<} = D \otimes G_0^{<}$$

$$G_1^{<} = G_1^R \Sigma_0^{<} G_1^A$$

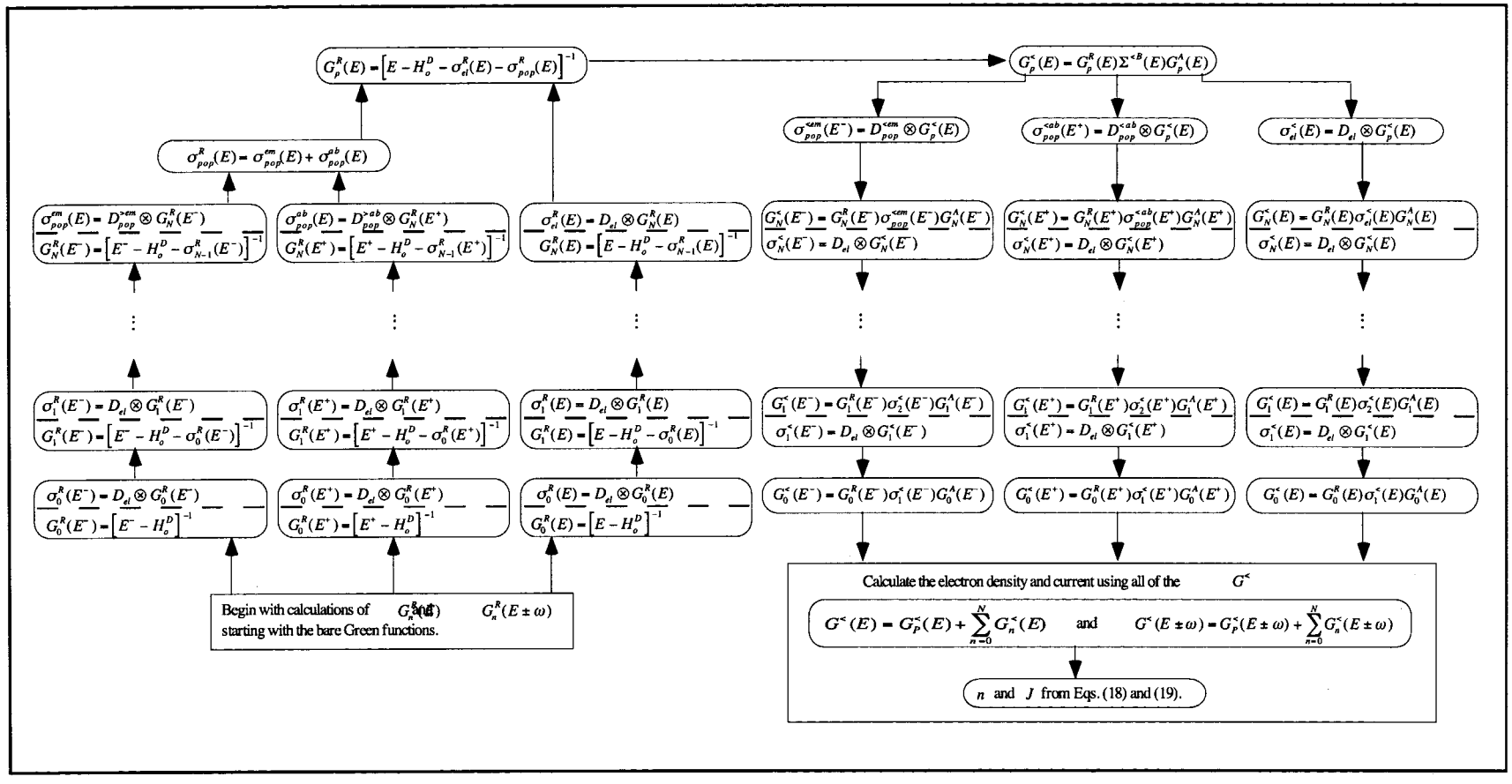
Computation ↓

↑ Transport

Multiple Sequential Scattering

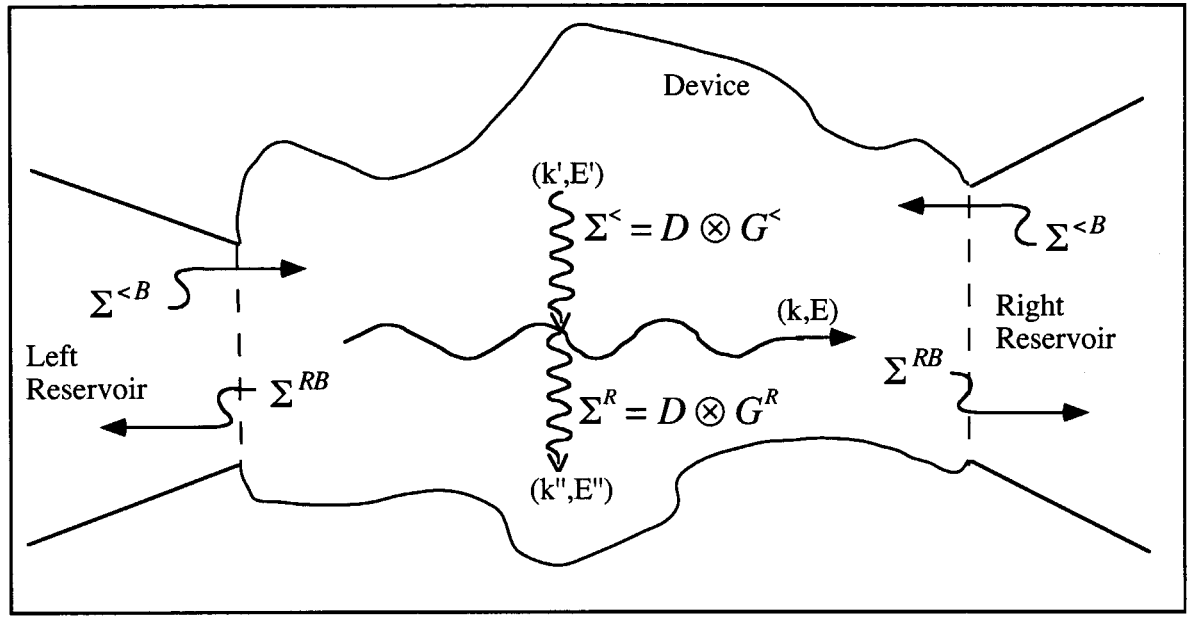


Multiple Sequential Scattering with POP



- **Elastic scattering couples all momenta (k)**
- **Inelastic scattering couples different total energies (E,E+hv,E-hv)**
- **Polar optical phonons are treated as a single scattering event in NEMO**

