High Bias Quantum Transport in Resonant Tunneling Diodes

Gerhard Klimeck

Transport in Resonant Tunneling Diodes

- Resonant Tunneling Diodes – Motivations
- Nanoelectronic Modeling Tool at TI – History and Key Insights

Use PCPBT on nanoHUB.org

- RTDs without bias – double barrier structures

Use RTDnegf on nanoHUB.org

- RTDs with linear potential drops
- RTDs with realistic doping profiles
- Resonant Tunneling Diodes with Relaxation in the Reservoirs
- RTDs with Quantum Charge Self-consistency (Hartree Model)

(Hopefully soon) use a new NEMO code on nanoHUB.org

- High performance RTDs – with bandstructure

Resonant Tunneling Diodes - NEMO1D: Motivation / History / Key Insights

Gerhard Klimeck

Thanks to: NEMO Core Team Members

NEMO 1-D – 1994-1998

Roger Lake, Texas Instruments / UC Riverside
R. Chris Bowen, Texas Instruments / JPL / TI
Tim Boykin, U Alabama in Huntsville
Dan Blanks, Texas Instruments
William R. Frensley, UT Dallas

NEMO 1-D – 1998-2003

R. Chris Bowen, JPL
Tim Boykin, U Alabama in Huntsville

Post Docs / Students / Developers / Consultants:

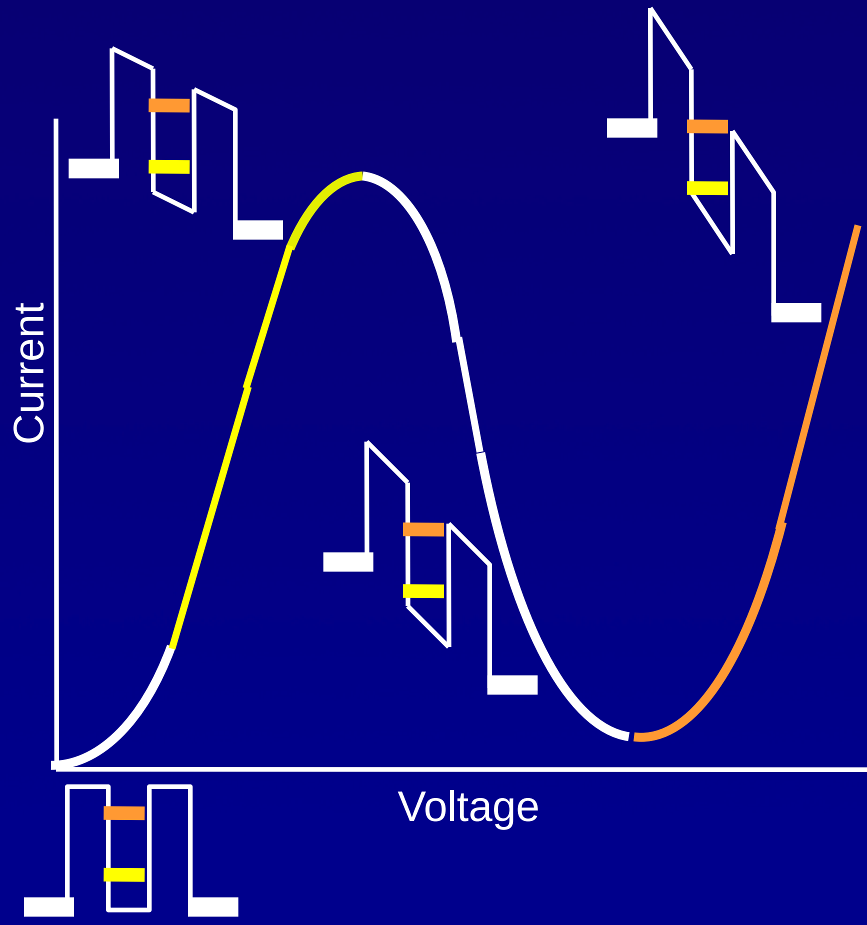
Manhua Leng, Chenjing Fernando, Paul Sotirelis, Carlos Salazar-Lazaro, Bill McMahon, Daniela Francovicchio, Mukund Swaminathan, Dejan Jovanovic

Experimentalists:

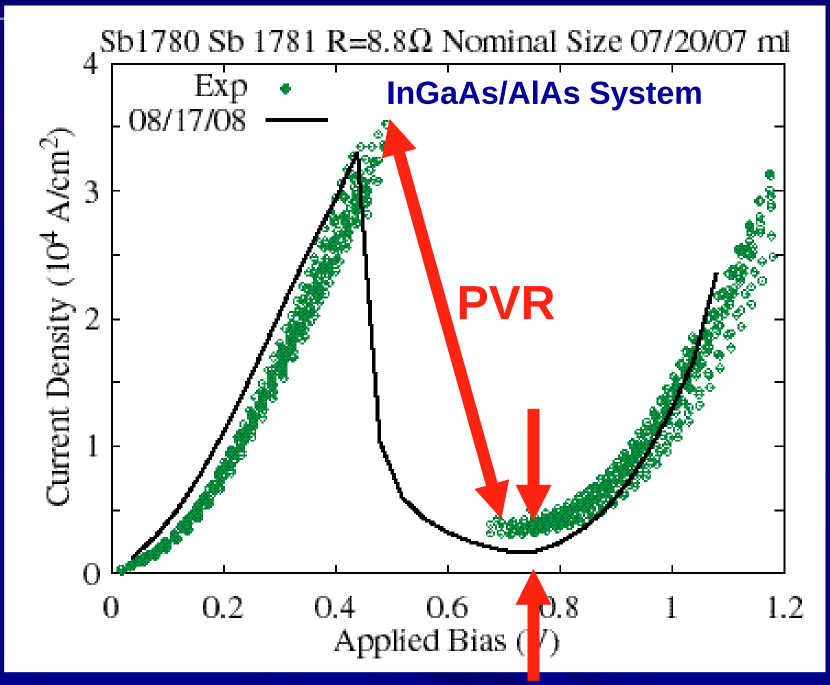
Alan Seabaugh, Ted Moise, Ed Beam, Tom Broekaert, Paul van der Wagt, Bobby Brar, Y. Chang (all TI), David Chow (HRL)

Funding by NRO, ARDA, ONR, NASA, JPL

Basic Operation of a 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

PVR – Peak-to-Valley-Ratio

1994: Best experiment PVR=80
=> On-Off-Ratio should to be >1,000

1994: What is the valley current physics?

1997: Can overlay experiment and theory.
What are the key insights?

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Resonant Tunneling Diodes in 1994

Potential:

- THz operation – limited only by tunneling time
- NDR => fast oscillations
- NDR => stable latches, digital logic

Challenges:

- Valley current too high => high “off” state current
- No production-like experiments => repeatability issues
- No generally accepted device modeling theory

⇒**Nanoelectronic Modeling – NEMO**

⇒Software tool that:

- Quantitative modeling
- Predictive design
- Physics-based understanding

State-of-the-art RTD Modeling and Simulation Knowledge 1994

Knowledge / Availability:

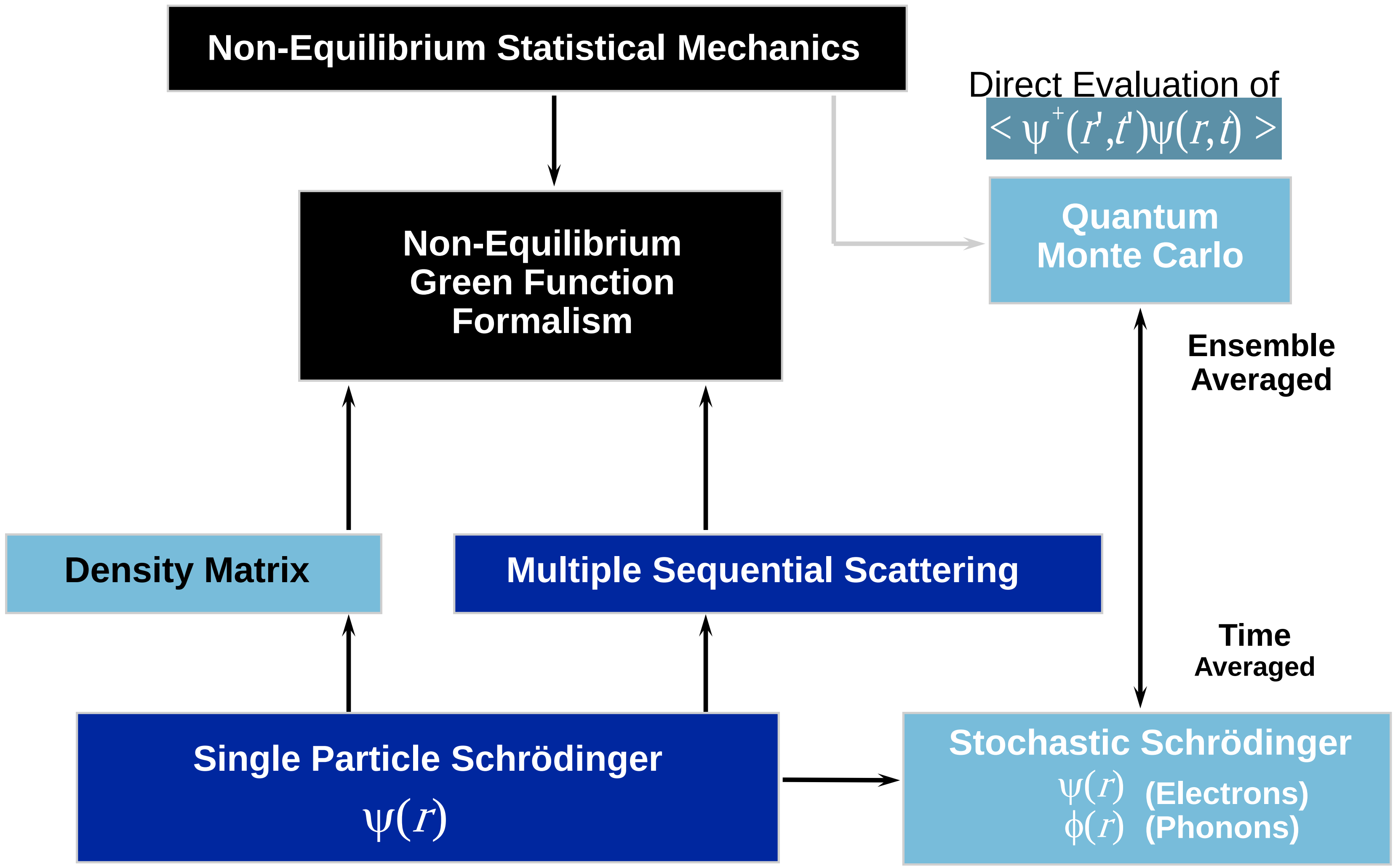
- 1-D Poisson Schrödinger
  - » Quantum transmitting boundary conditions (QTBM), flatband (Lent)
  - » Single band, effective mass, no scattering (“everyone”)
  - » Multiple Sequential Scattering (Roblin)
  - » Tight binding, no scattering (Boykin, Ting)
- Density Function
  - » Single band, no scattering, time dependent (Ferry)
- Wigner Function
  - » Single band with empirical scattering (Frensley)
- NEGF
  - » Single band with scattering (Lake, Jauho)
  - » Single band with charge self-consistency (Klimeck)
- **SCATTERING is the source of the valley current**

Limitations:

- Tiny device simulation domains – no extended contact regions
- No realistic scattering models
- Computation too expensive for engineering (we can build this in one month)
- No predictive theory, modeling, and simulation

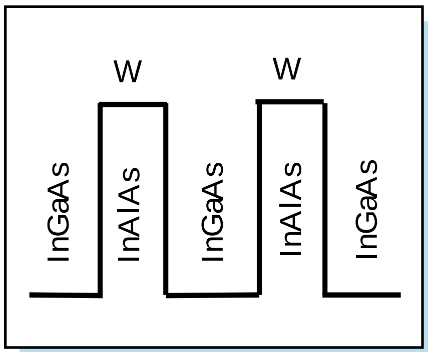
Available and Explored Theories

- **The non-equilibrium Green function formalism underlies NEMO.**
- **All of the approaches shown were considered.**
- **Approaches in light blue were dropped. Approaches in dark blue were incorporated.**

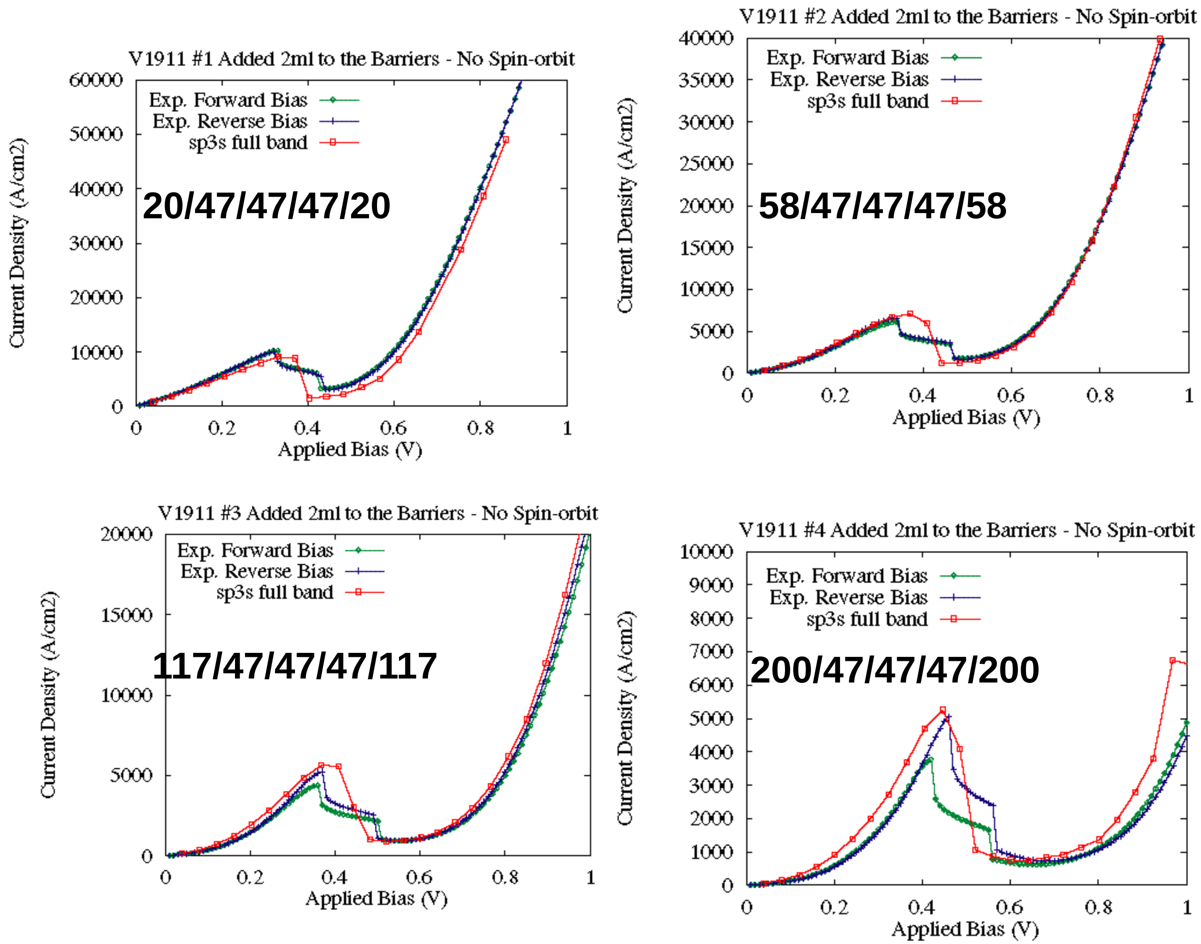


4 Stack RTD with Spacer Variation

Vary Spacer Length

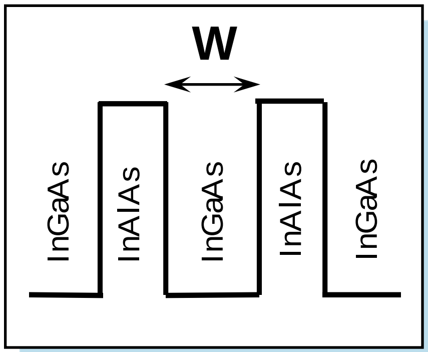


Four nominally symmetric devices:
20/47/47/47/20 A [1]
58/47/47/47/48 A [2]
117/47/47/47/117 [3]
200/47/47/47/200 [4]



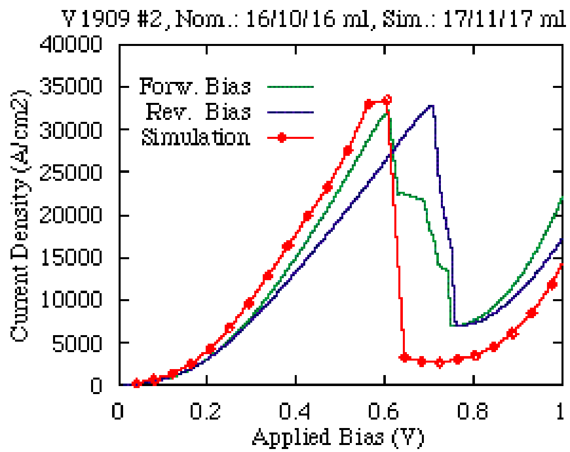
4 Stack RTD with Well Width Variation

Vary Well Width

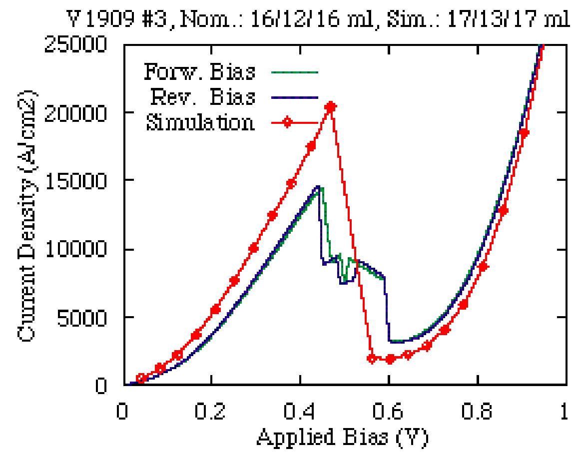


Three nominally symmetric devices:
47/29/47 A [1]
47/35/47 A [2]
47/47/47 A [3]

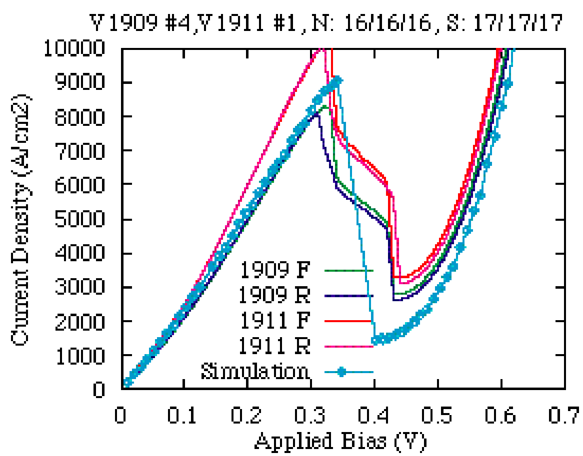
One asymmetric device:
35/47/47 A



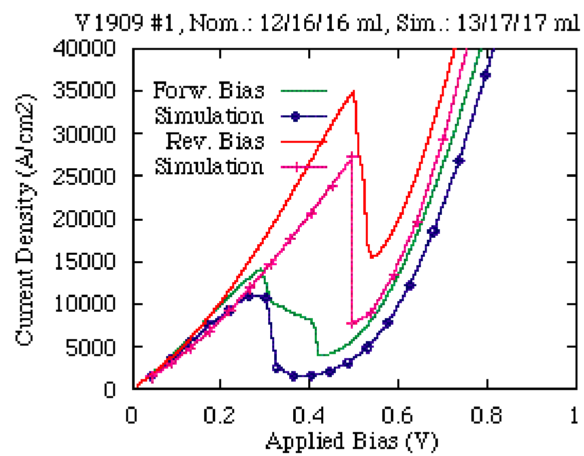
20/47/29/47/20



20/47/35/47/20



20/47/47/47/20

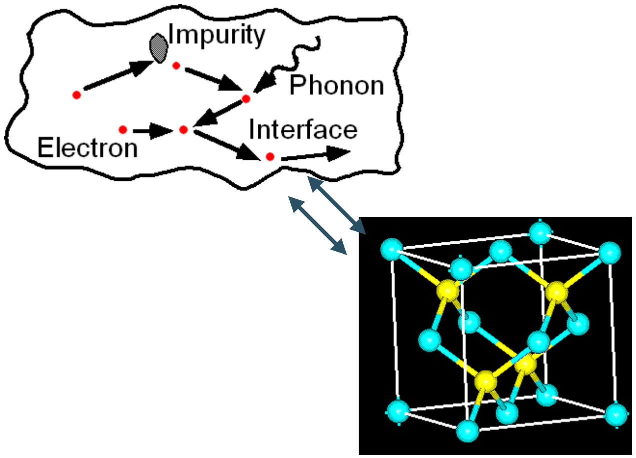


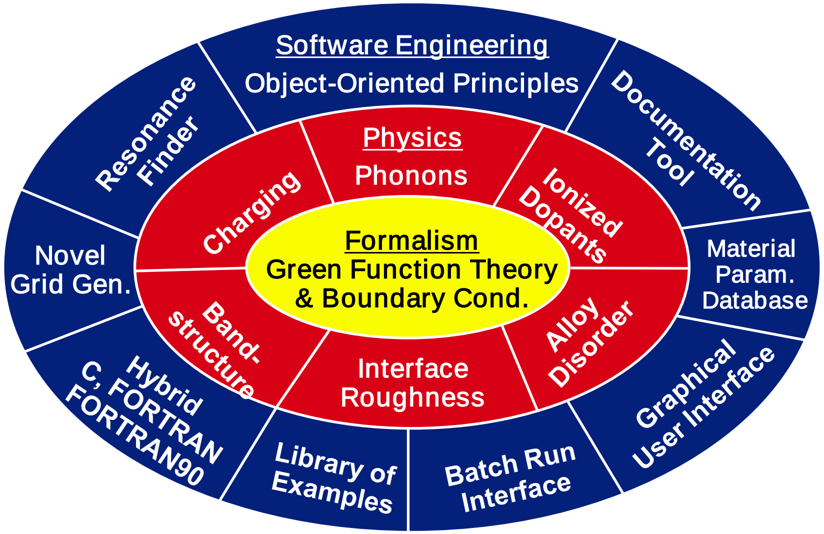
20/35/47/47/20

NEMO: A User-friendly Quantum Device Design Tool

- NEMO 1-D was developed under a NSA/NRO contract to Texas Instruments and Raytheon from '93-'98 (>50,000 person hours, 250,000 lines of code).
- NEMO 1-D maintained and NEMO 3-D developed at JPL '98-'03 (>14000 person hours) under NASA, NSA, and ONR funding.

- NEMO is THE state-of-the-art quantum device design tool.
  - » First target: transport through resonant tunneling diodes (high speed electronics).
  - » Second target: electronic structure in realistically large nano devices (detectors).
  - » Third target: qbit device simulation.
  - » Ultimate target: Educational tool - heterostructures, bandstructure, transport.
- Bridges the gap between device engineering and quantum physics.
- Based on Non-Equilibrium Green function formalism NEGF - Datta, Lake, Klimeck.
- Currently used by limited number of government labs and few Universities.





State-of-the-art RTD Modeling and Simulation Knowledge 1998

Knowledge:

- Scattering inside RTD
  - » Only important at low temperatures
  - » Not important for room temperature, high performance
- Scattering inside extended contacts
  - » Of critical importance at any temperature
- Charge self-consistency
  - » Critical everywhere, contacts and central device
- Bandstructure – atomistic device resolution
  - » Critical for understanding high temperature, high performance devices
- NEGF is the baseline of an industrial strength simulator

Availability:

- An engineering modeling and design tool for 1D heterostructures
- Experimentally verified – **analysis and design**

Releasing NEMO1-D has been a Struggle

Even a movie was made!

Currently only available through JPL for government use!

We need public-domain codes as field develops!

NEMO 3-D can be found for free at: https://nanohub.org/groups/nemo_3d_distribution

The other Nemo has also been found:

Open 1D Systems: Transmission through Double Barrier Structures - Resonant Tunneling

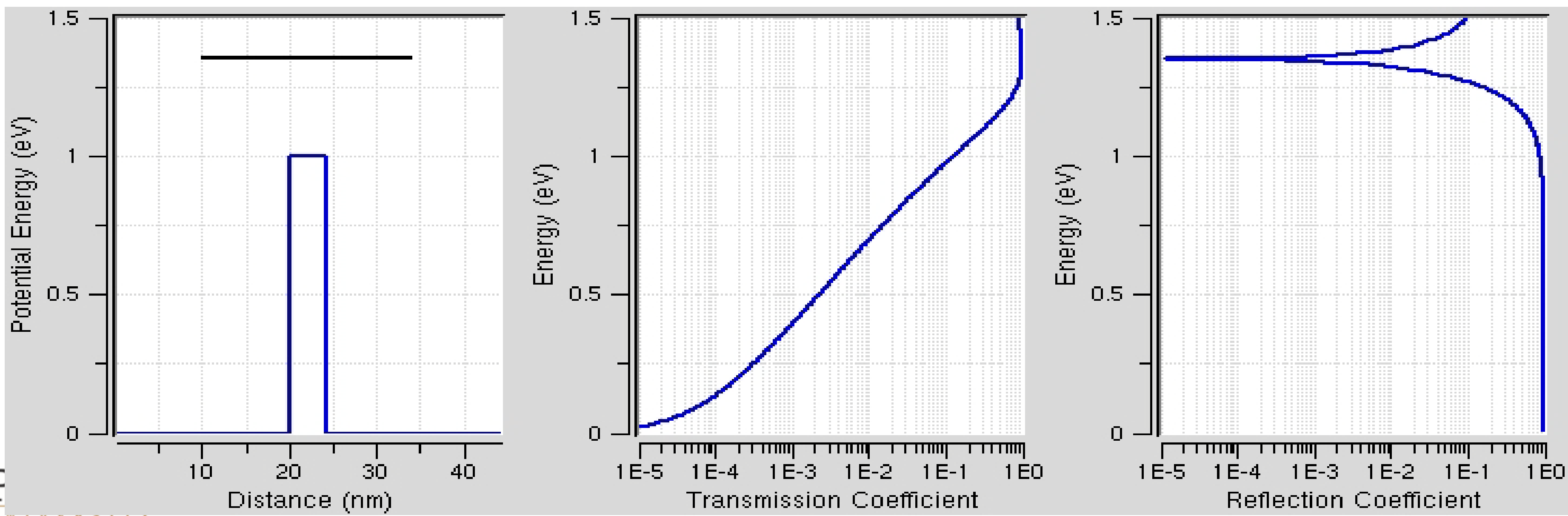
NCN

Gerhard Klimeck,
Dragica Vasileska,
Samarth Agarwal

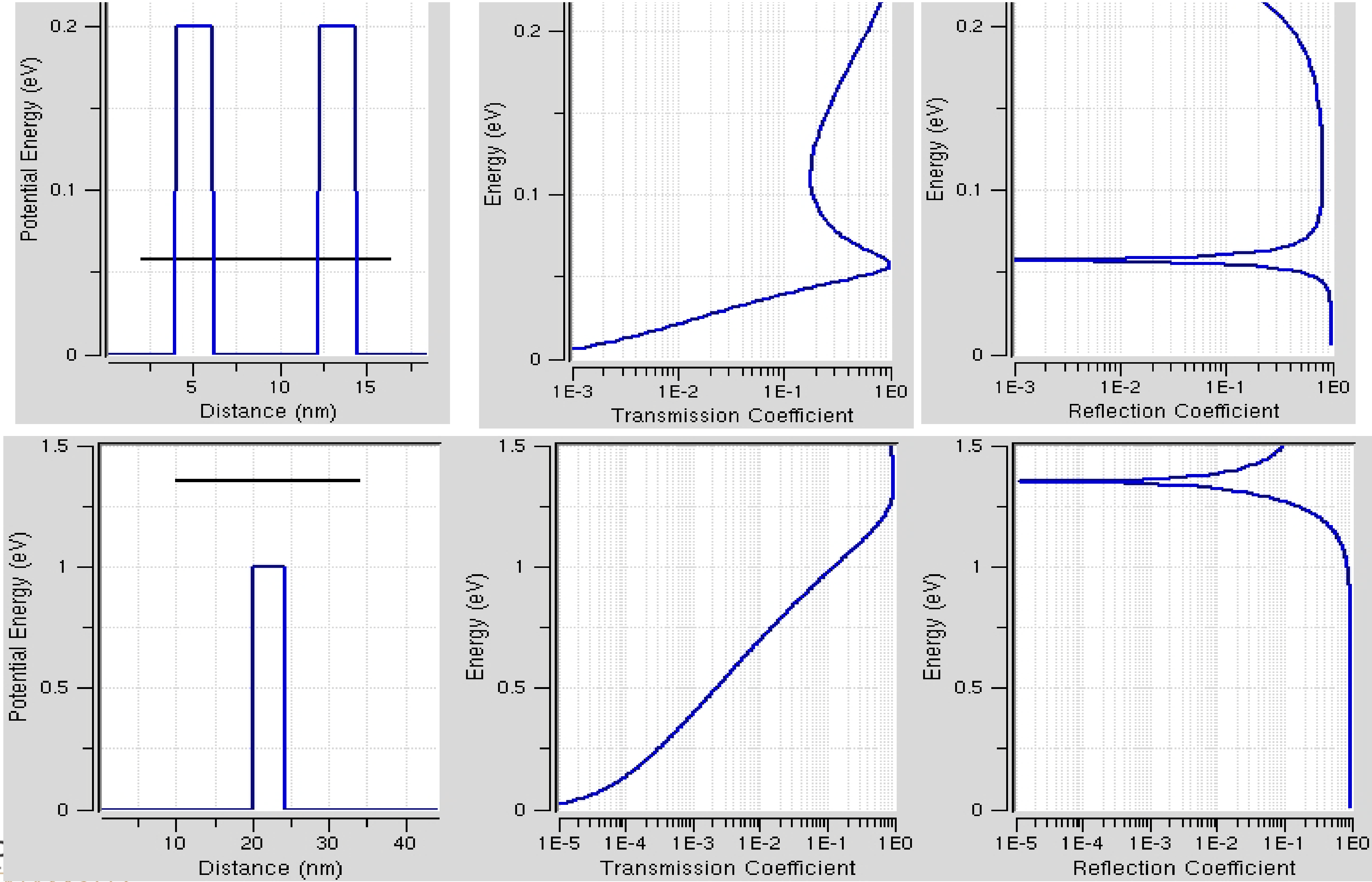
PURDUE
UNIVERSITY

Reminder: Single barrier

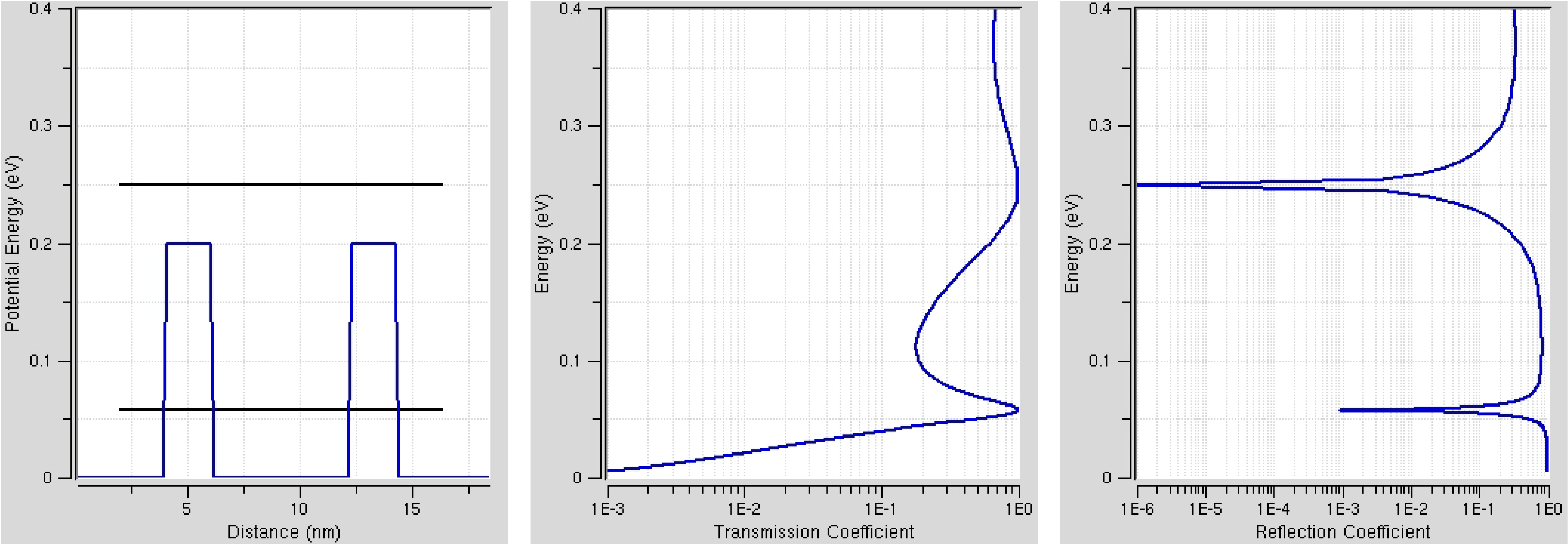
- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier.
  Transmission goes to one.



- Double barriers allow a transmission probability of one / unity for discrete energies
- (reflection probability of zero) for some energies below the barrier height.
- This is in sharp contrast to the single barrier case
- Cannot be predicted by classical physics.

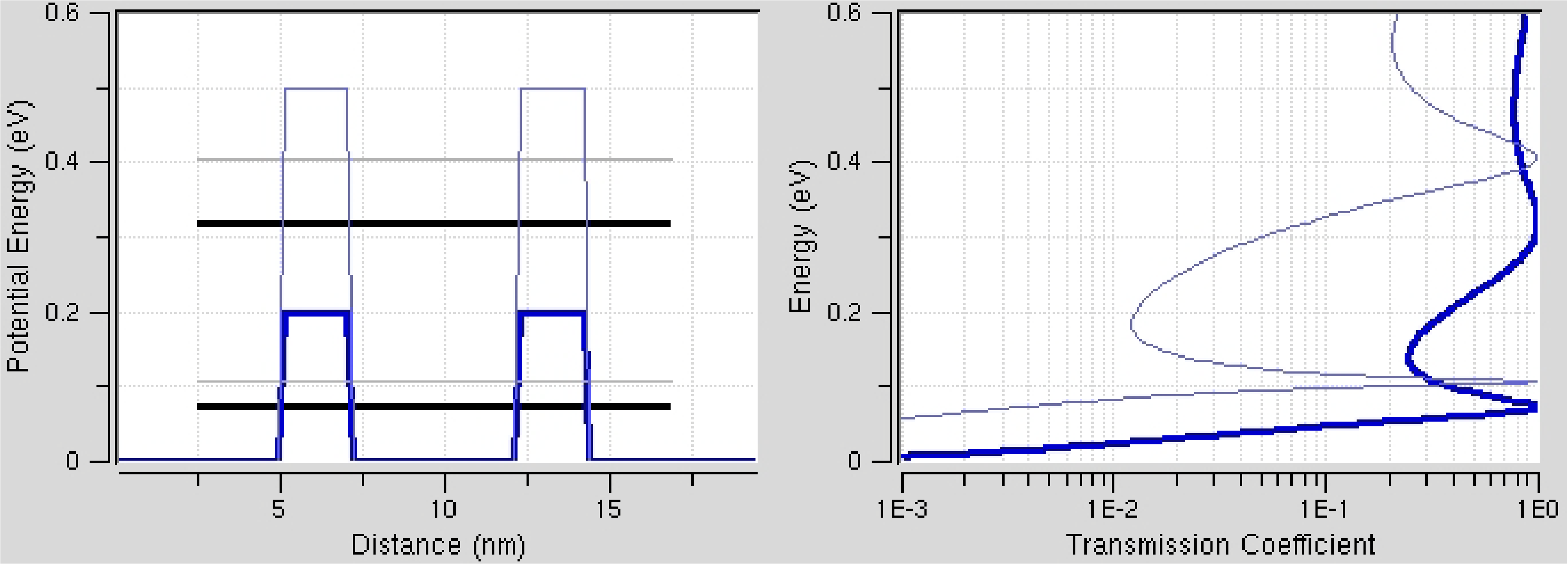


Double barrier: Quasi-bound states



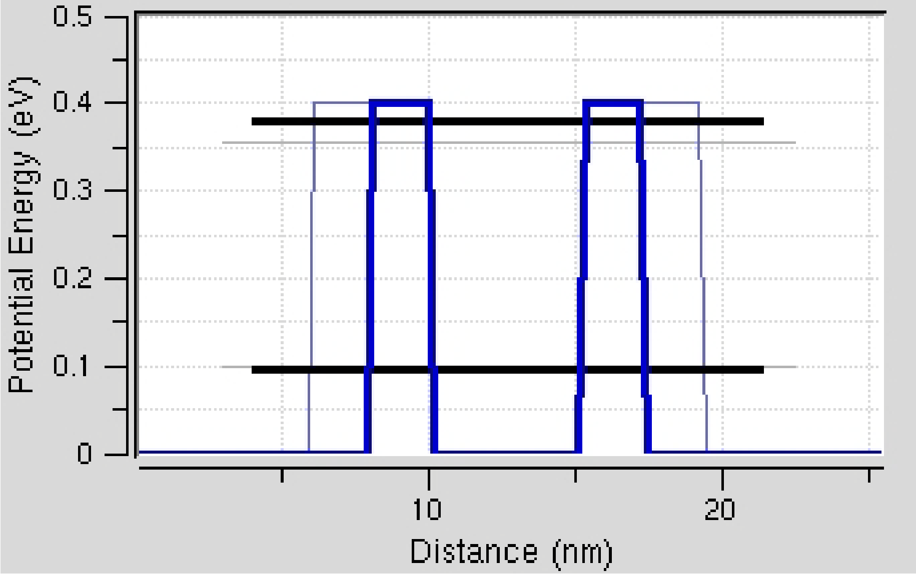
- In addition to states inside the well, there could be states above the barrier height.
- States above the barrier height are quasi-bound or weakly bound.
- How strongly bound a state is can be seen by the width of the transmission peak.
- The transmission peak of the quasi-bound state is much broader than the peak for the state inside the well.

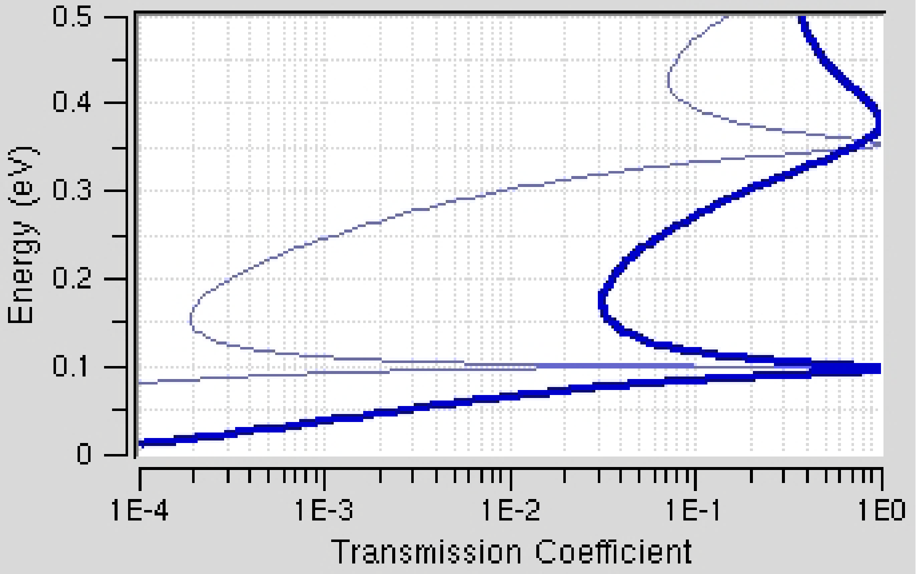
Effect of barrier height



- Increasing the barrier height makes the resonance sharper.
- By increasing the barrier height, the confinement in the well is made stronger, increasing the lifetime of the resonance.
- A longer lifetime corresponds to a sharper resonance.

Effect of barrier thickness





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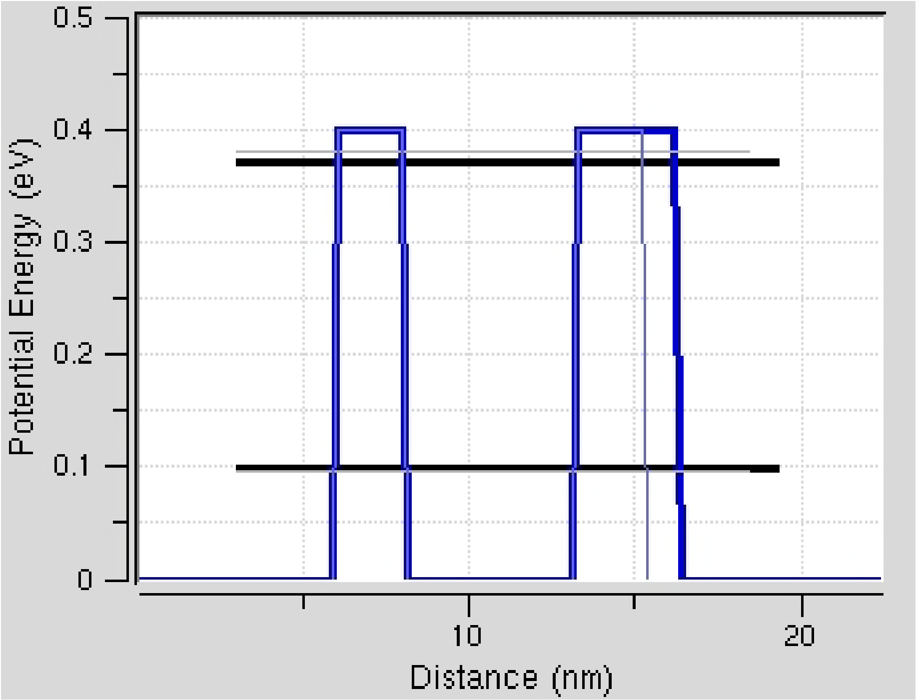
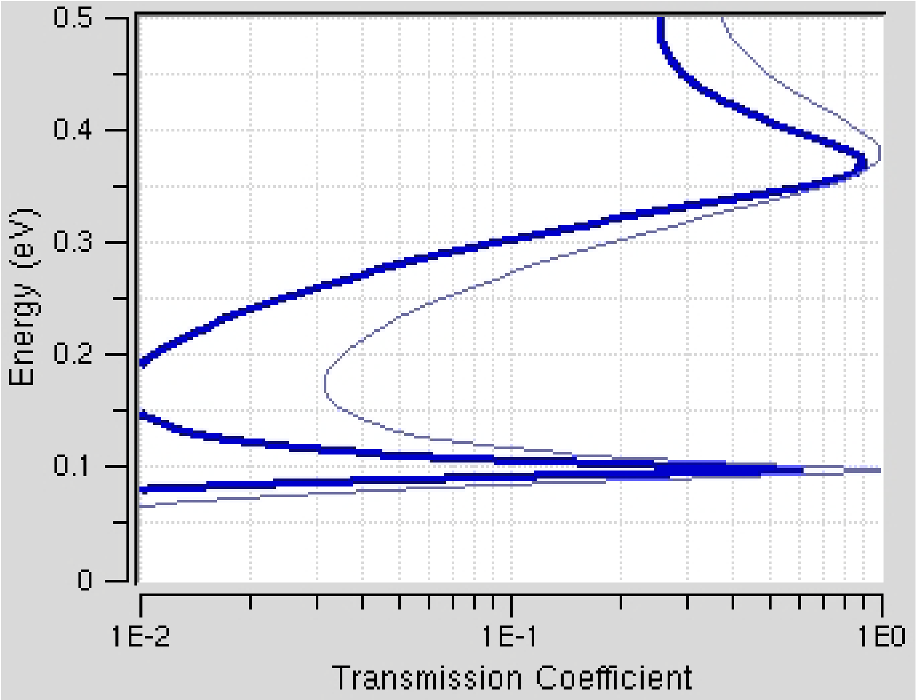
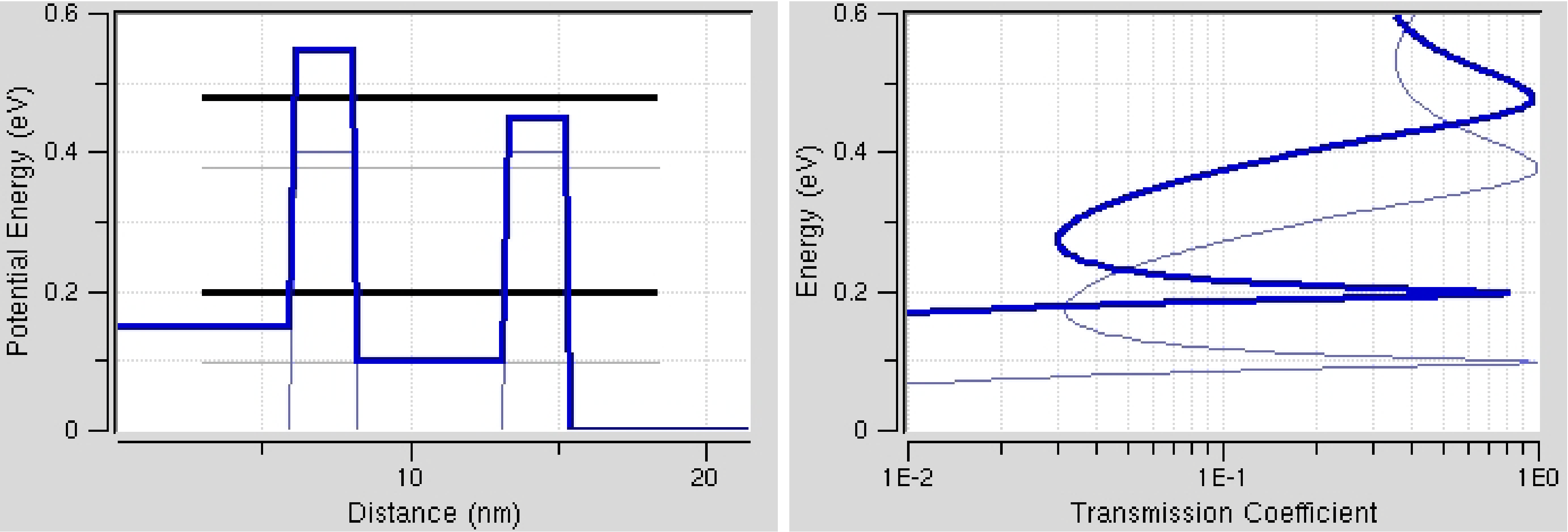
Asymmetric barriers





- Transmission in the symmetric case goes to one for resonance energies.
- Transmission in the non-symmetric case (second barrier is thicker) does not go to one for resonance energies.
- Current in the non-symmetric case will always be less than the symmetric case.

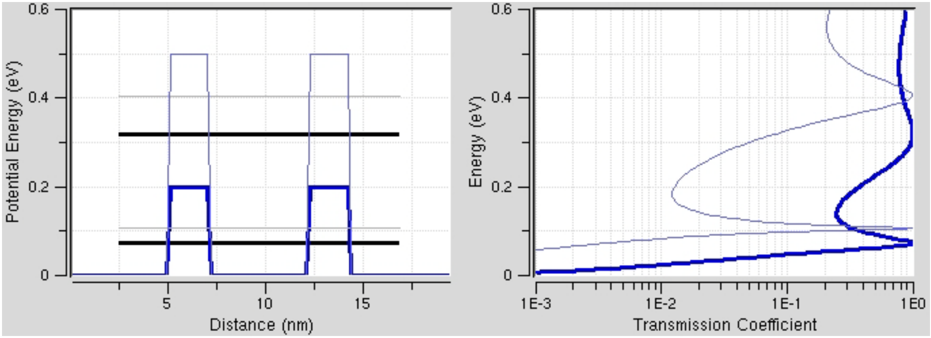
Potential Drop



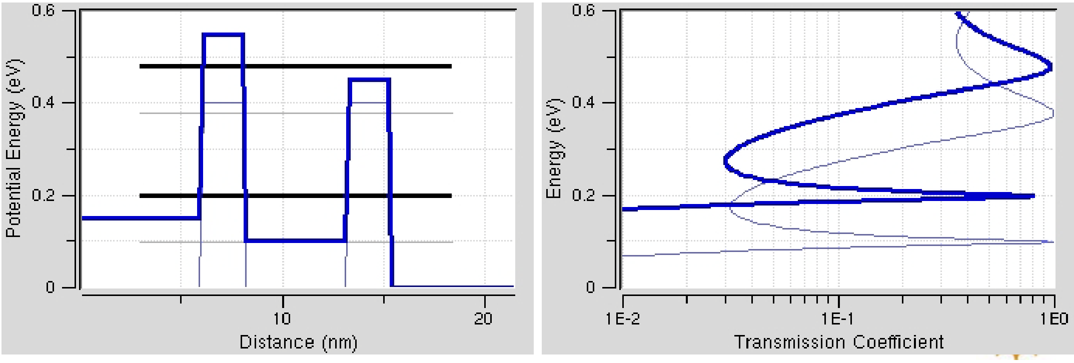
- Symmetric structure (no bias) exhibit unity transmission on resonance.
- Potential drop introduces asymmetry
  => transmission never reaches unity anymore
- Increased asymmetry reduces resonance transmission / current.