Scattering: Self-Consistent Born Treatment



Dynamics

$$\left(E - H_0 - \Sigma^R_{SCATT} - \Sigma^R_{BOUND}\right)G^R = 1$$

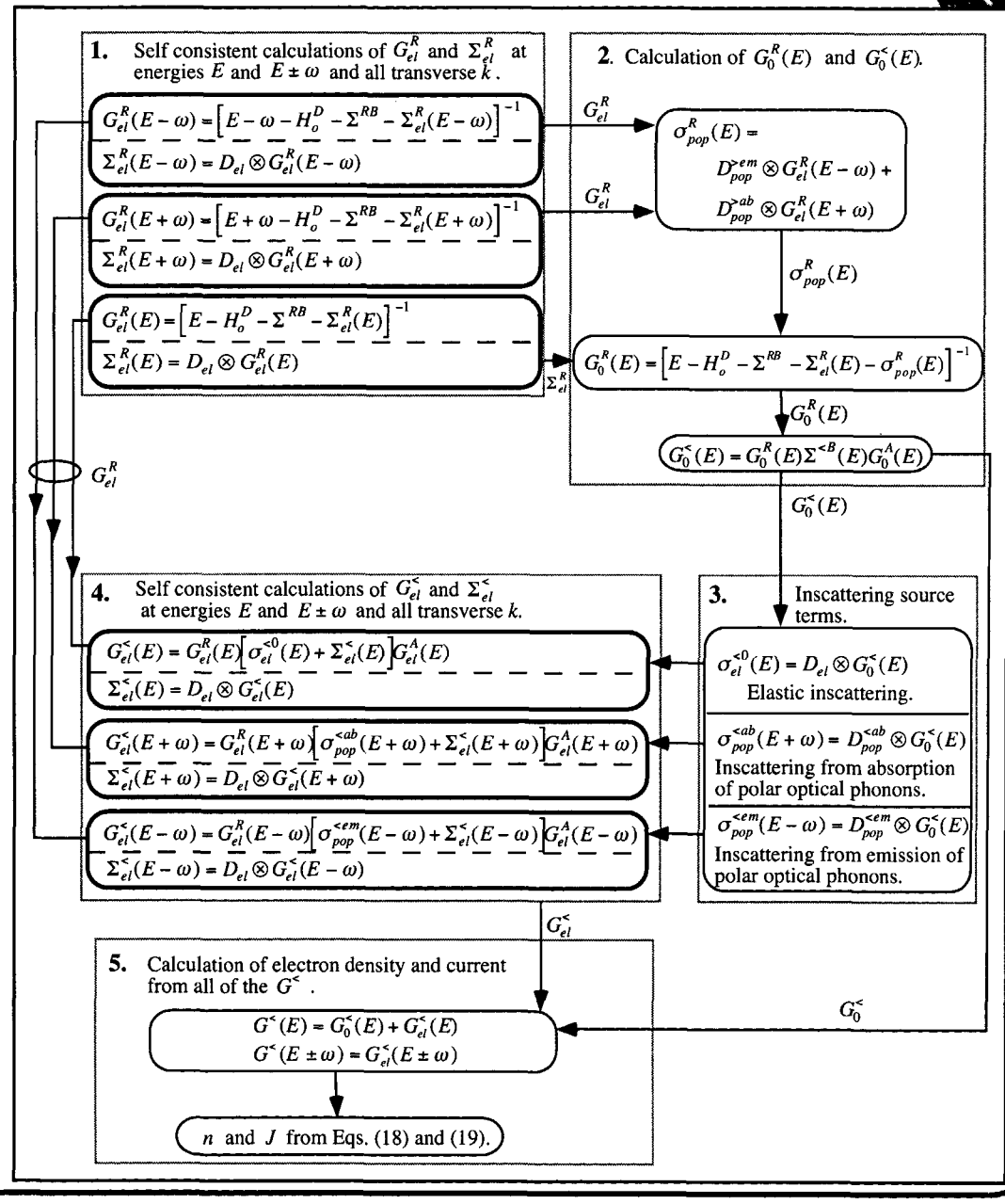
Kinetics

$$\left(E - H_0 - \Sigma^R_{SCATT} - \Sigma^R_{BOUND}\right)G^< = \left(\Sigma^<_{SCATT} - \Sigma^<_{BOUND}\right)G^A$$

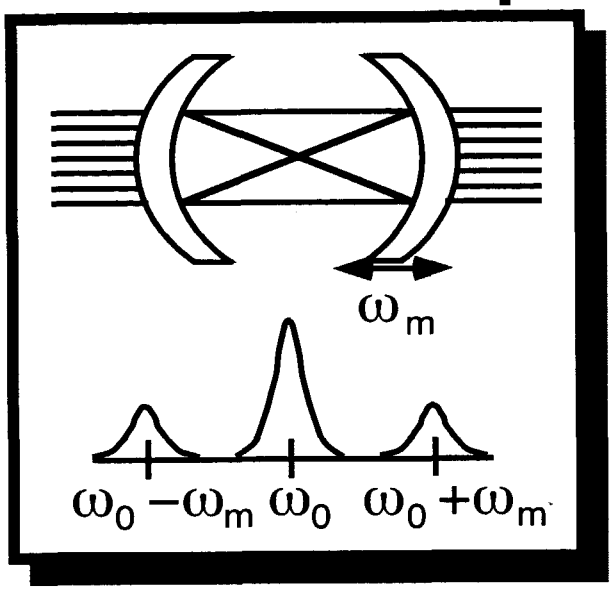
Infinite number of uncorrelated single scattering events.