Key Summary

- Double barrier structures can show unity transmission for energies BELOW the barrier height
  - » Resonant Tunneling



- Resonance can be associated with a quasi bound state
  - » Can relate the bound state to a particle in a box
  - » State has a finite lifetime / resonance width
  - » Open and closed systems differ significantly for realistic barrier heights/widths
- Increasing barrier heights and widths:
  - » Increases resonance lifetime / electron residence time
  - » Sharpens the resonance width
- Asymmetric barriers
  - » Reduce the unity transmission

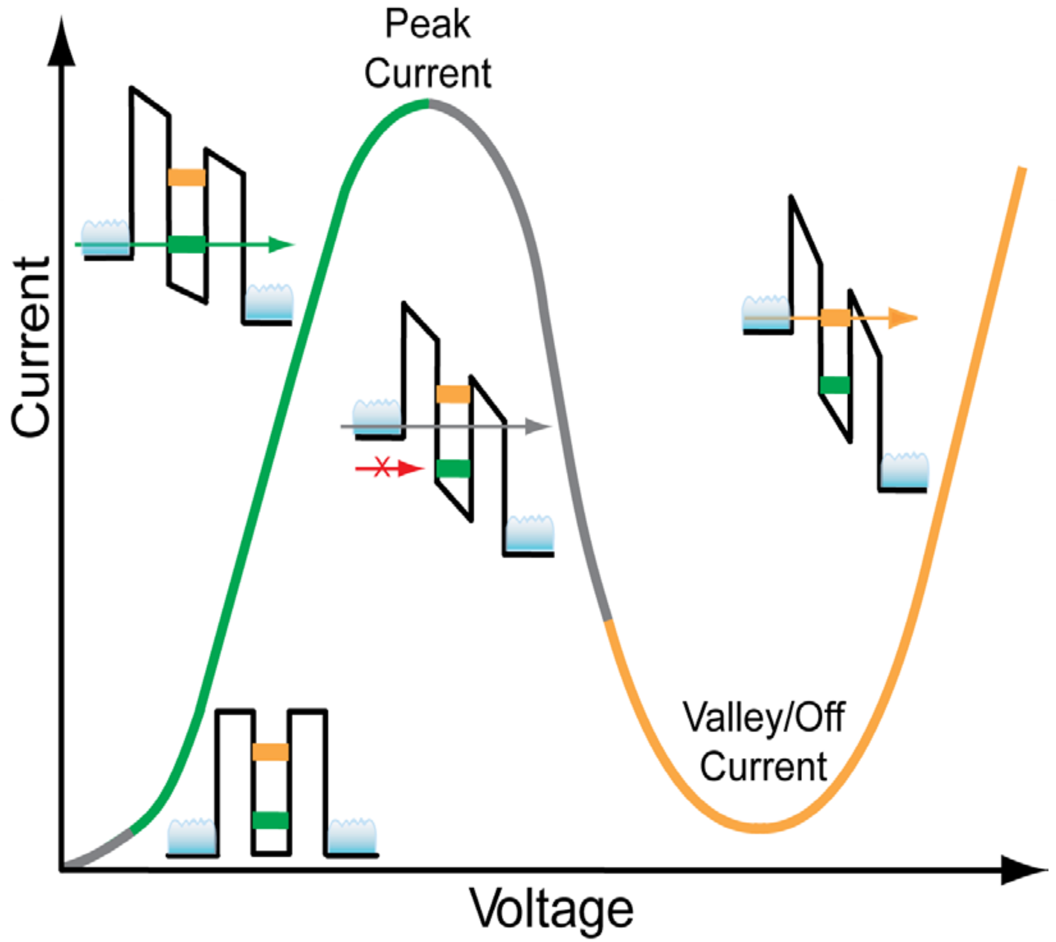


Introduction to RTDs: Linear Potential Drop

Gerhard Klimeck

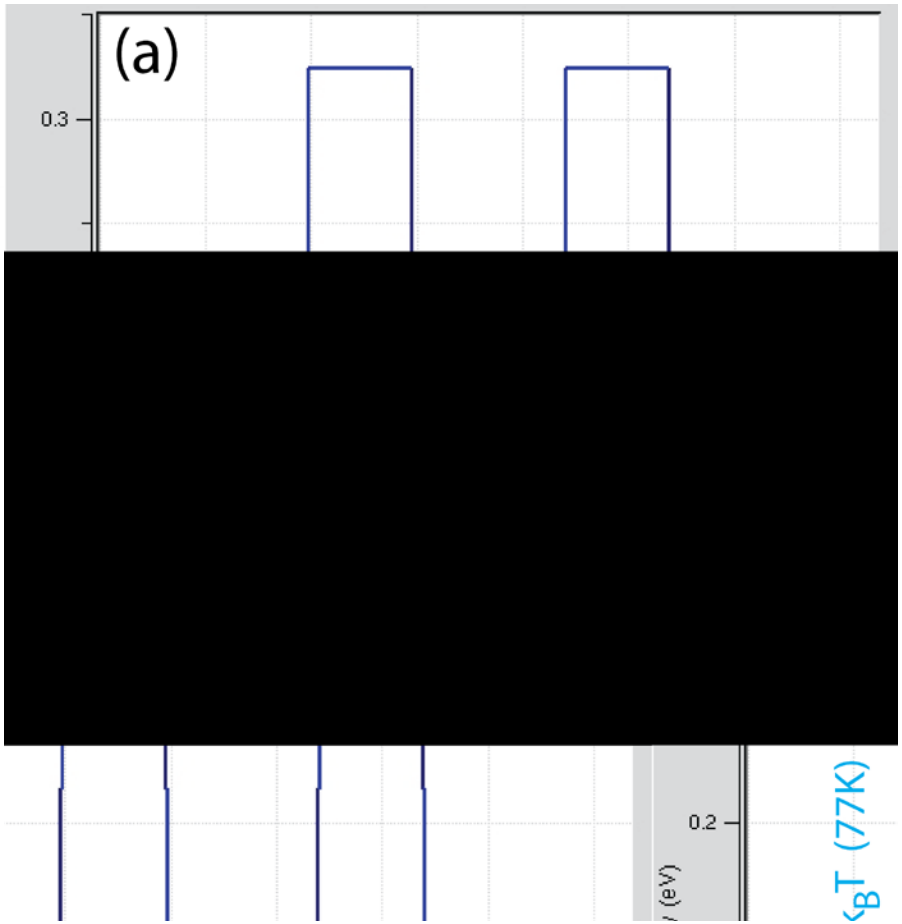
NCN

Schematic description of the operation of a RTD



- An RTD is formed as a single quantum well structure surrounded by very thin layer barriers.
- The current reduction acts like a negative differential resistance (NDR).

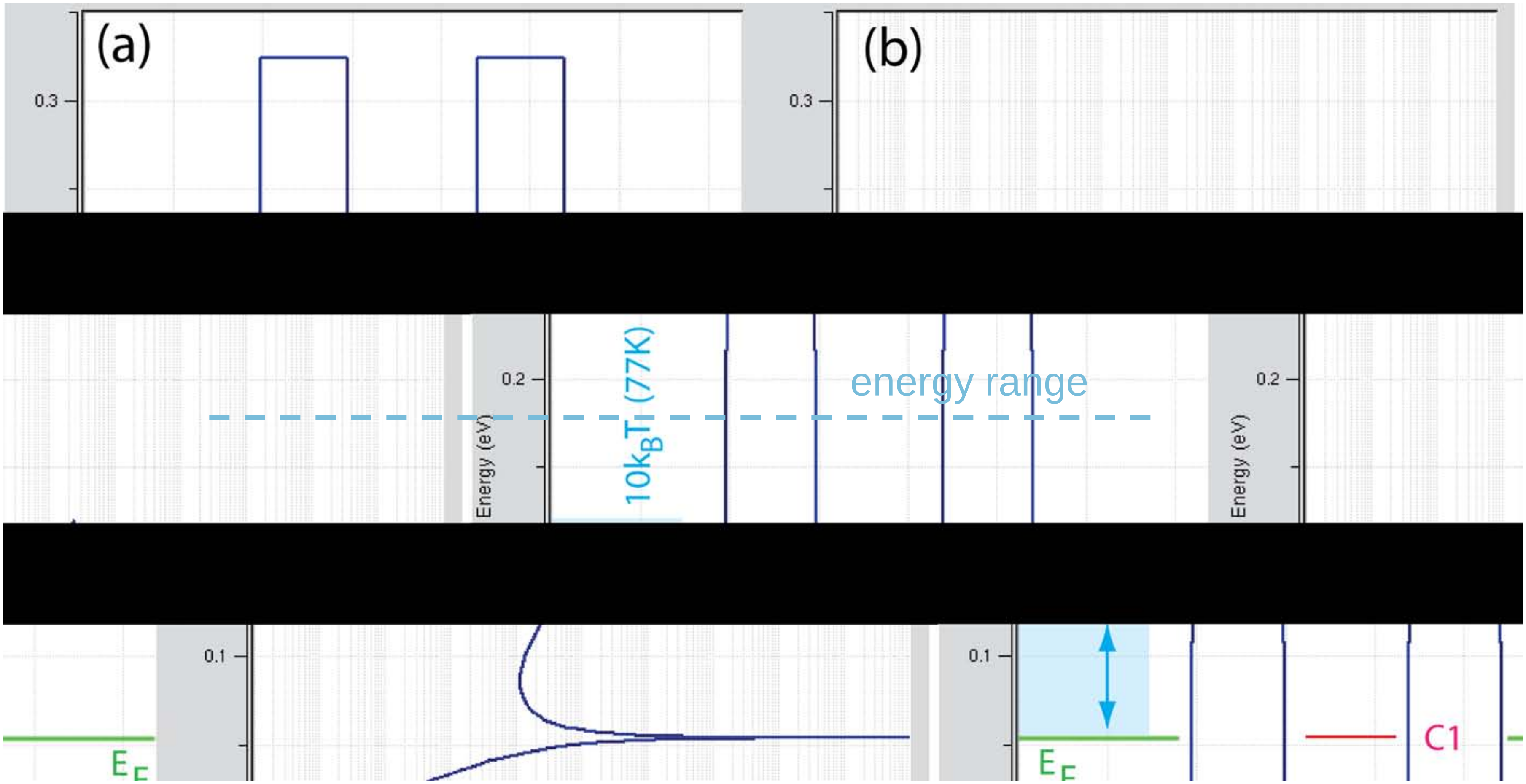
A GaAs-based RTD with AlxGa1-xAs barriers



- Well 7nm
- Barriers 5nm
- *x*=0.3 Al   ΔEc=324meV
- T=77K.

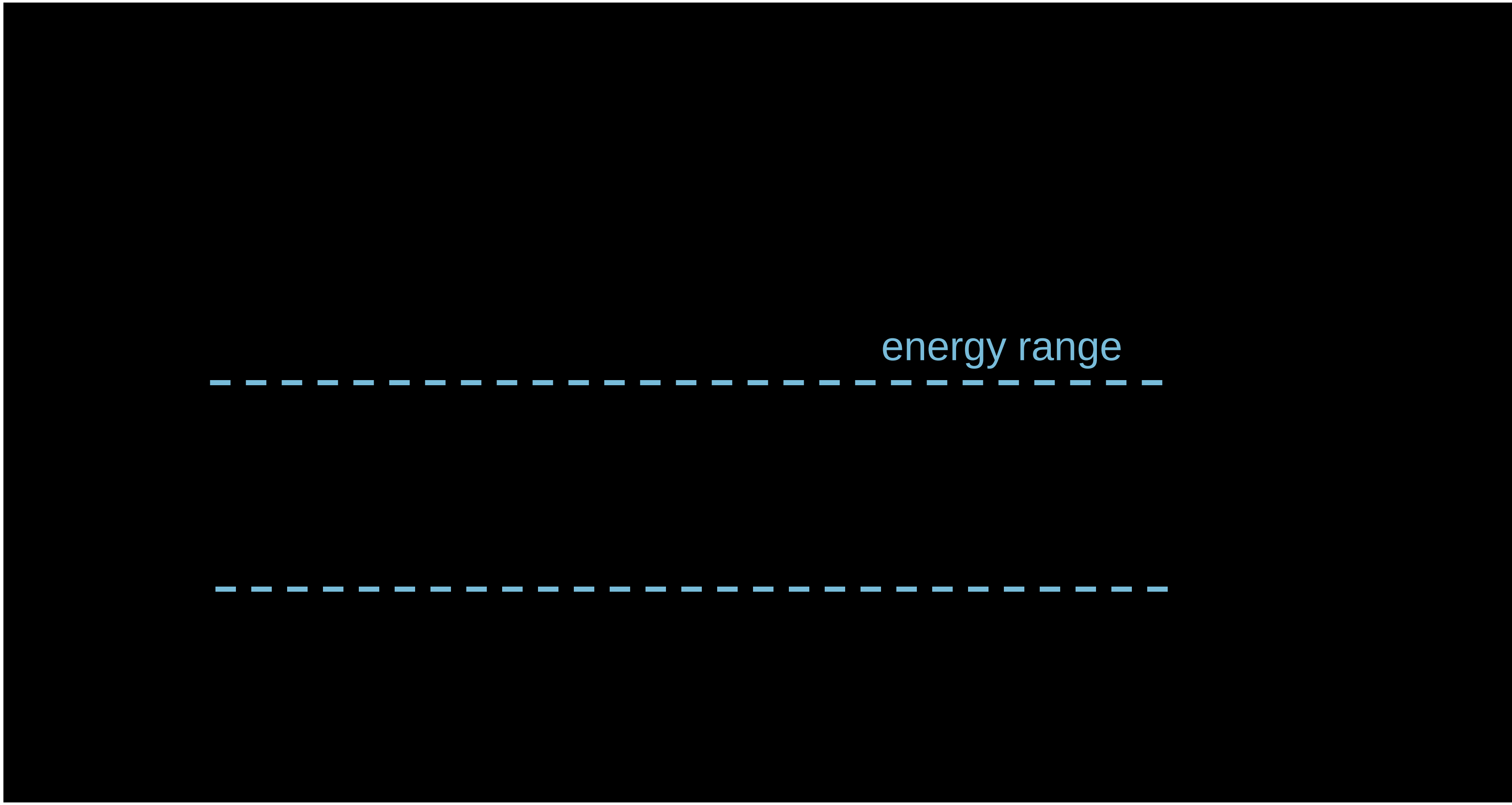
- Assume linear potential drop.
  - » a flat electrostatic potentials in the emitter and the collector
  - » a linear potential drop in the central device region across the barriers and the central well

RTD with Transmission in Equilibrium



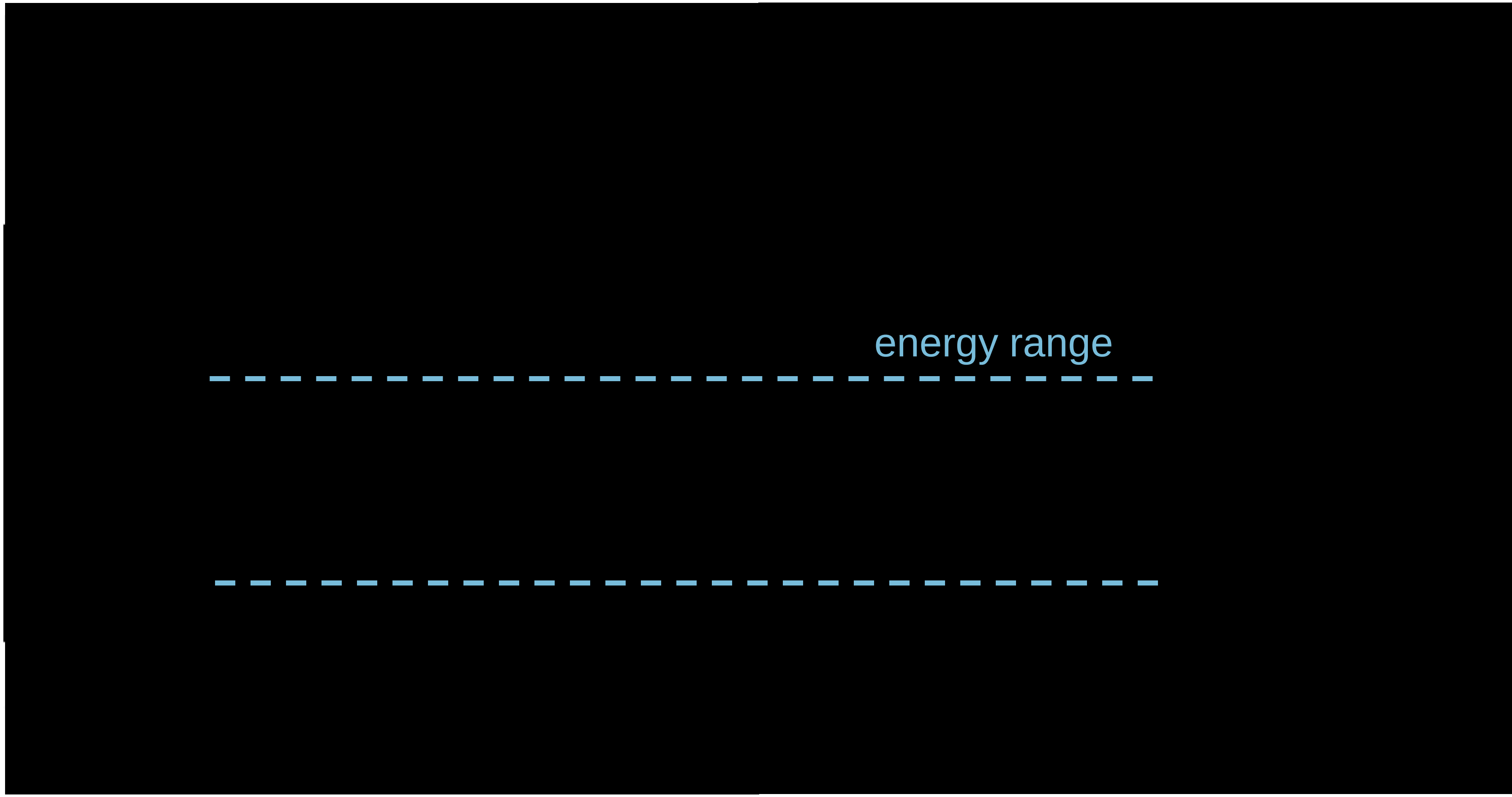
- Transmission sharply spiked at resonance energy => T=1
- Relevant energy range determined by $10k_BT$

RTD with 0.08V Linear Drop Bias



- 0.08V applied bias - Fermi Levels separate
- Resonance moves down in energy
- Transmission sharply spiked at resonance energy => T<1 asymmetric

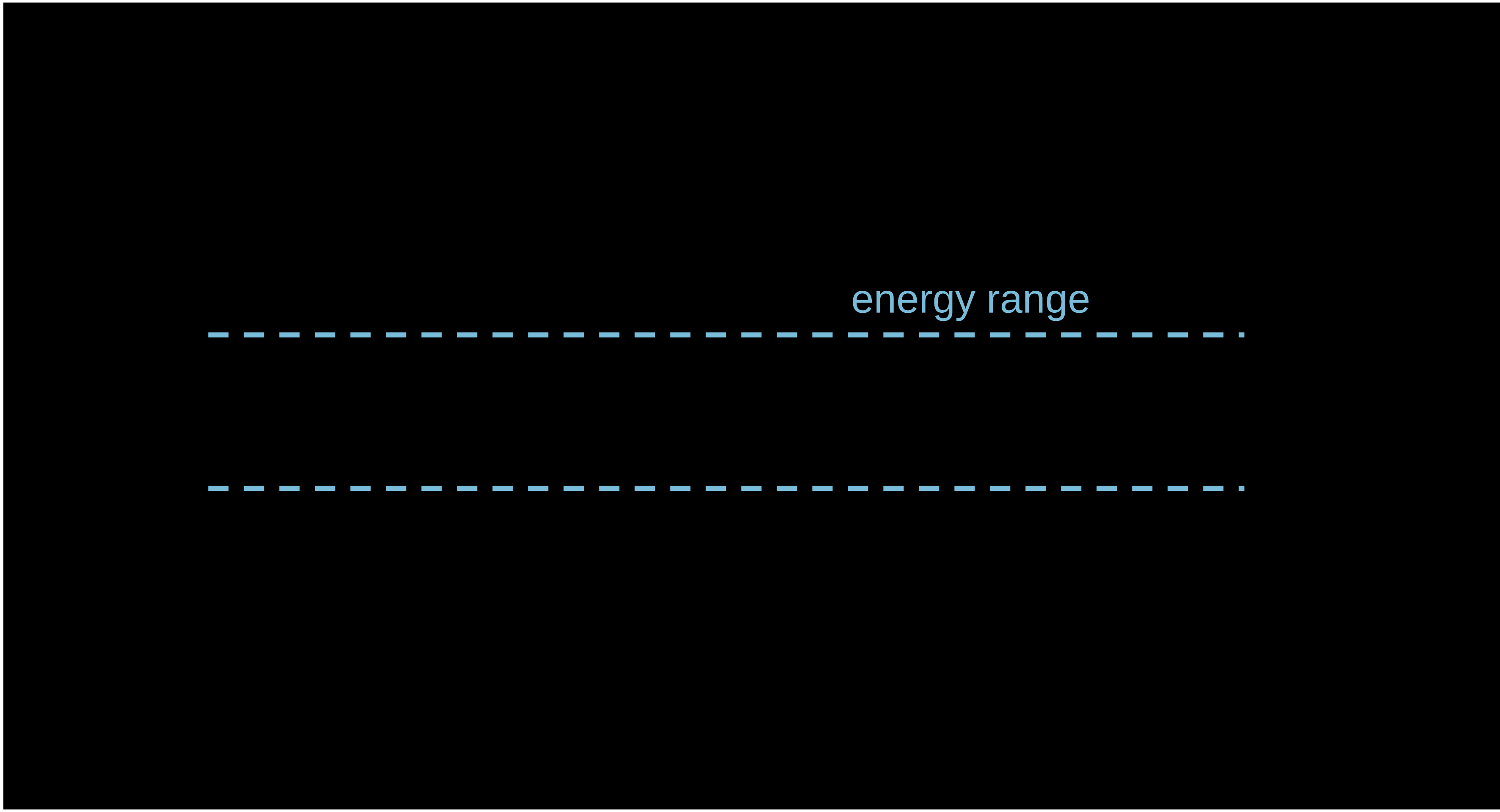
Current Density J(E)



- 0.08V applied bias - Fermi Levels separate
- $J(E) = T(E) * (f_L(E) – F_R(E))$
- Green Line – Running Integral of J(E)

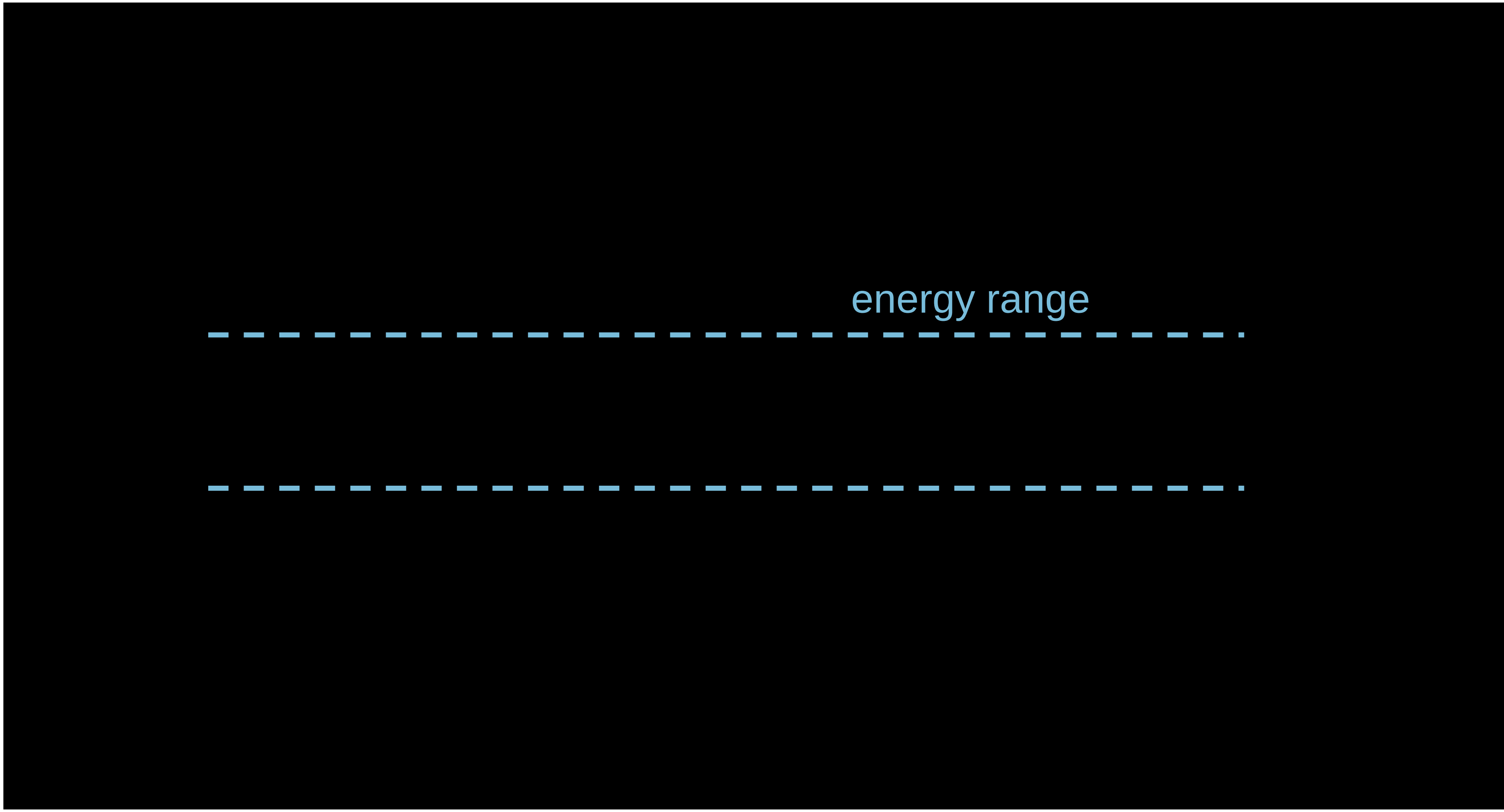
$$I(E) = \int_{-\infty}^{E} dE' J(E') / \int_{-\infty}^{\infty} dE' J(E')$$

RTD with 0.16V Linear Drop Bias



- 0.16V applied bias - Fermi Levels separate
- Resonance has no supply from the left – no resonance transmission
- Just off-resonant transmission