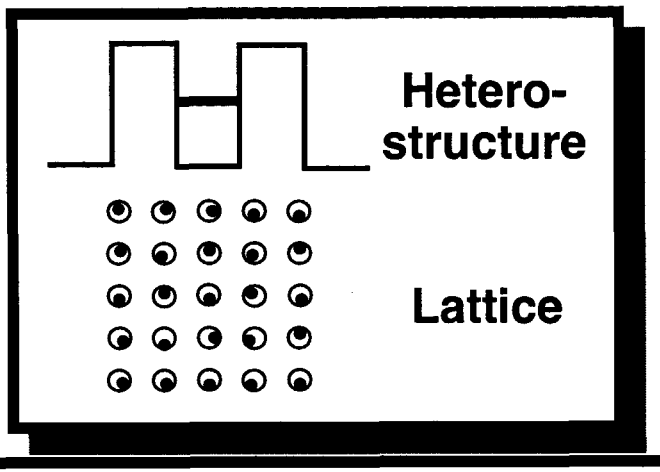
Self-Consistent Born Scattering with POP

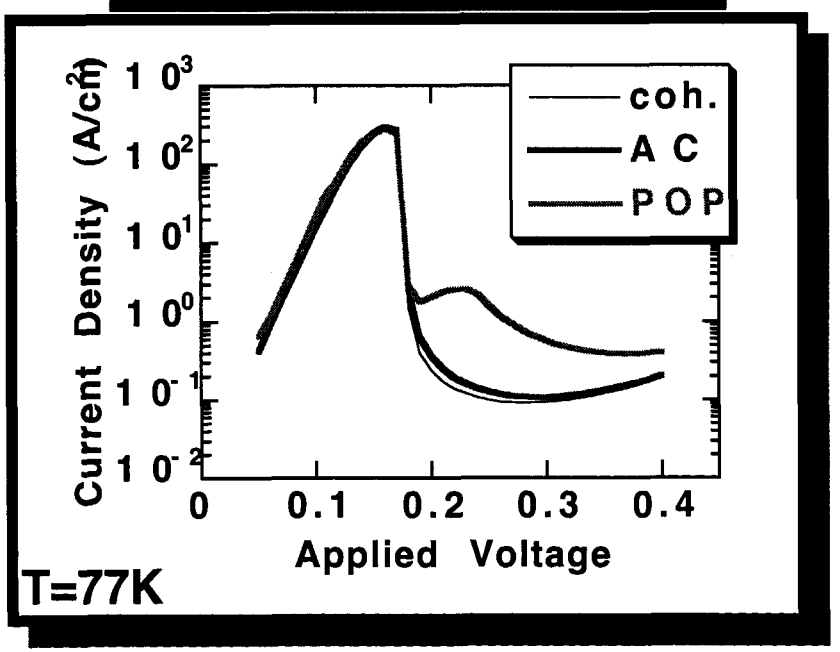
- Elastic scattering couples all momenta (k)
- Inelastic scattering couples different total energies (E,E+hv,E-hv)
- Polar optical phonons are treated as a single scattering event in NEMO



Electron-Phonon Interactions
Coupled Resonators





Self-consistent Born
(infinite sequential scattering)
treatment of
acoustic phonon-scattering

Single sequential scattering
treatment of
polar optical phonon scattering