Current J(E) at 0.16V Bias



- 0.16V applied bias - Fermi Levels separate
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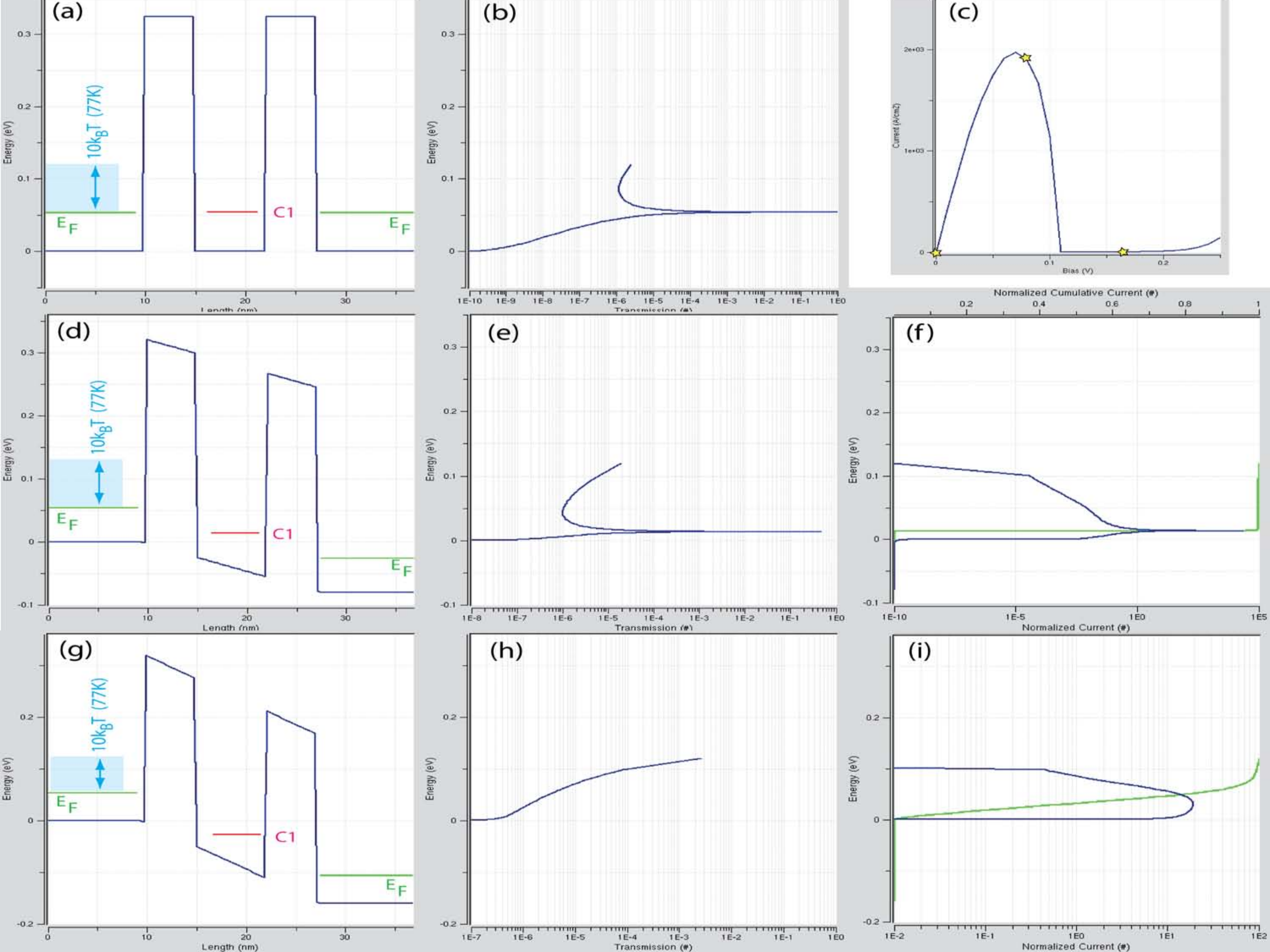
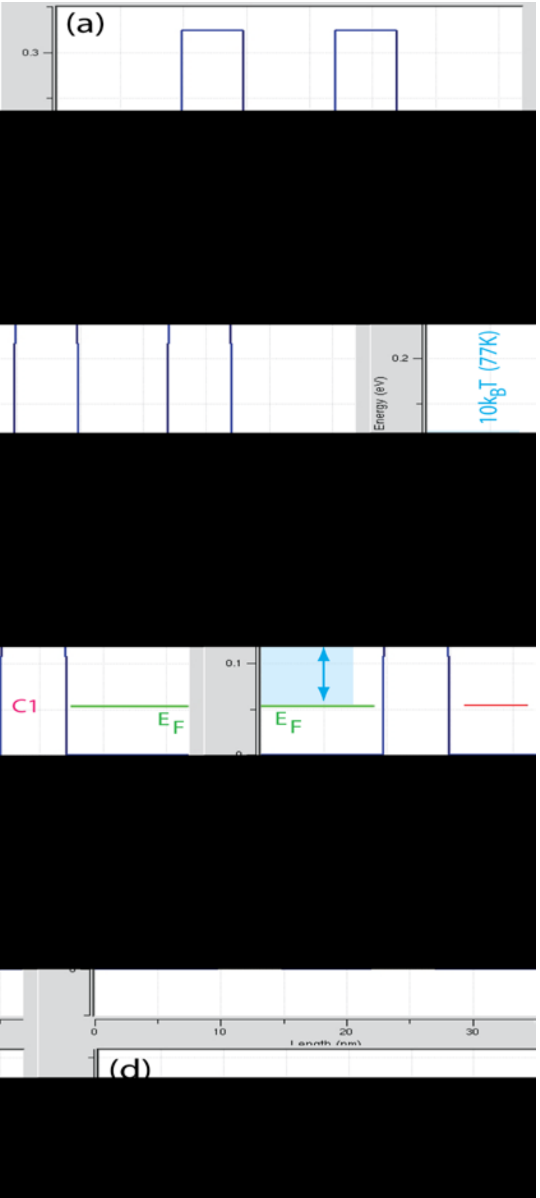
- Green Line – Running Integral of J(E)

$$I(E) = \int_{-\infty}^{E} dE' J(E') / \int_{-\infty}^{\infty} dE' J(E')$$


(a)
Energy (eV)
10k_BT (77K)
E_F
C1
E_F
Length (nm)
(b)
Energy (eV)
Transmission (#)
(c)
Current (A/cm2)
Bias (V)
Normalized Cumulative Current (#)
(d)
Energy (eV)
10k_BT (77K)
E_F
C1
E_F
Length (nm)
(e)
Energy (eV)
Transmission (#)
(f)
Energy (eV)
Normalized Current (#)
(g)
Energy (eV)
10k_BT (77K)
E_F
C1
E_F
Length (nm)
(h)
Energy (eV)
Transmission (#)
(i)
Energy (eV)
Normalized Current (#)

IV characteristic with linear potential drop



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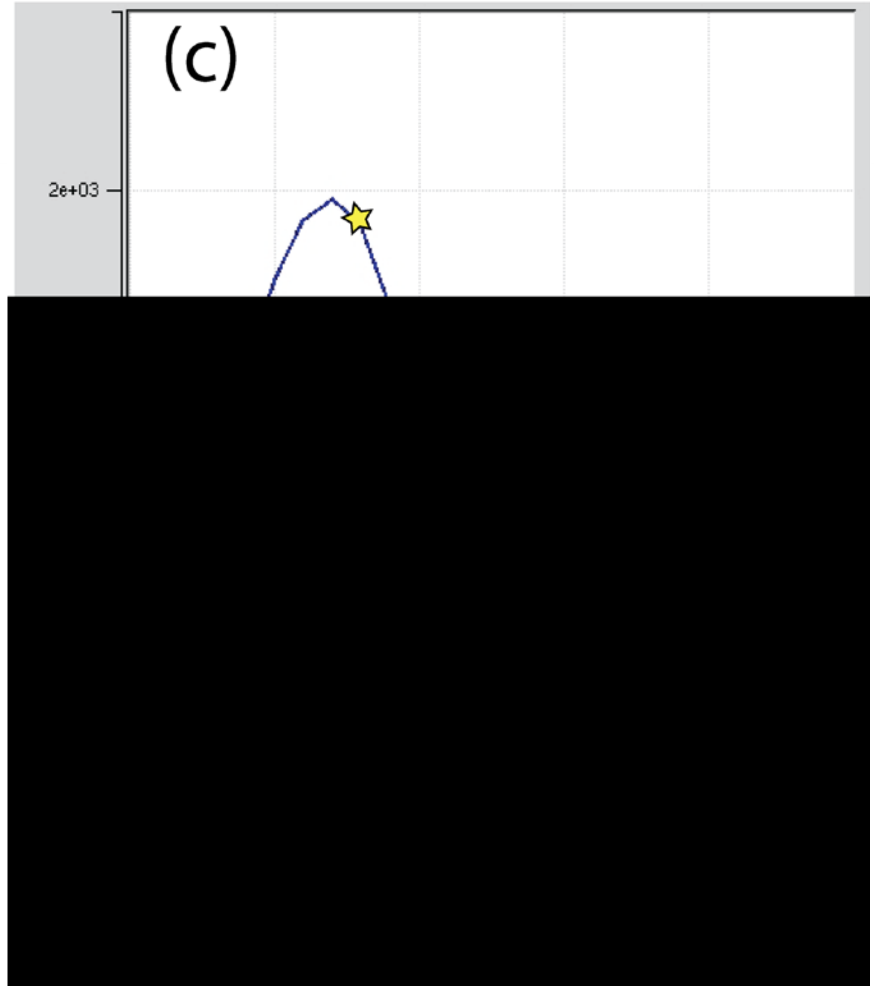

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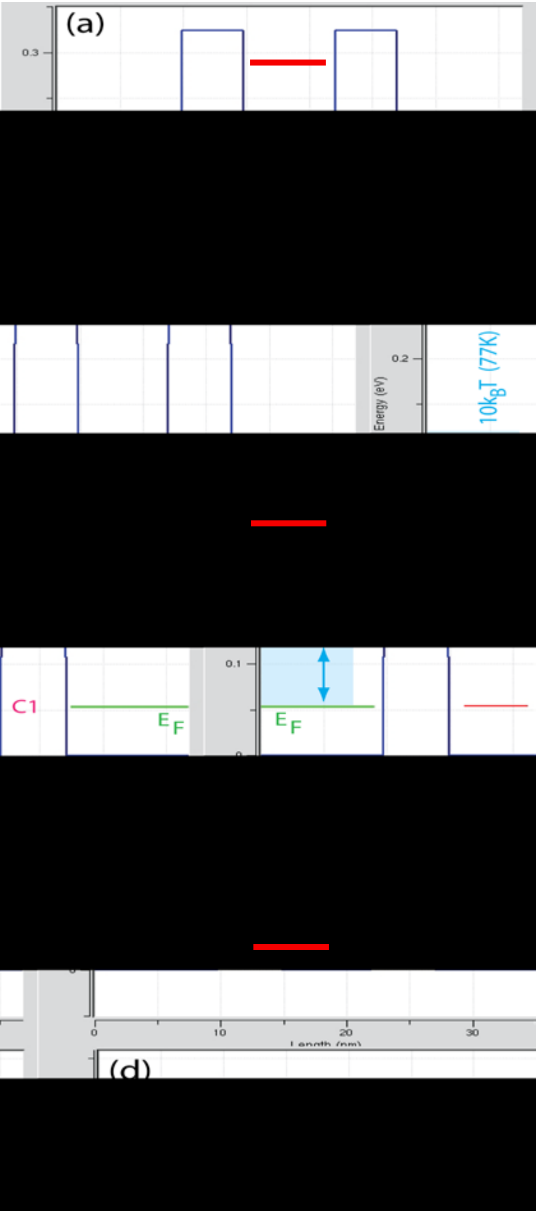
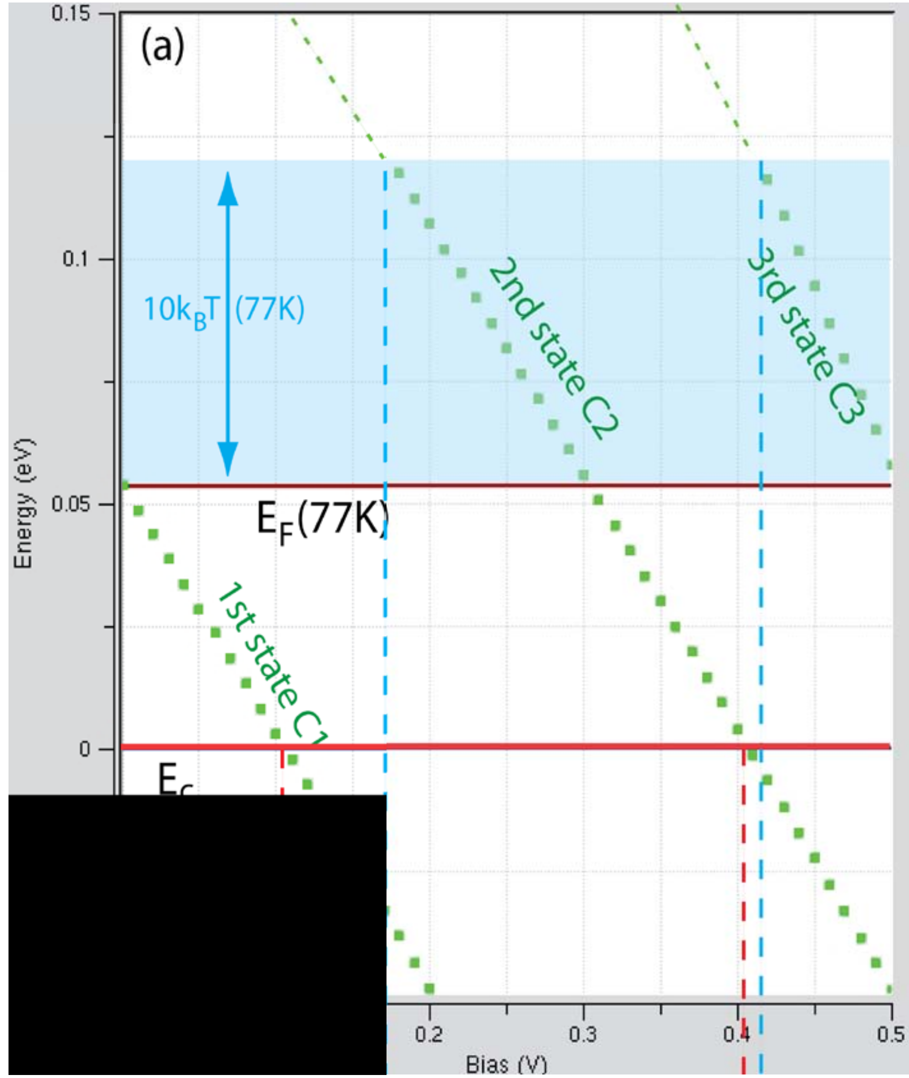
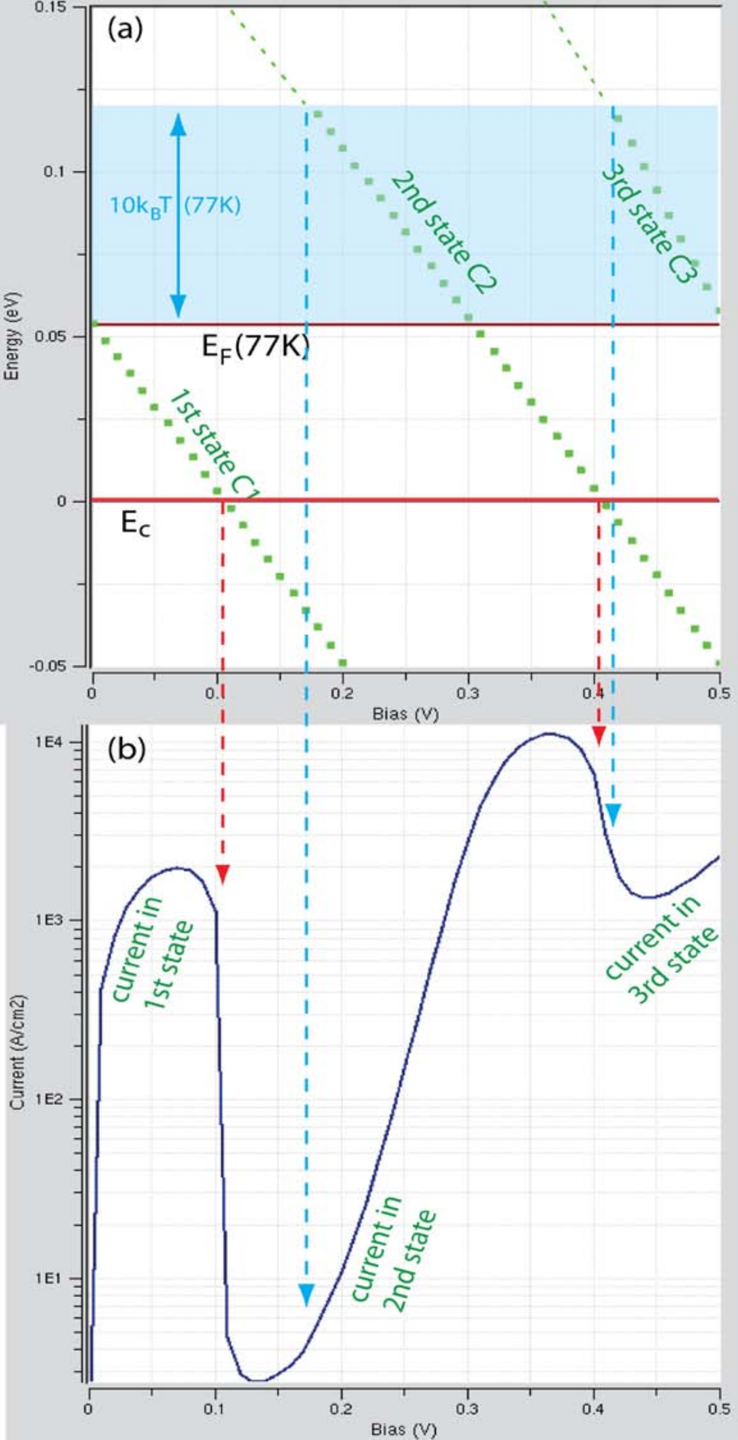
- ideal N-shaped Current Voltage (I-V) characteristic

Resonance Energies as a Function of Bias



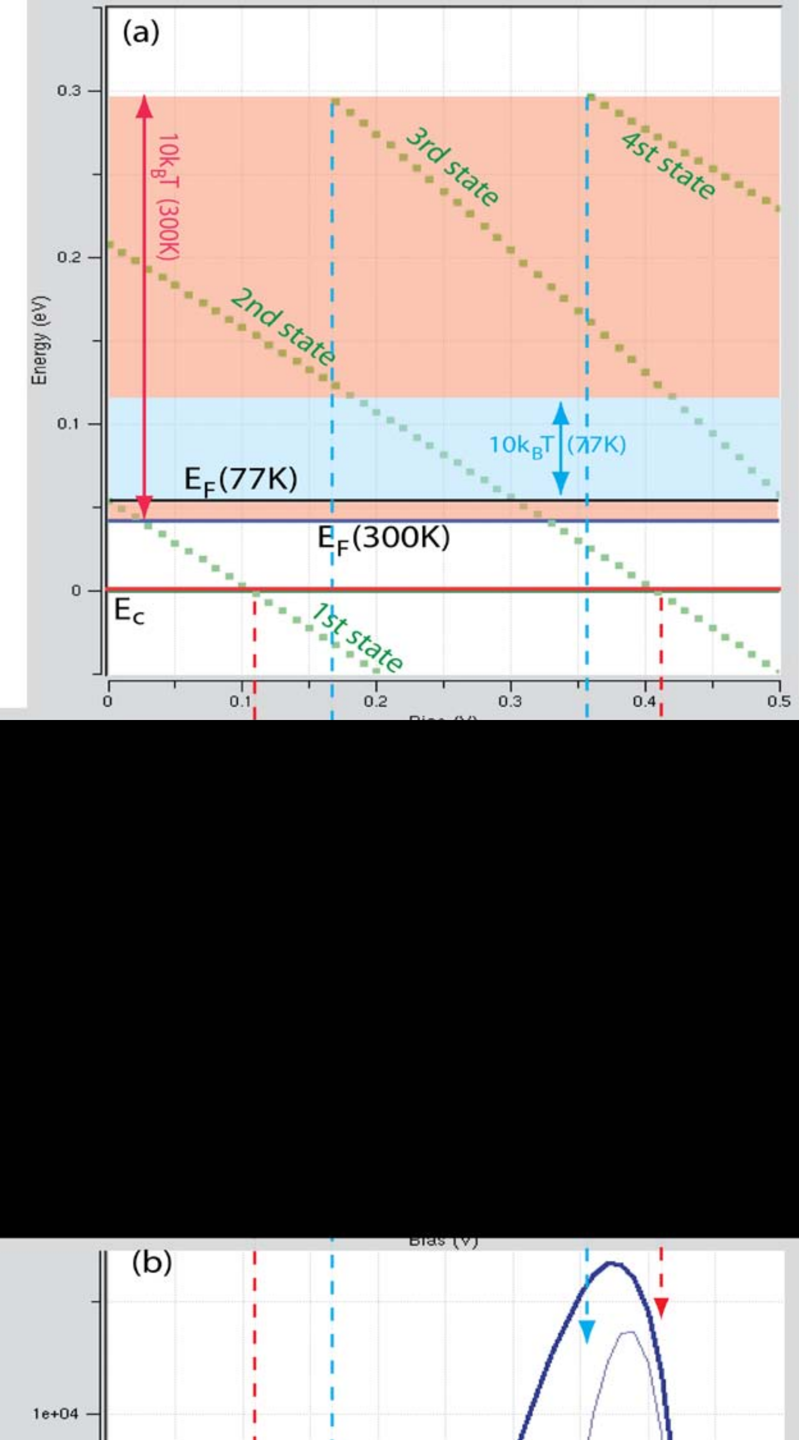


- Resonances drop linearly with Bias



Resonance energy, Fermi-level and conduction band (77K)

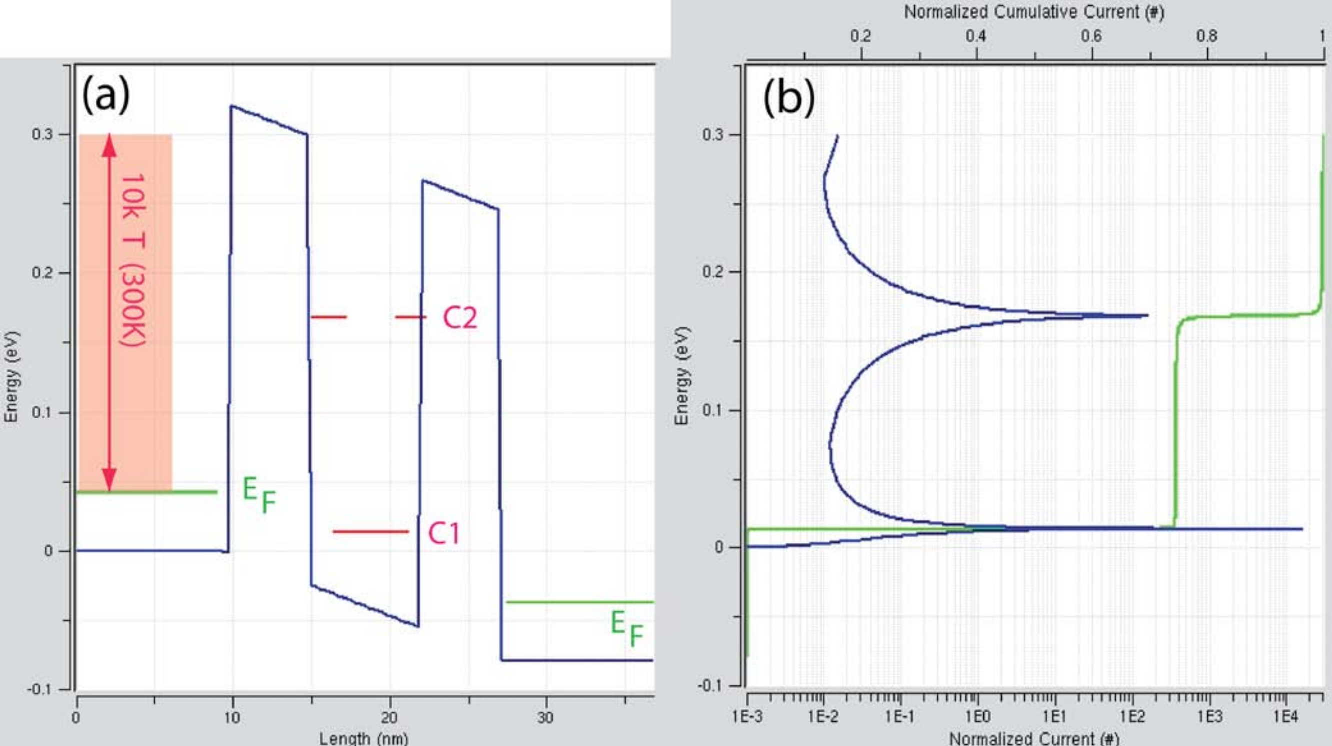
- Current turn-offs are associated with resonances dipping under the conduction band edge (red dashed arrows from (a)).
- Current turn-ons are associated with resonances dipping into the thermally excited sea of electrons 10kBT above the Fermi level (blue dashed arrows from (a)).
- Conduction band edge and electron temperature define energy window of carrier supply.

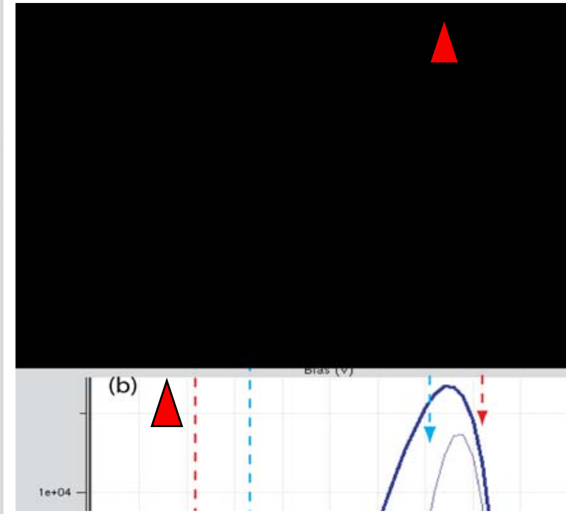


Resonance energy, Fermi-level and conduction band (300K)

- (a) Energies of the 1st, 2nd, 3rd, and 4th state in the RTD.
- The rose shaded field corresponds now to the energy range of 10kBT at 300K.
- (b) Current voltage characteristic at 300K and 77K on a linear scale.
- Resonances number 3 and 4 reach into that energy window.

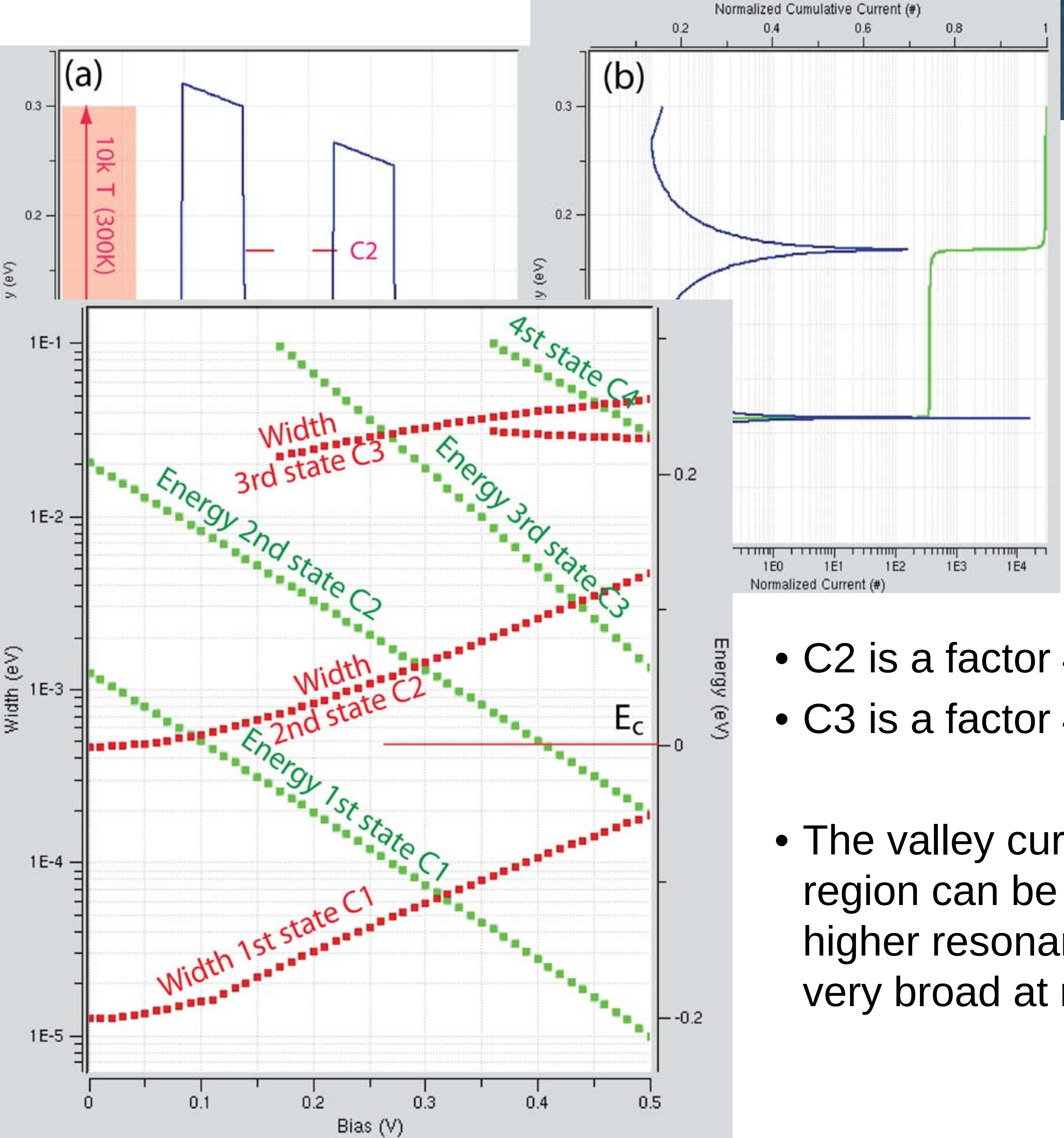
Peak currents





- Bias: 0.08V / 0.38V
- Highly excited states carry significant current densities at biases 0.08V and 0.38V.

Resonance Widths

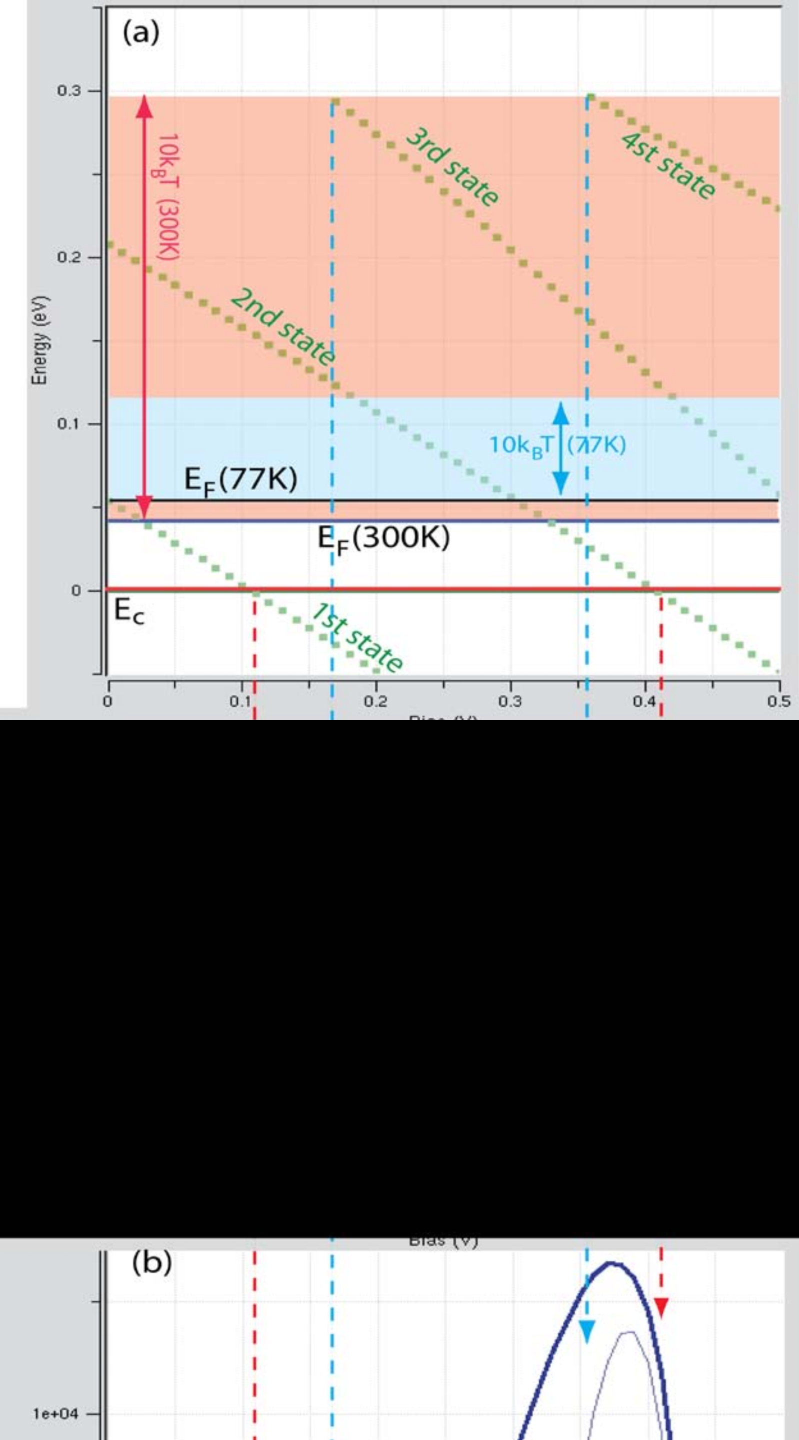


- Resonances have different widths!!!
- Higher energy resonance C2 broader than the lower C1

- C2 is a factor 40 broader than C1
- C3 is a factor 40 broader than C2

- The valley current in the turn-off region can be carried through higher resonance states that are very broad at room temperature.

Broad Excited Resonances Carry a LOT of Current



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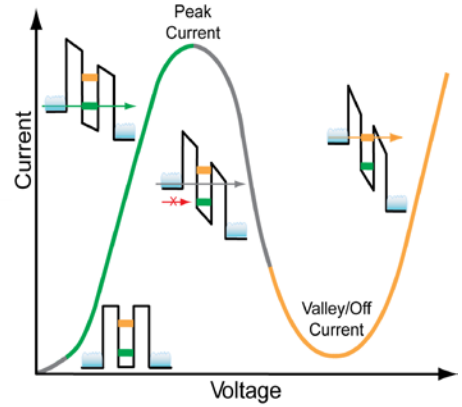
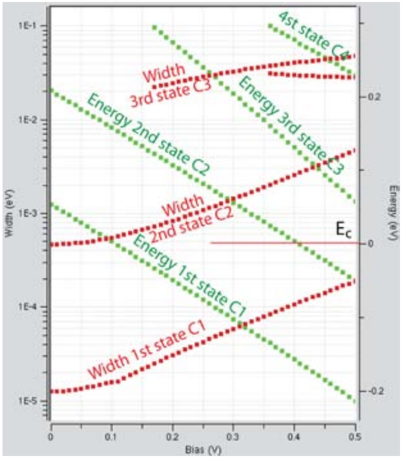
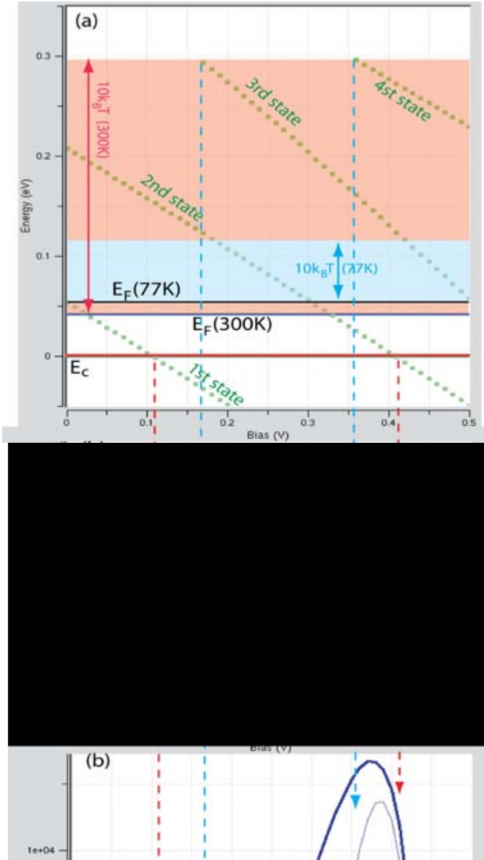
Conclusions

- RTDs can be built in realistic material systems such as GaAs/AlGaAs
- Ideal current-voltage characteristics show an N-shaped behavior of current turn-on and turn off with increasing bias
- The current turns off when a resonance state is pulled under the conduction band of the emitter
- Doping, Fermi-Levels, and temperature determine the relevant energy ranges in which carriers can be injected from the emitter
- Excited states are generally much broader than the ground states – they can carry more current
- The valley current in the turn-off region can be carried through higher resonance states that are very broad at room temperature.



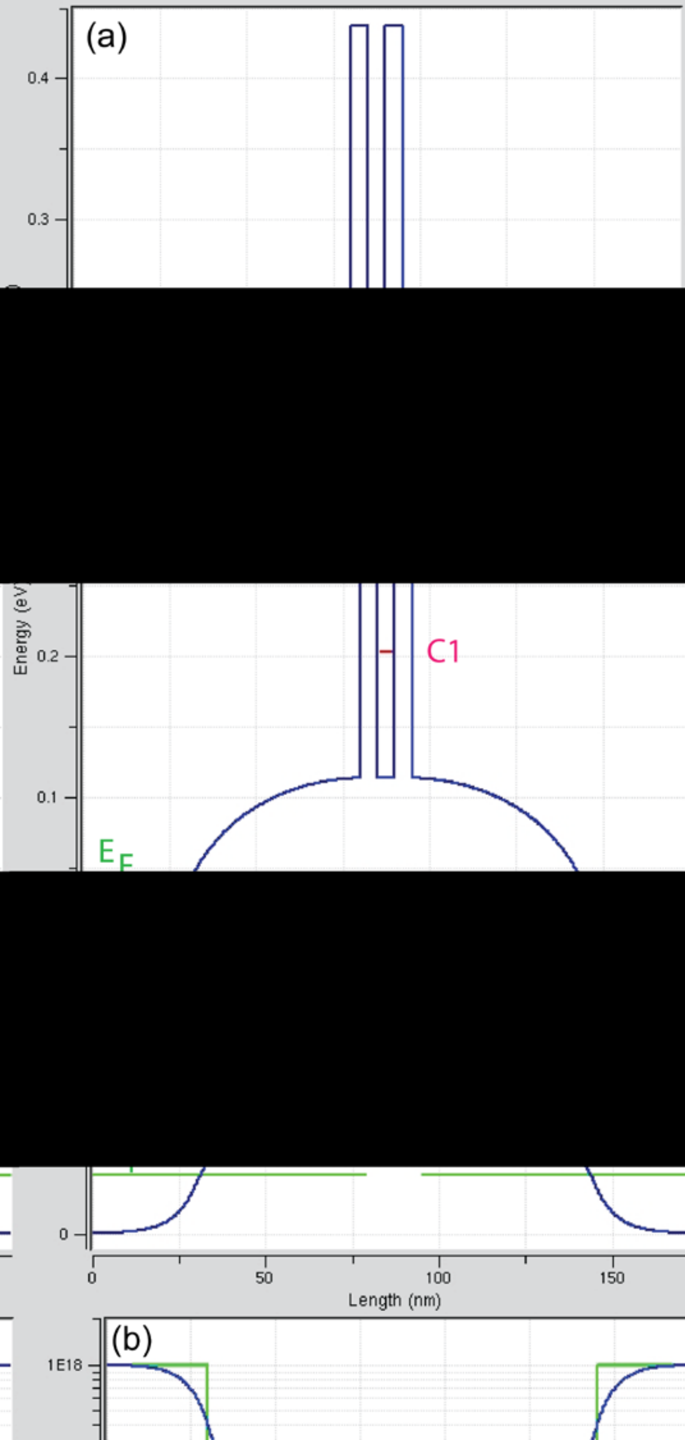




Introduction to RTDs: Realistic Doping Profiles

Gerhard Klimeck

NCN



RTD Conduction band profile with realistic doping profile

- Need extremely high doping for high current densities
- Impurity scattering can destroy the RTD performance

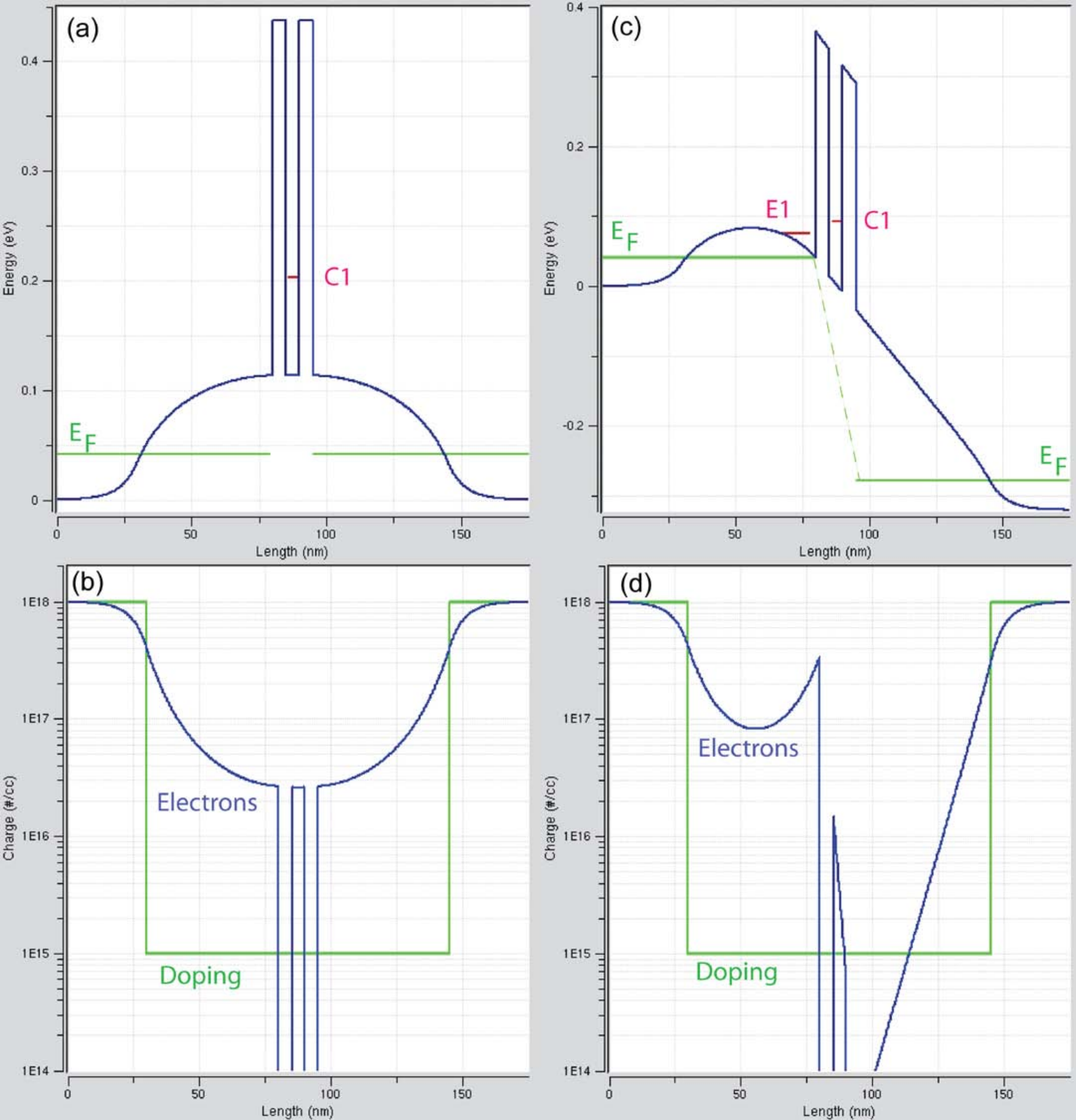
=> undoped spacer 20-100nm

- Electrons diffuse from high density contacts to low density RTD

- Potential floats up to repel the electrons

- Overall RTD is raised above the Fermi levels

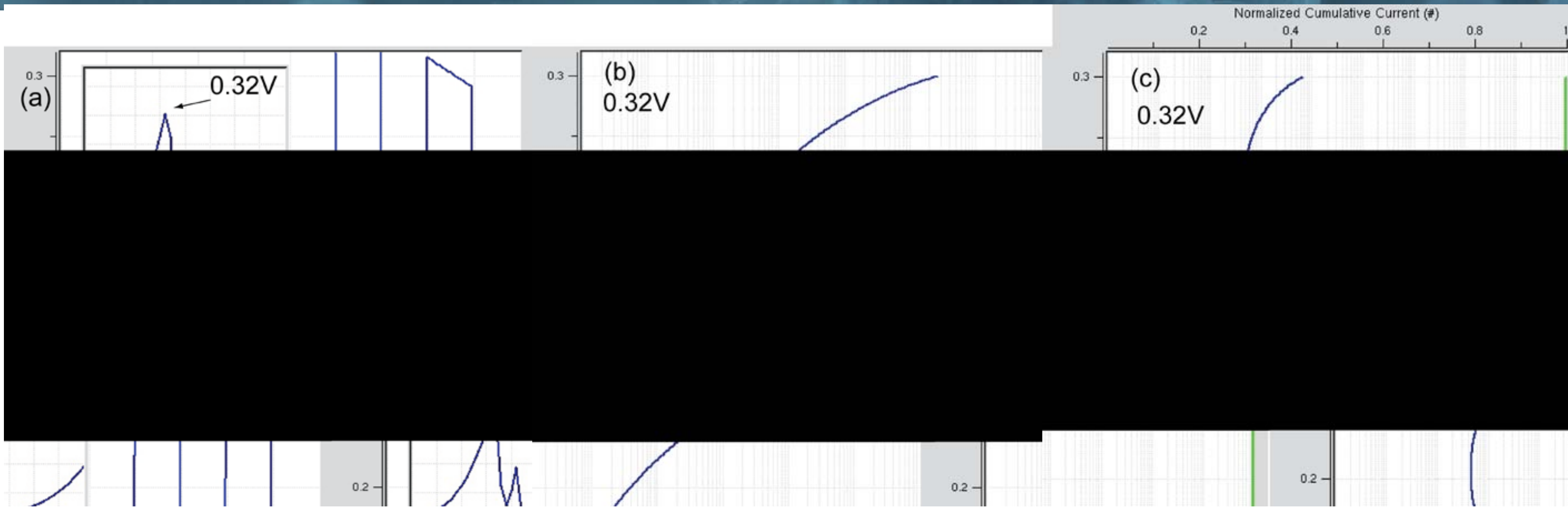
0 and 0.32V bias



Under Bias;

- triangular quantum well in emitter.
- charge build-up against the RTD in emitter
- charge depletion on the collector side.
- charge shows a strong spike which cannot occur in reality due to the wave-nature of the carriers.

Interaction the triangular well states and the central RTD



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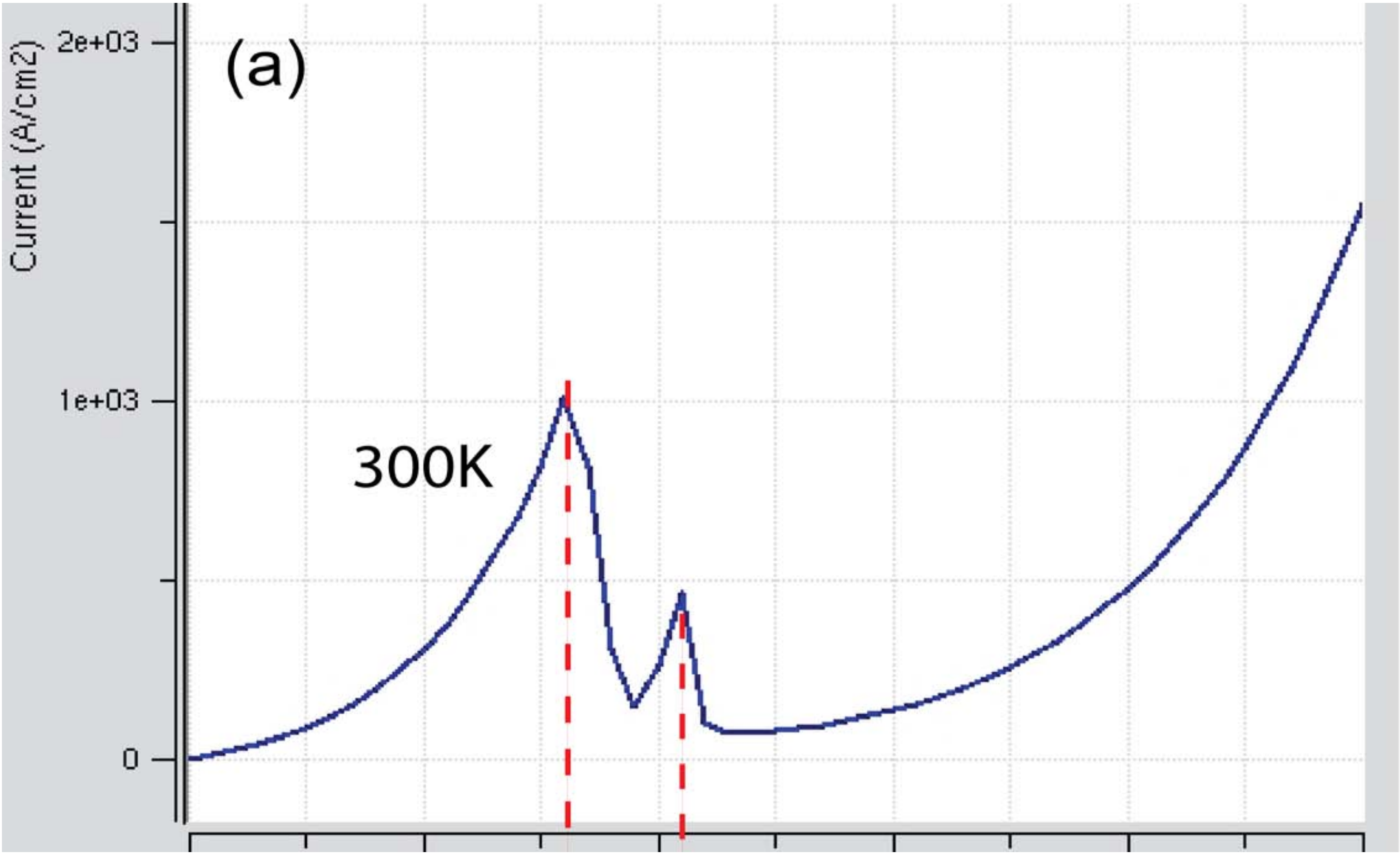
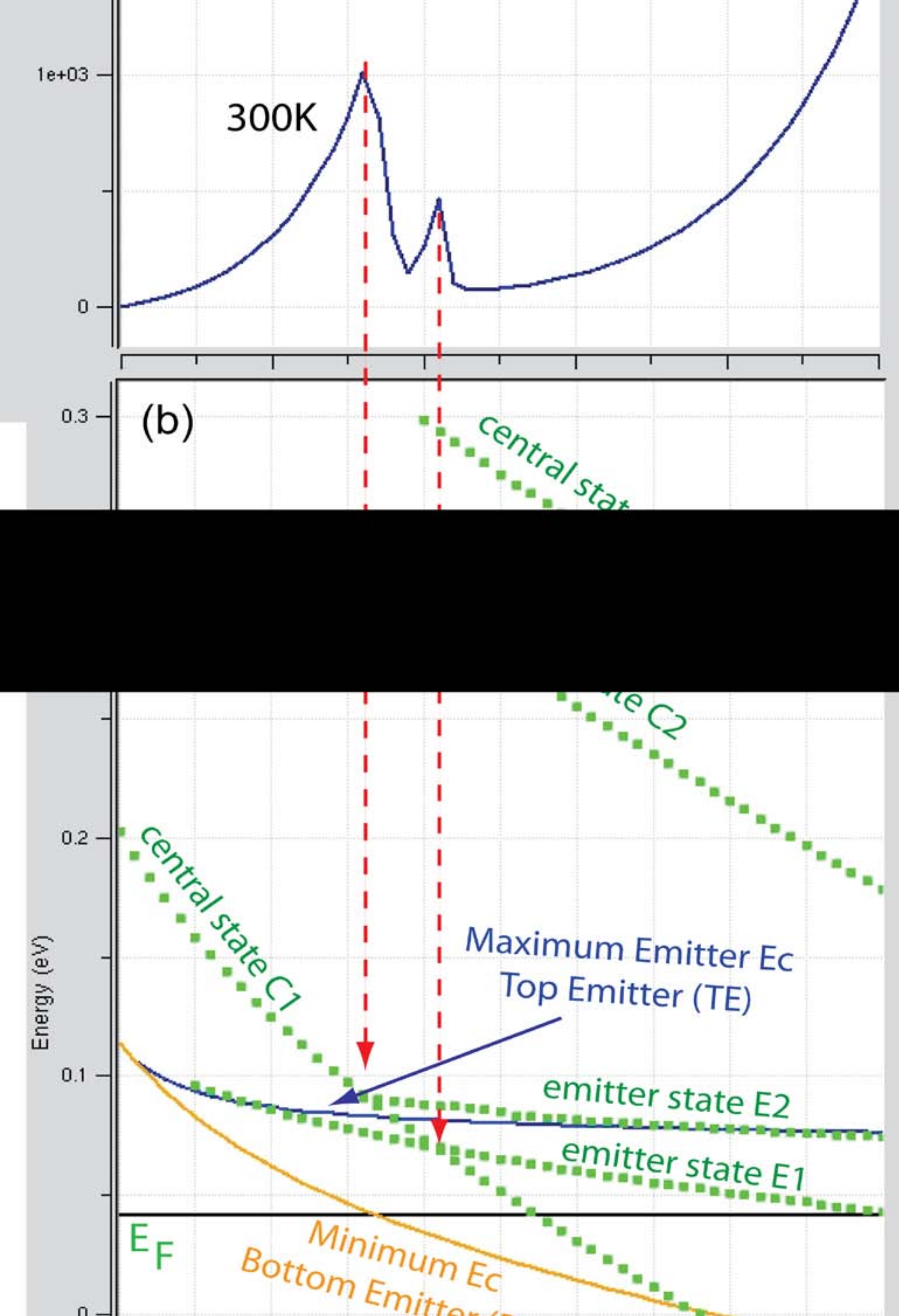
Current-Voltage characteristic

- Multiple peaks are visible.
- Central resonance probes the states in the emitter



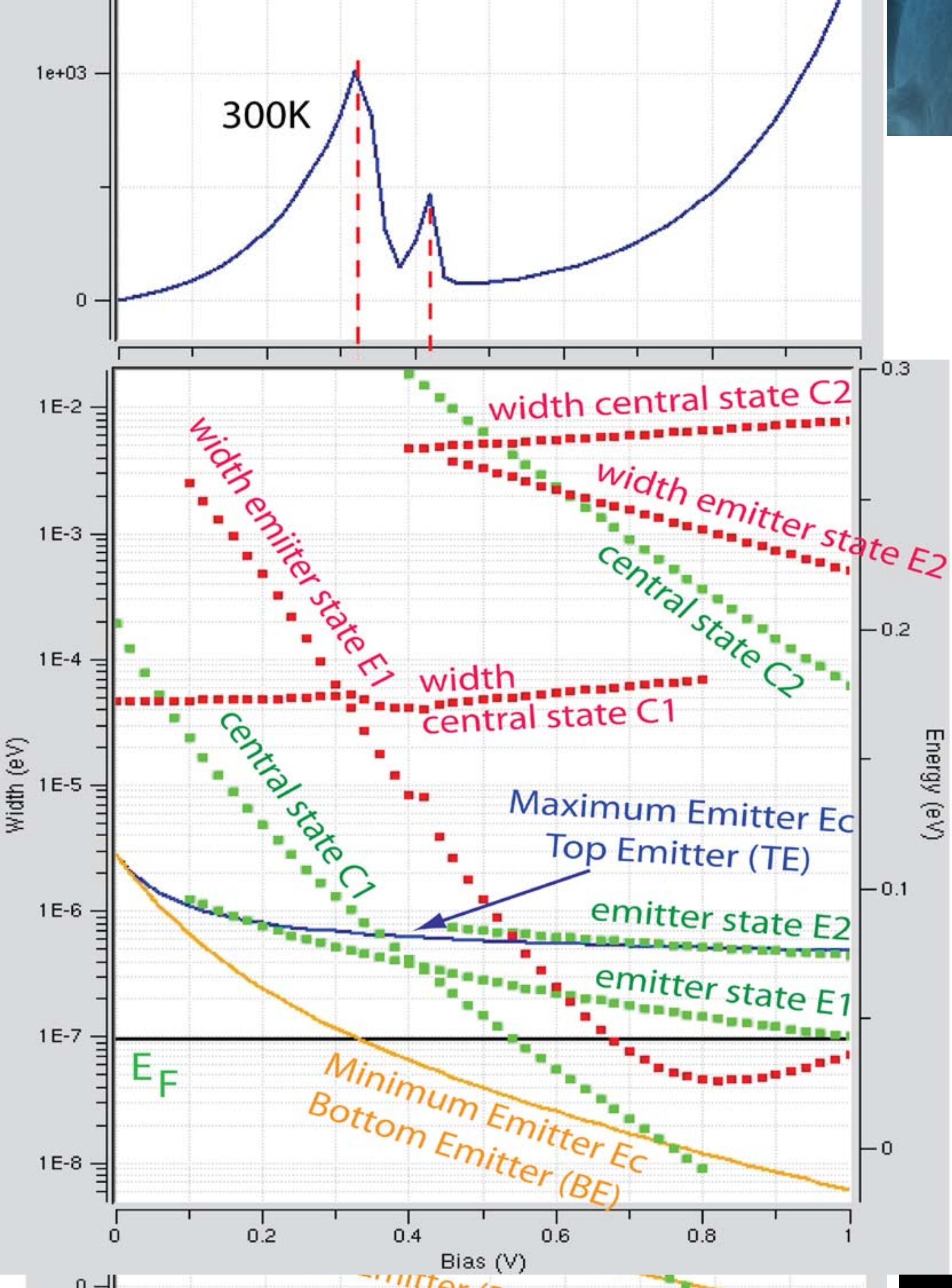
Current-Voltage characteristic and trace of resonance energies



- Multiple peaks are visible.
- Central resonance probes the states in the emitter

[redacted]

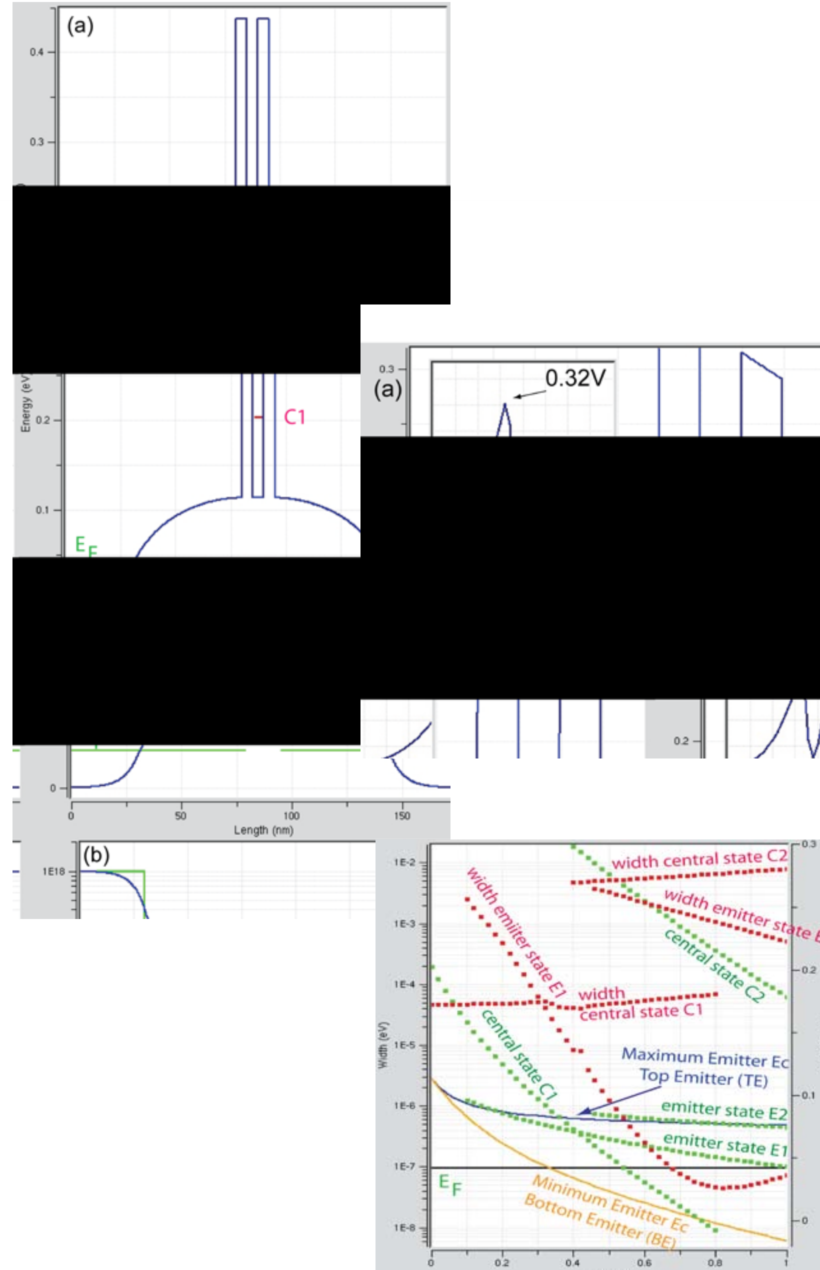
Bias Dependence of Resonance Widths



- Width of C1 ~0.4meV weak bias dependence
- Width of E1 varies exponentially with bias! Can become VERY narrow Truly bound state!

Conclusions

- Realistic RTDs have a non-uniform doping profile that keeps dopants away from the central RTD to avoid ionized impurity scattering
- The non-uniform doping profile results in a non-uniform electrostatic potential profile above the Fermi levels in the high contact regions
- An applied bias causes a potential drop not only in the central RTD region but also in parts of the emitter. That potential drop in the emitter creates a triangular potential well.
- The tri-angular potential well in the emitter binds quantum mechanical states which can interact with the central RTD states.
- The quasi-bound emitter states resonance widths vary exponentially with the applied bias and can become extremely narrow.



Introduction to RTDs: Relaxation Scattering in the Emitter

Gerhard Klimeck

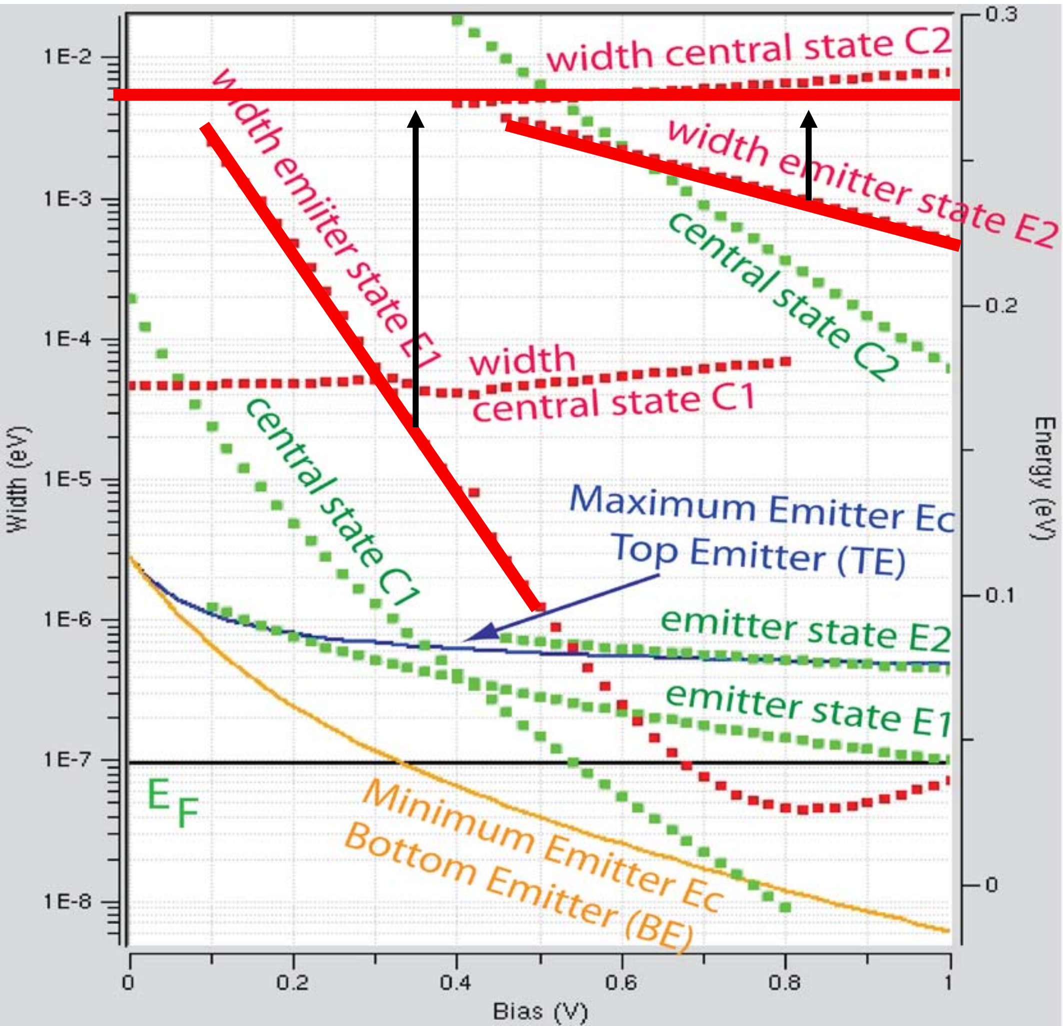
NCN

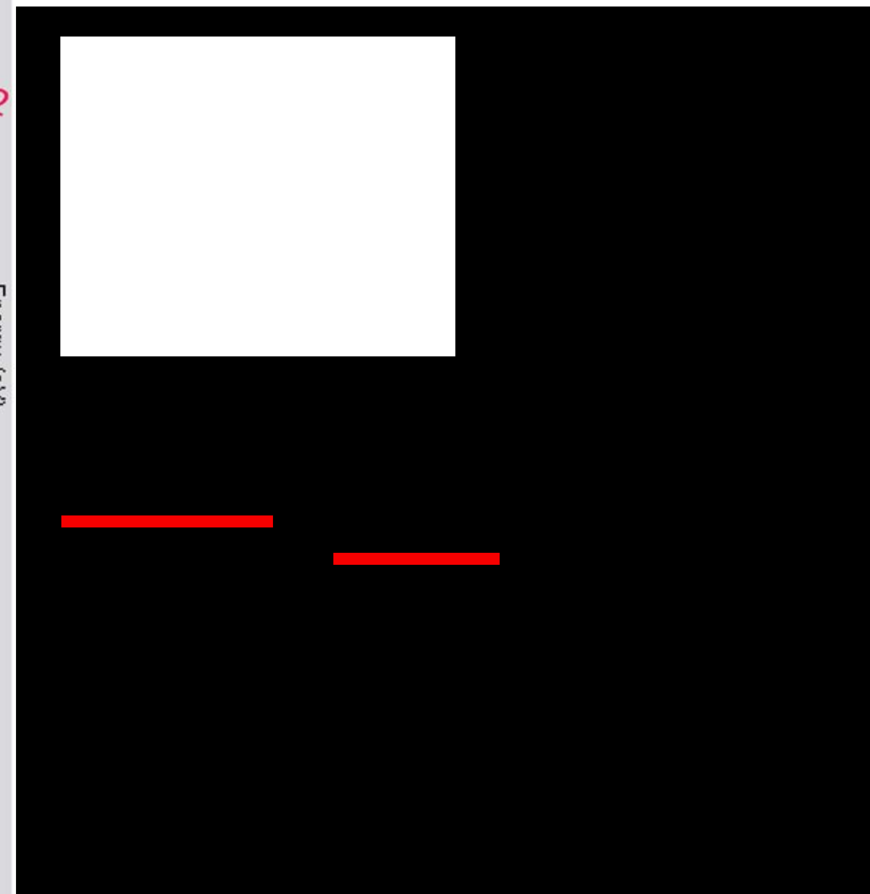
Resonance Widths / Lifetimes in the Emitter

- Width of E1 varies exponentially with bias!   => truly bound state!
- Electron sheet density in the emitter is 10^{10}-10^{12}/cm^2
  => strong electron-electron and electron-phonon scattering
  => state is broadened

$$\tau = 0.1 ps$$

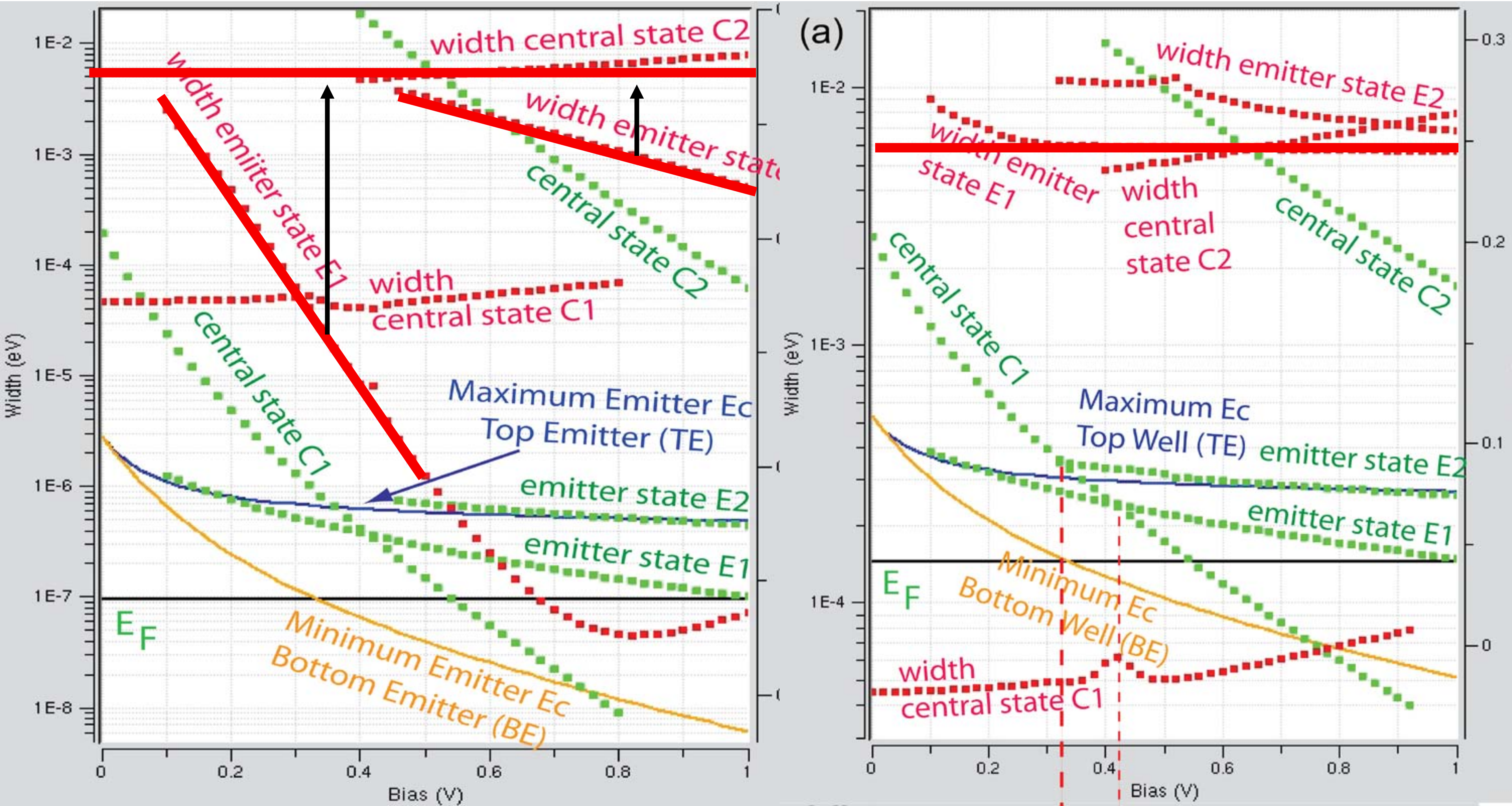
$$\Gamma = \hbar / 2\tau = 6.6 meV$$



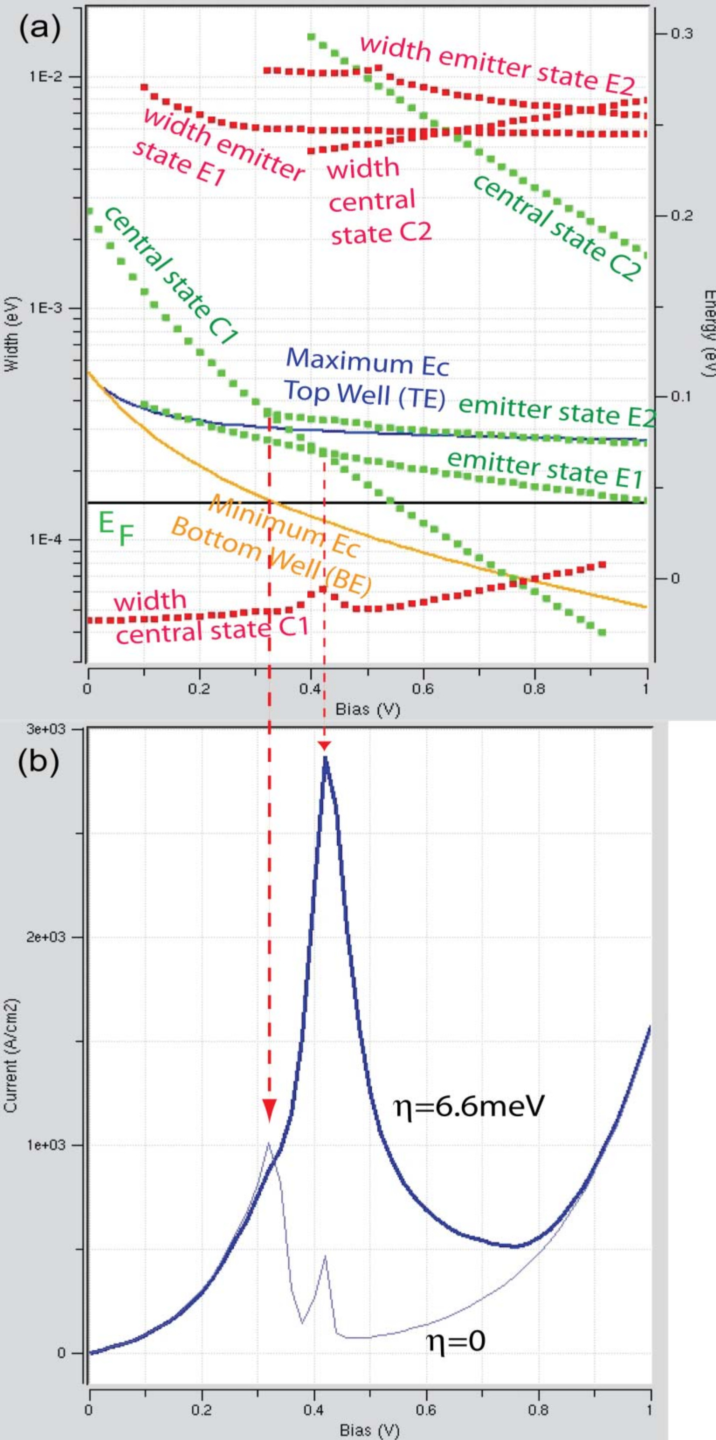


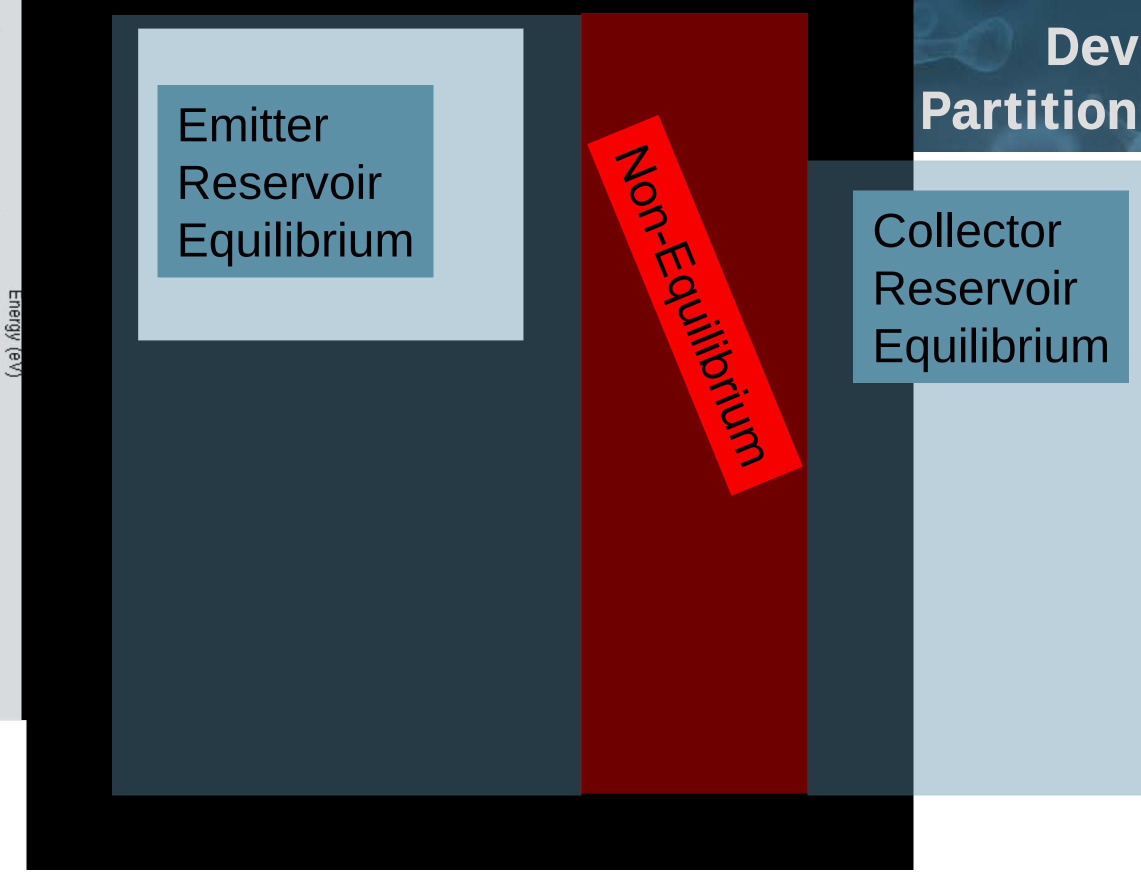
Relaxation in the Emitter - *η=6.6meV*

- NEMO [APL94] introduced the relaxation in the reservoirs $\eta = \hbar / 2\tau = 6.6meV$
- Mimics the broadening through scattering
- Critical item in the understanding of RTD transport



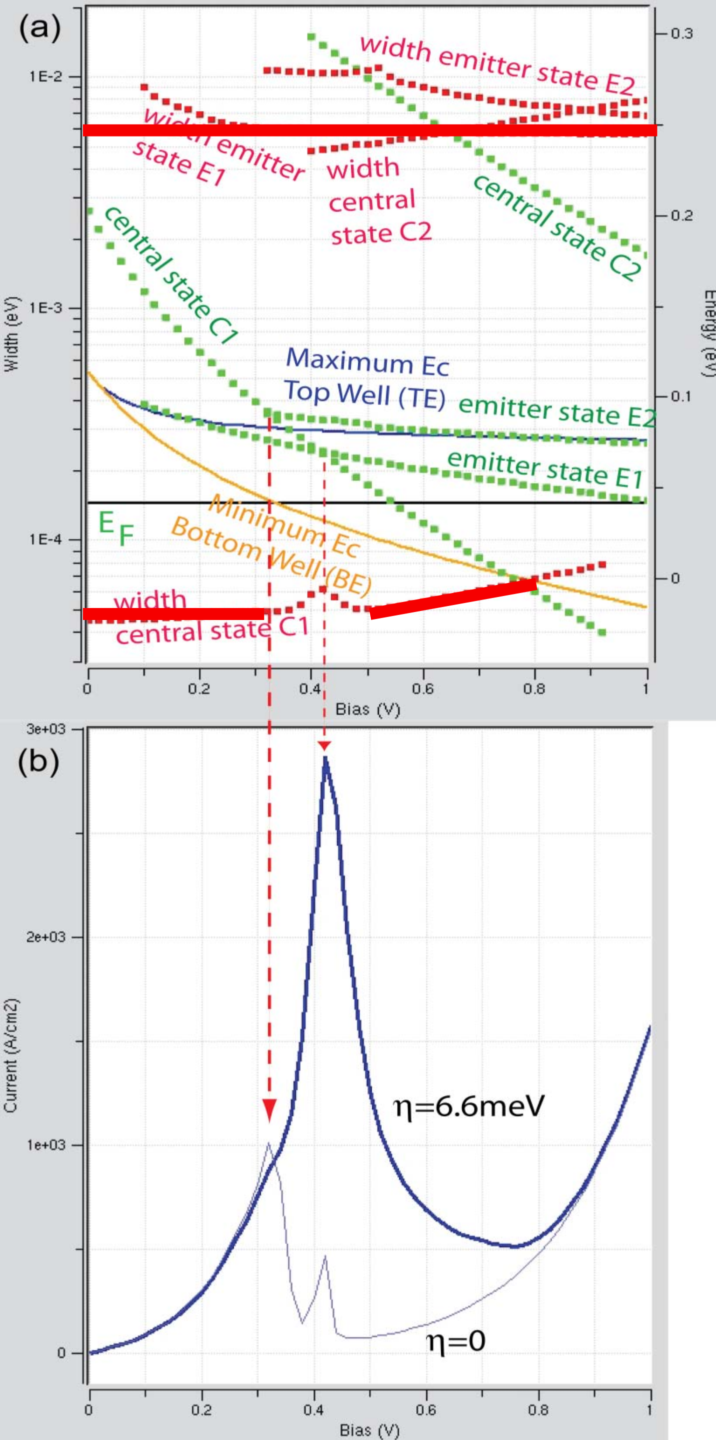
Device Partitioning

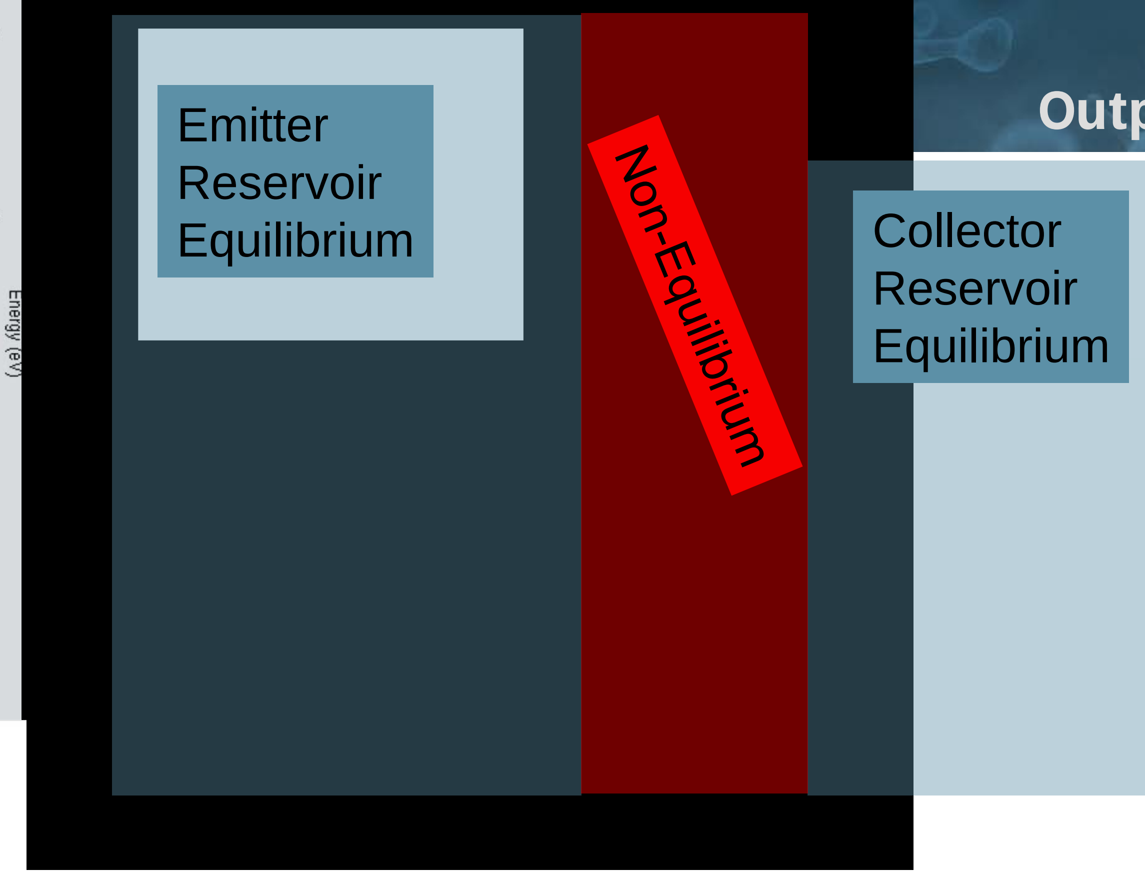




- Emitter and collector ASSUMED to be in equilibrium
  => Reservoirs => STRONG scattering
- iη=i 6.6meV is added to Hamiltonian in reservoirs
  => non-Hermitian
  => current not conserved AND NOT computed
  => only compute equilibrium charge
- Central device region treated with NEGF
  => non-equilibrium charge and current

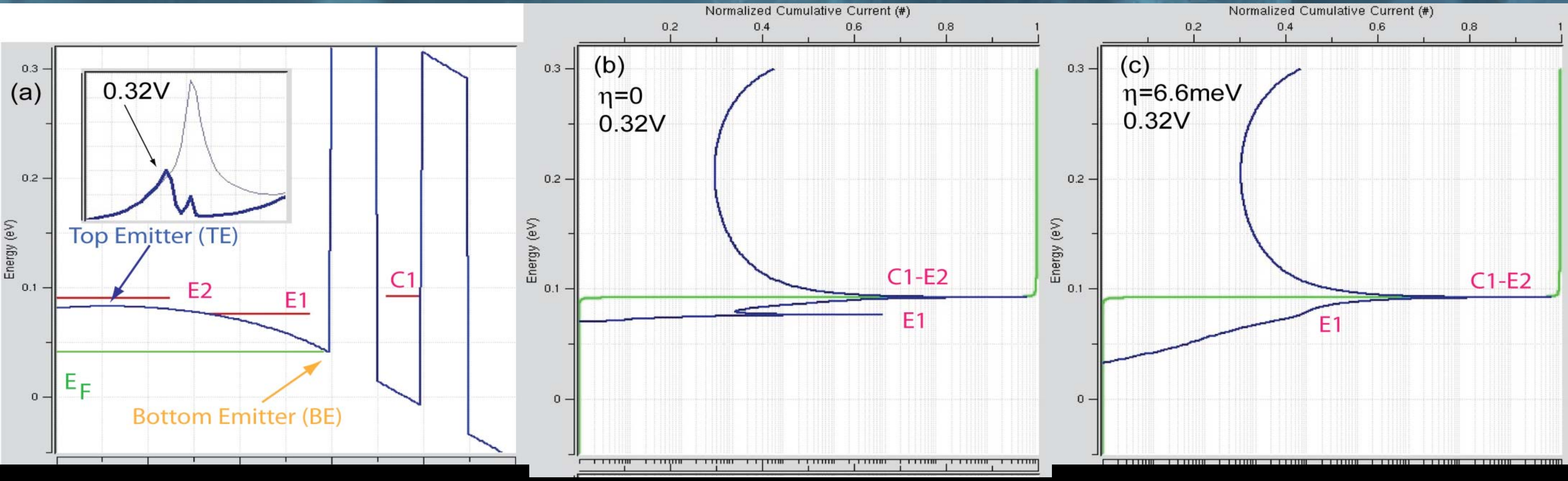
I-V Output

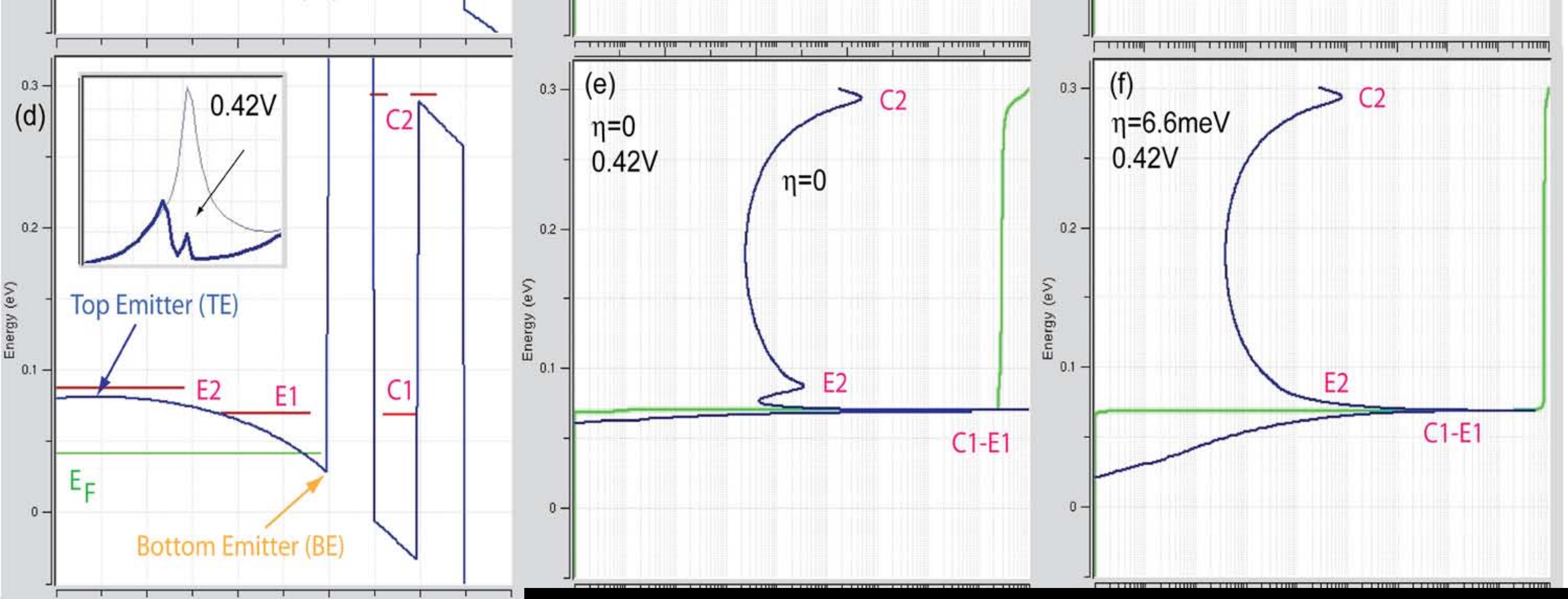




- Central resonance C1 almost unaffected
- Emitter resonances E1 significantly broadened >6.6meV
- The relatively narrow central resonance is probing the states in the emitter
- Overall current increases

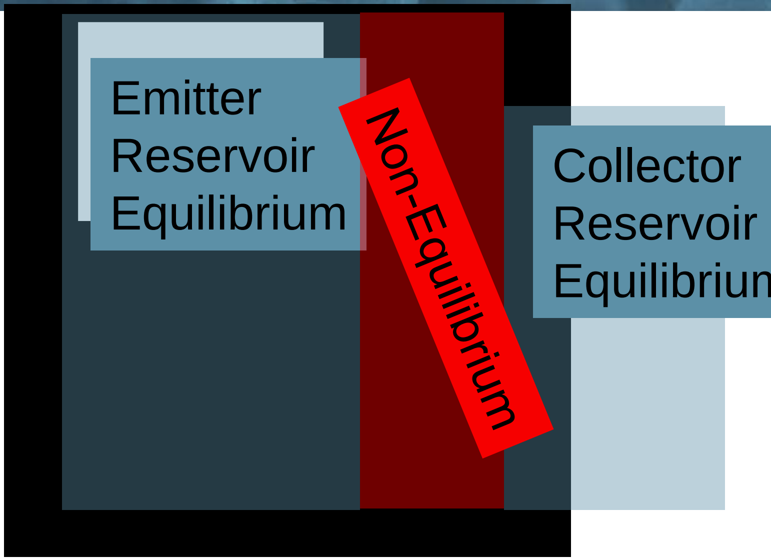
Conduction band edge, transmission, and current density



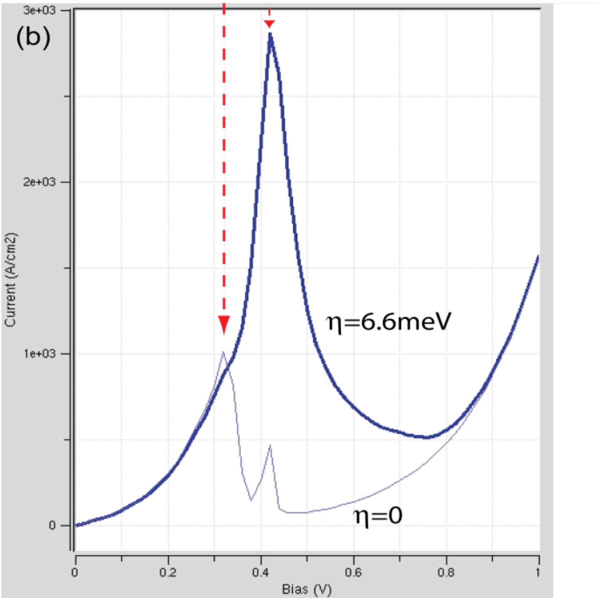


(d)
0.42V
Top Emitter (TE)
E2
E1
C1
C2
E_F
Bottom Emitter (BE)
Energy (eV)
0.3
0.2
0.1
0
(e)
η=0
0.42V
η=0
C2
E2
C1-E1
Energy (eV)
(f)
η=6.6meV
0.42V
C2
E2
C1-E1
Energy (eV)

Conclusions



- Realistic doping profiles
  => triangular quantum wells in the emitter.
  => confined states in the emitter
  very long lifetime / very narrow states in the mathematically ideal case
- High electron density in the emitter, Equilibirum conditions!
  => strong equilibrating scattering
  => states are broadened
- NEMO introduced an empirical broadening model
  - » Partition the device into reservoirs and NEGF region
  - » Reservoirs are non-Hermitian – compute charge only
  - » Central NEGF region sees effects of thermalized states
- For typical high performance InGaAs/InAlAs RTDs: set the relaxation to η=*6.6meV*
  => scattering time of about t=0.1ps.
- The relaxation rate should not be used to match experimental data on a one-time basis.

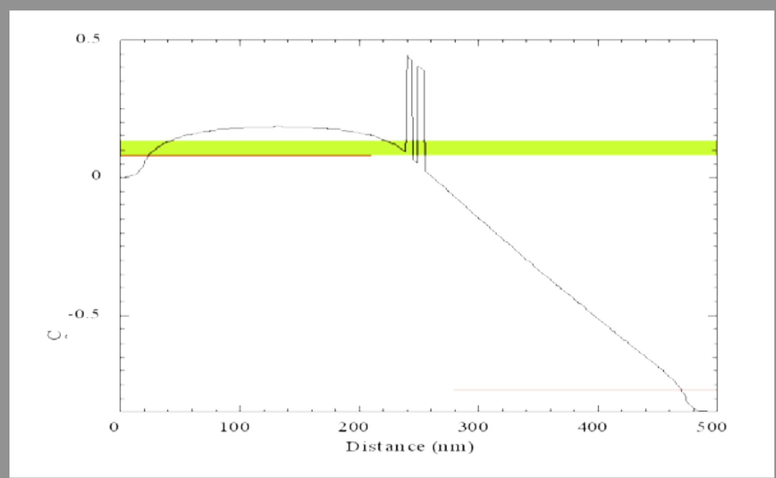


NEMO1D:
Full Bandstructure Effects
(quantitative RTD modeling at room temperature)

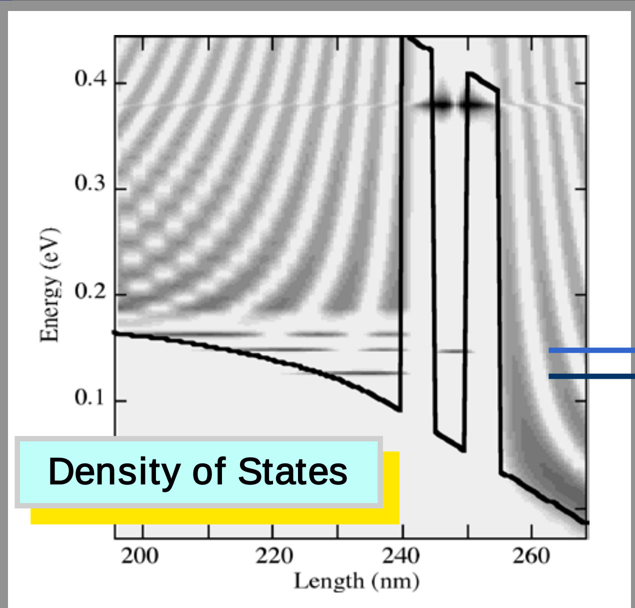
NCN

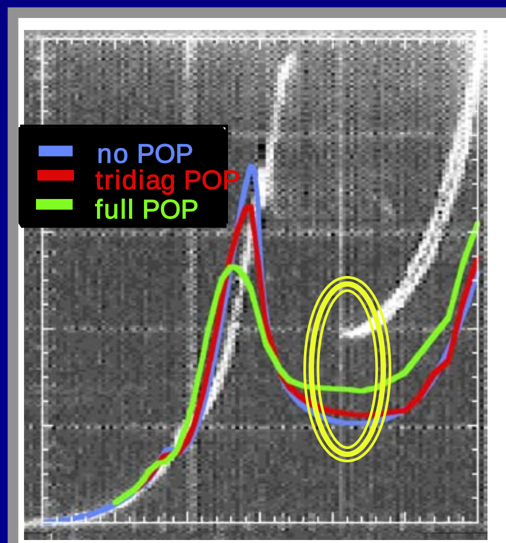
Gerhard Klimeck

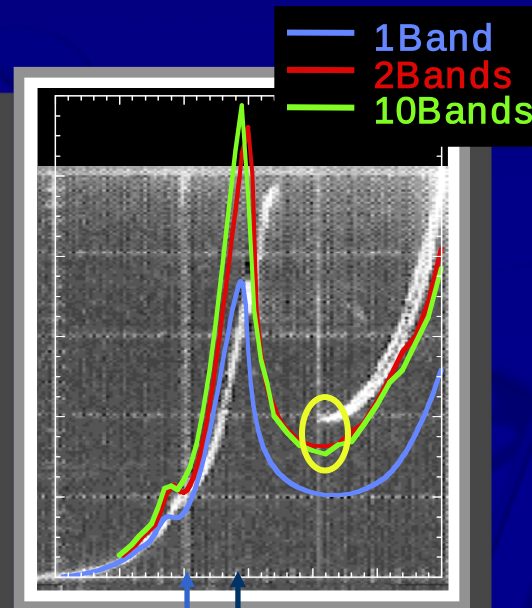
Where Does The Valley Current Come From? Bandstructure

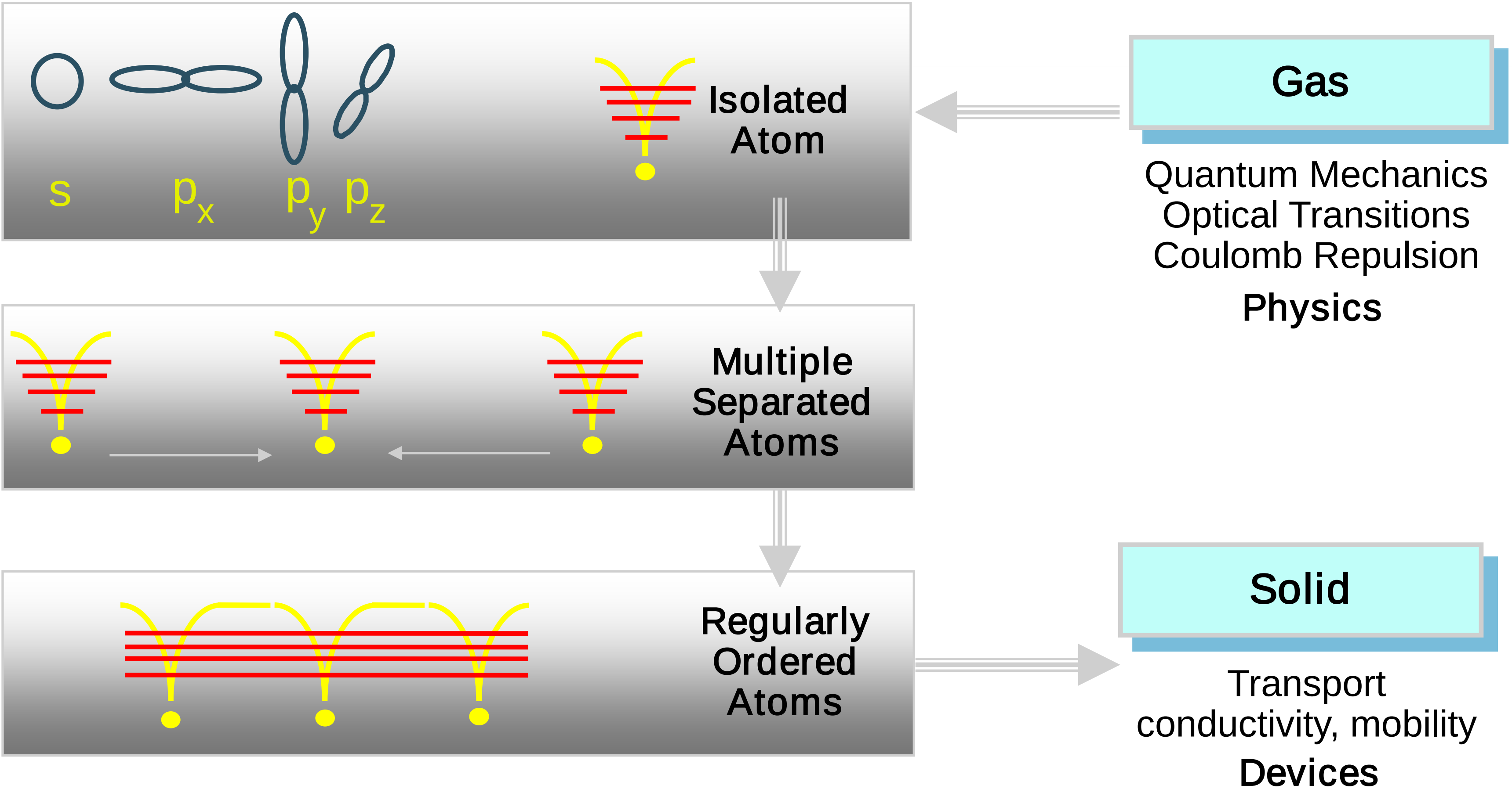


20 nm GaAs $N_D = 2\ 10^{18}\ cm^{-3}$
200 nm GaAs $N_D = 2\ 10^{15}\ cm^{-3}$
18 nm GaAs
5 nm $Al_{0.4}Ga_{0.6}As$
5 nm GaAs
5 nm $Al_{0.4}Ga_{0.6}As$
18 nm GaAs
200 nm GaAs $N_D = 2\ 10^{15}\ cm^{-3}$
20 nm GaAs $N_D = 2\ 10^{18}\ cm^{-3}$

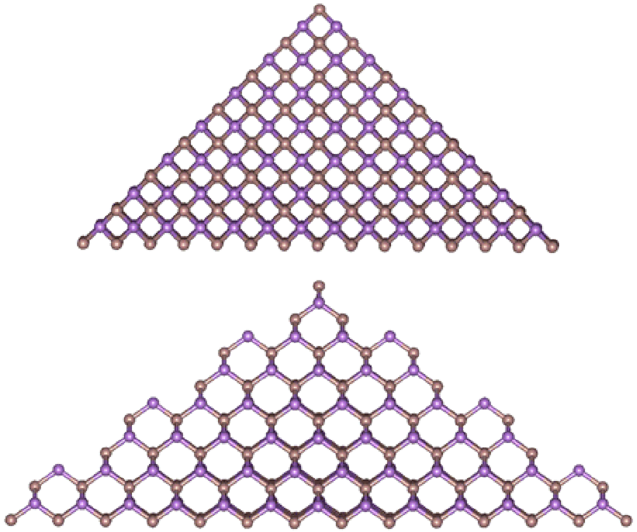


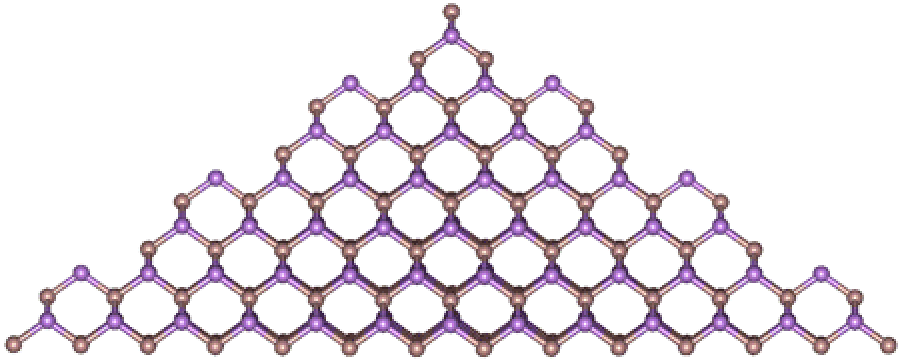




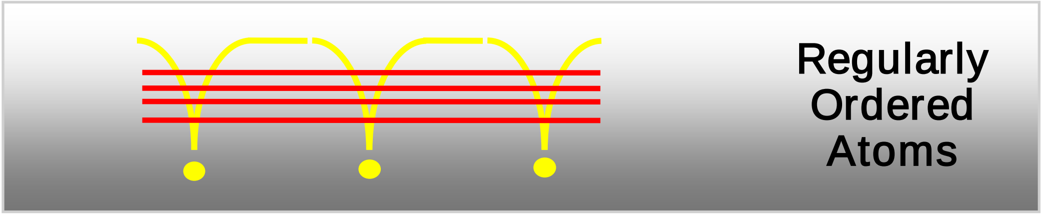


- Bands are channels in which electrons move “freely”.





- Crystal is not symmetric in all directions!



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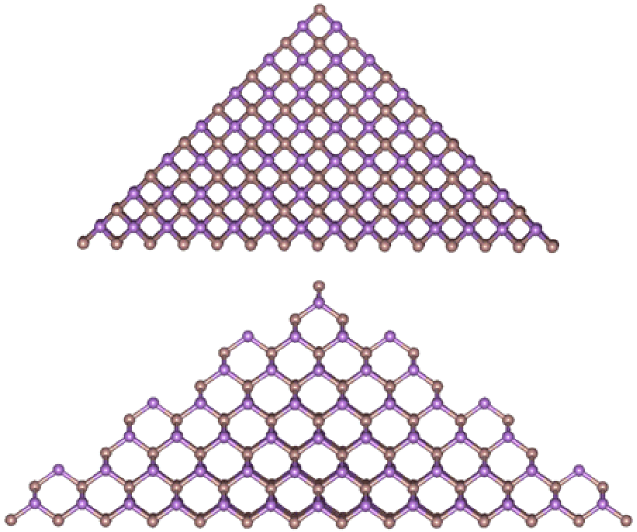
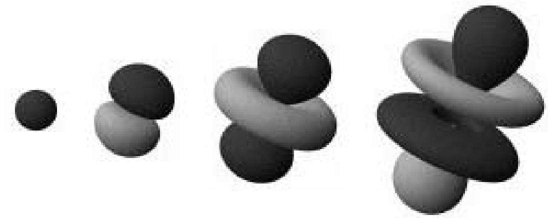
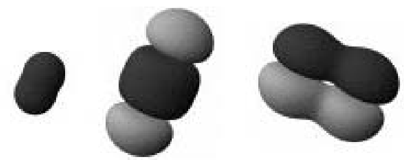
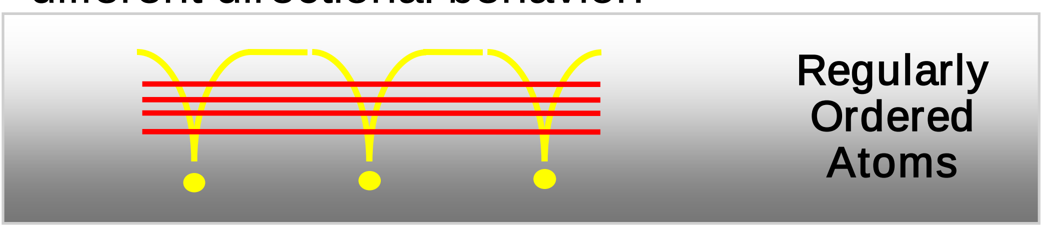






- Crystal is not symmetric in all directions!
- Orbitals on each atom give electrons different directional behavior!



Schrödinger Eq.

$$H\Psi = E\Psi$$

Ansatz: Plane Waves

$$\Psi \propto e^{ikr}$$

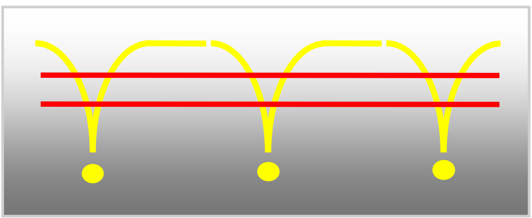
$$E = fct(k)$$

- Bands are channels in which electrons move “freely”.
- **What does “free” propagation really mean?**

Full Bandstructure vs. Parabolic Bands

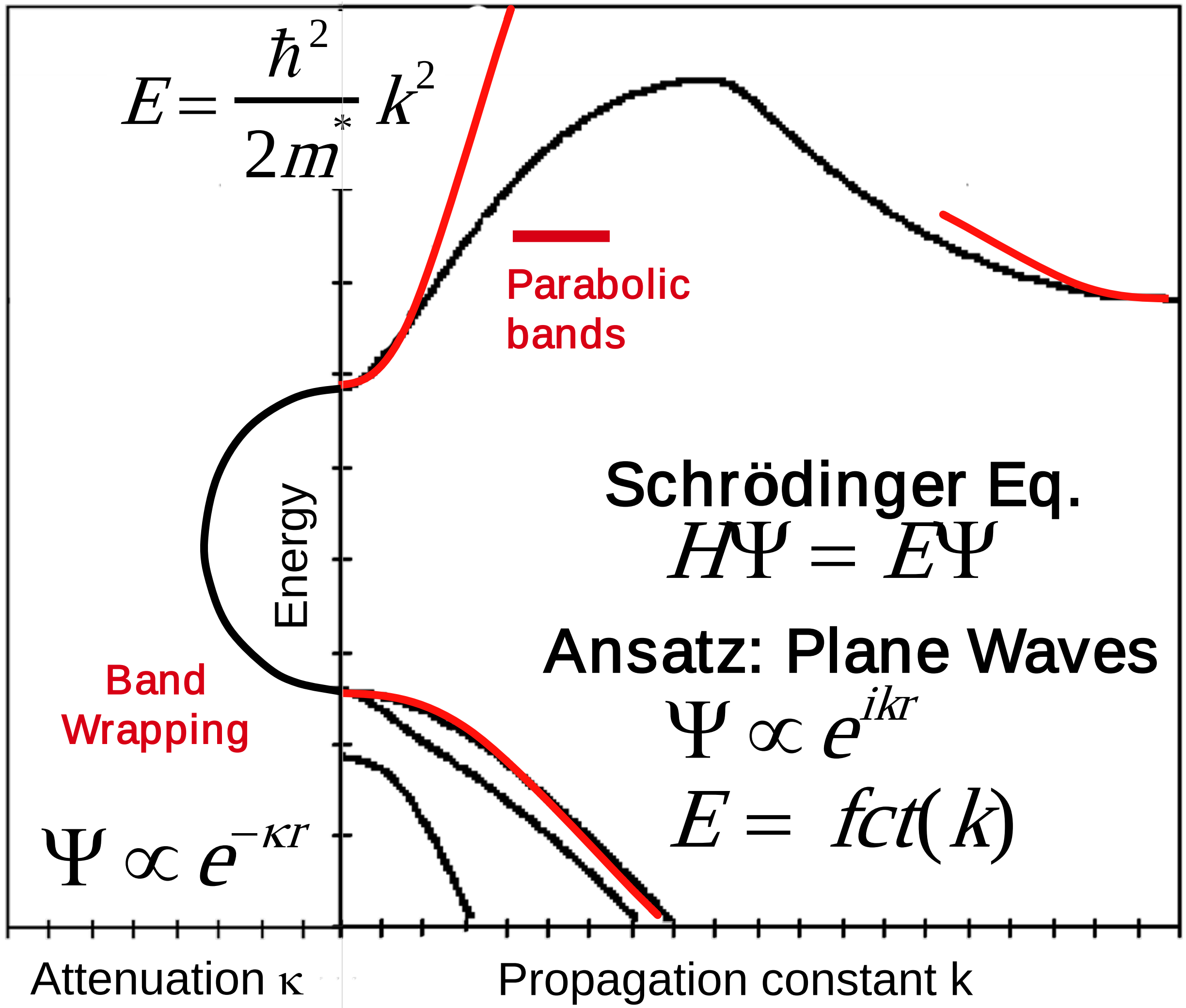
Realistic Material Properties:
- Non-parabolic cond. band
- States outside Γ at X, L
- Non-trivial valence band
- Coupled bands

Typical Assumption:
- Decoupled bands
- Parabolic bands



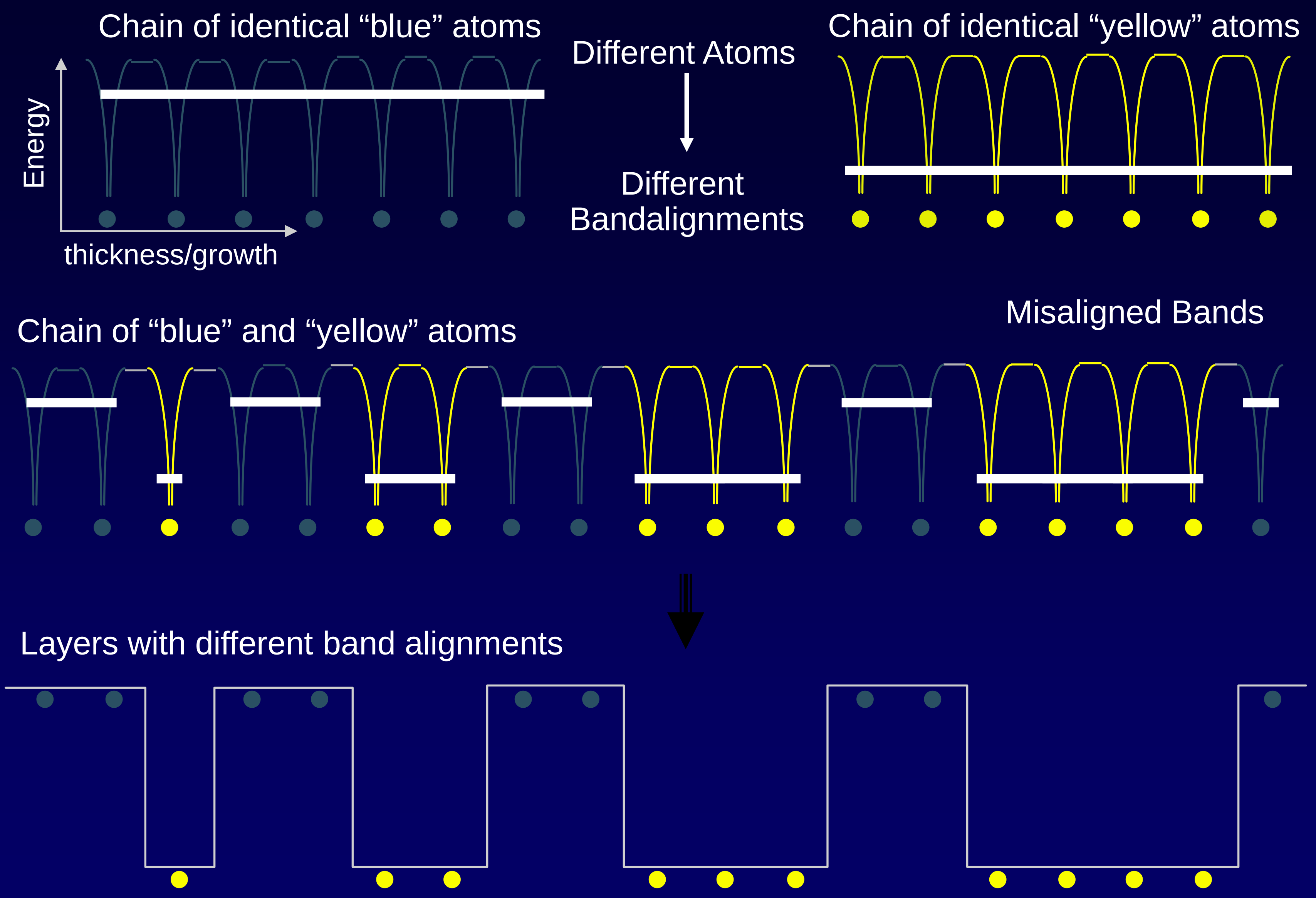
Well-Established:
- Ec, m* describes it all
  $\mu = \mu_0 \, \tau/m^*$
- Drift diffusion simulators
- Boltzmann Transport sim.
- Quantum transport sim.

Will Fail:
- Bands are coupled
- Material variations on nm-scale

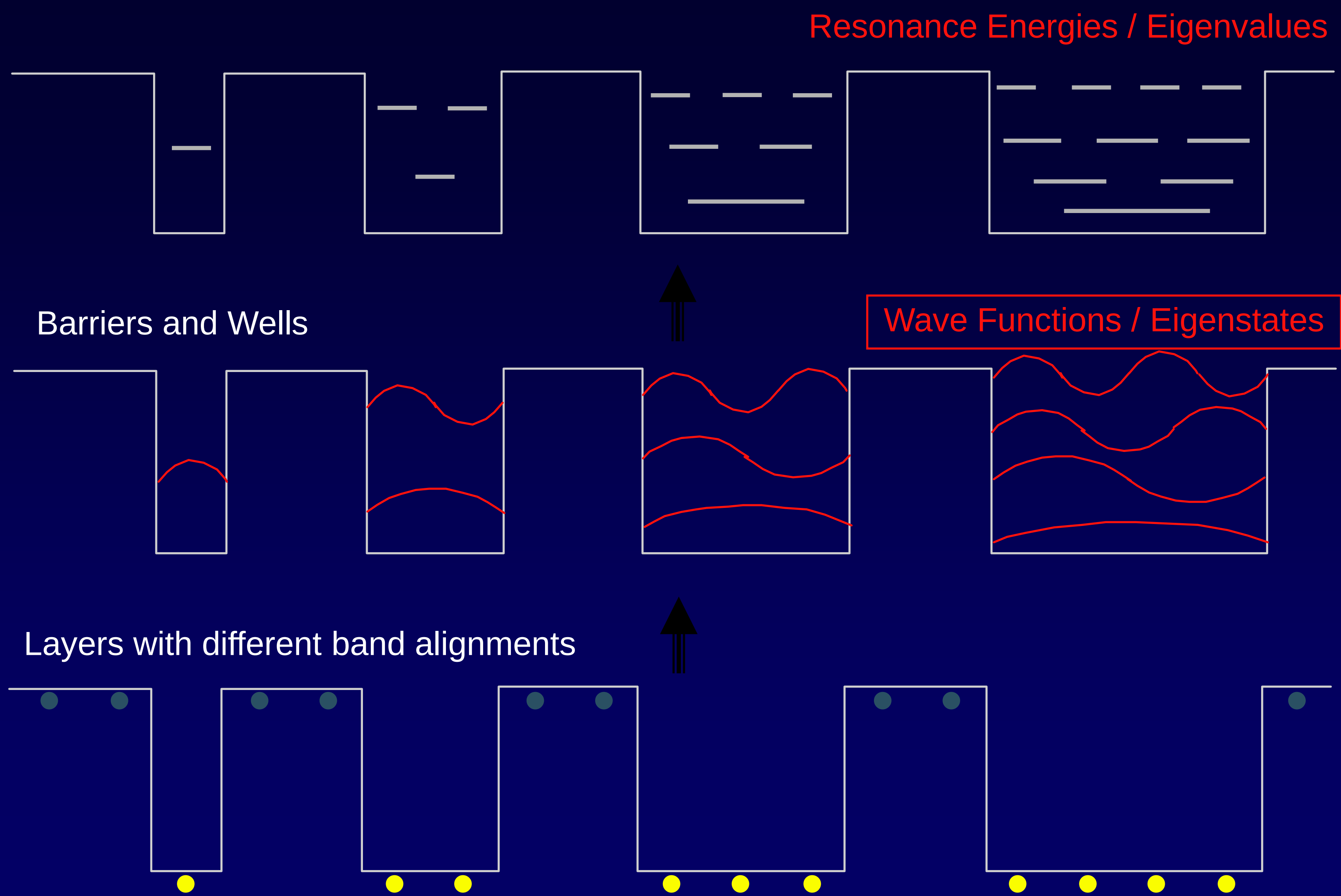


Bandstructure Engineering Basics

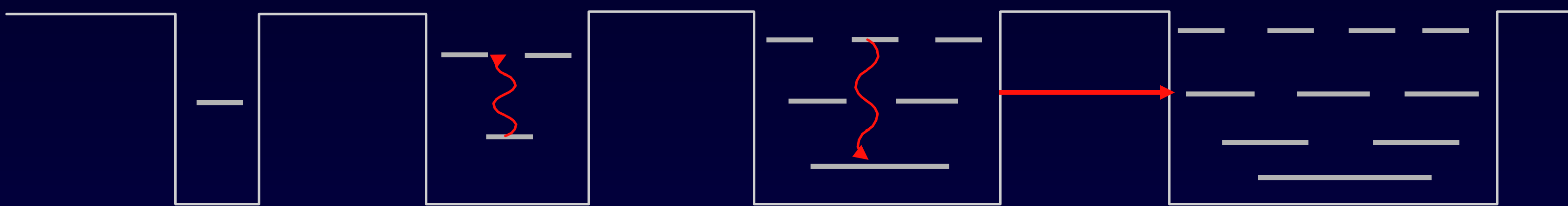
(page 1 of 2)



Bandstructure Engineering Basics
(page 2 of 2)



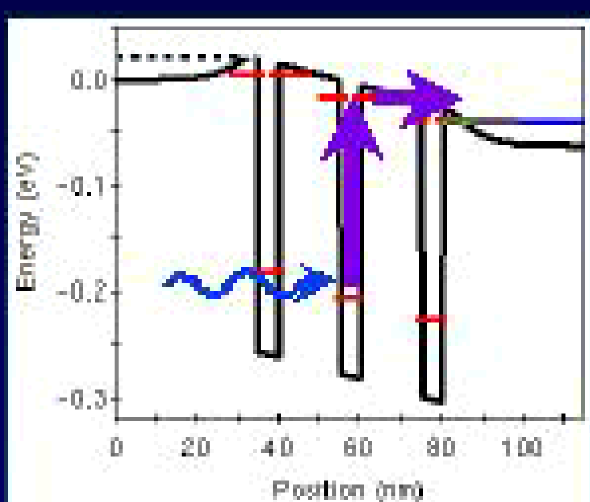
Transitions / Transport Controlled by Design
A Plethora of Capabilities



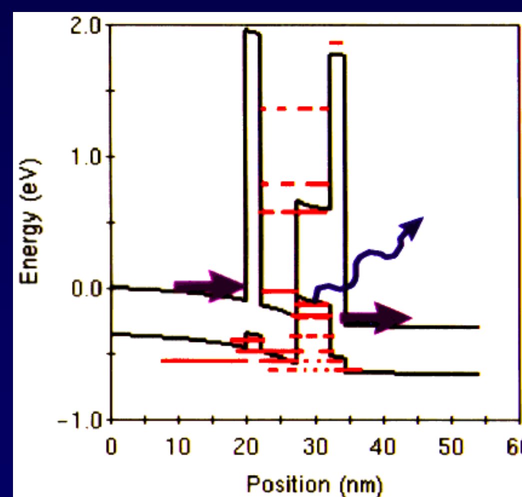
Photon Absorption → Detectors

Photon Emission → Lasers

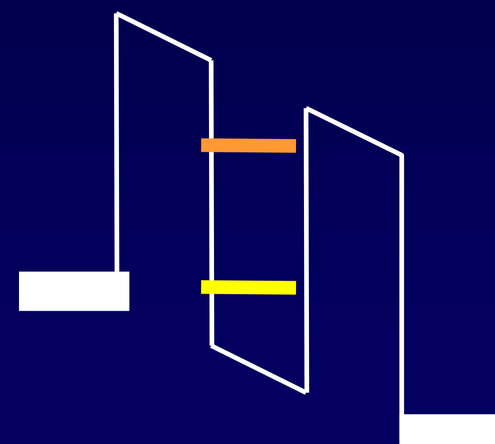
Tunneling → Logic / Memory



Quantum Well Infrared Detector



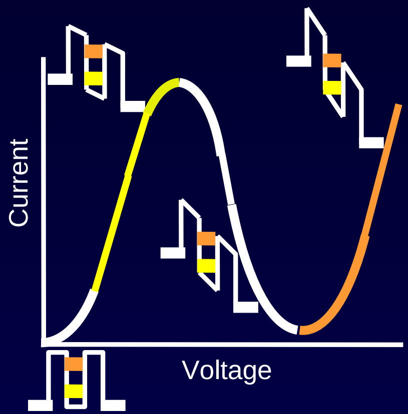
Quantum Cascade Laser



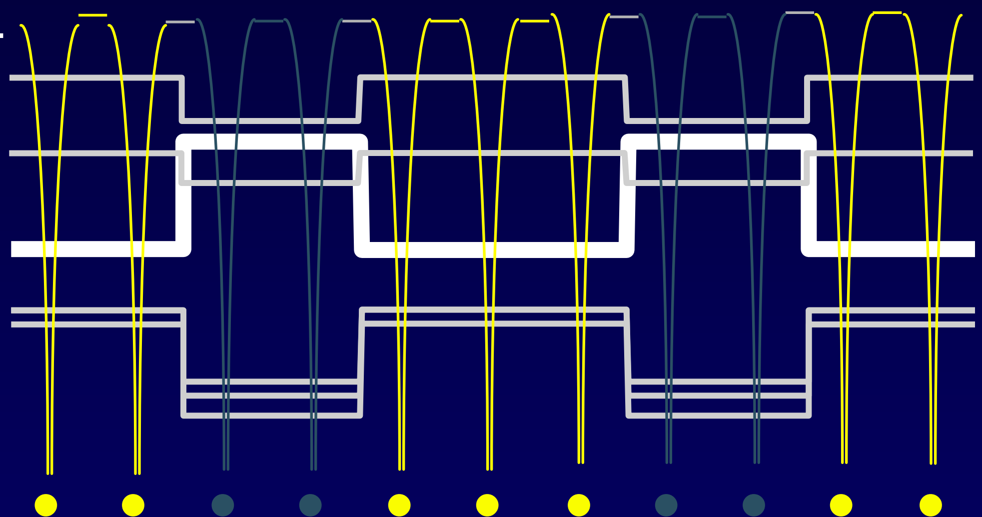
Resonant Tunneling Diode

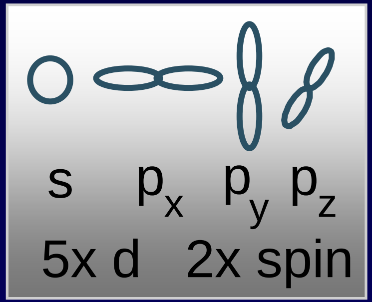
NEMO 1-D Resonant Tunneling Diode Simulation
Atomistic Representation is the Key!

Atomistic Basis Sets



Concepts

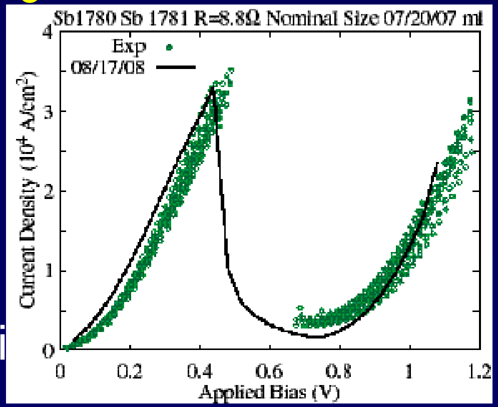




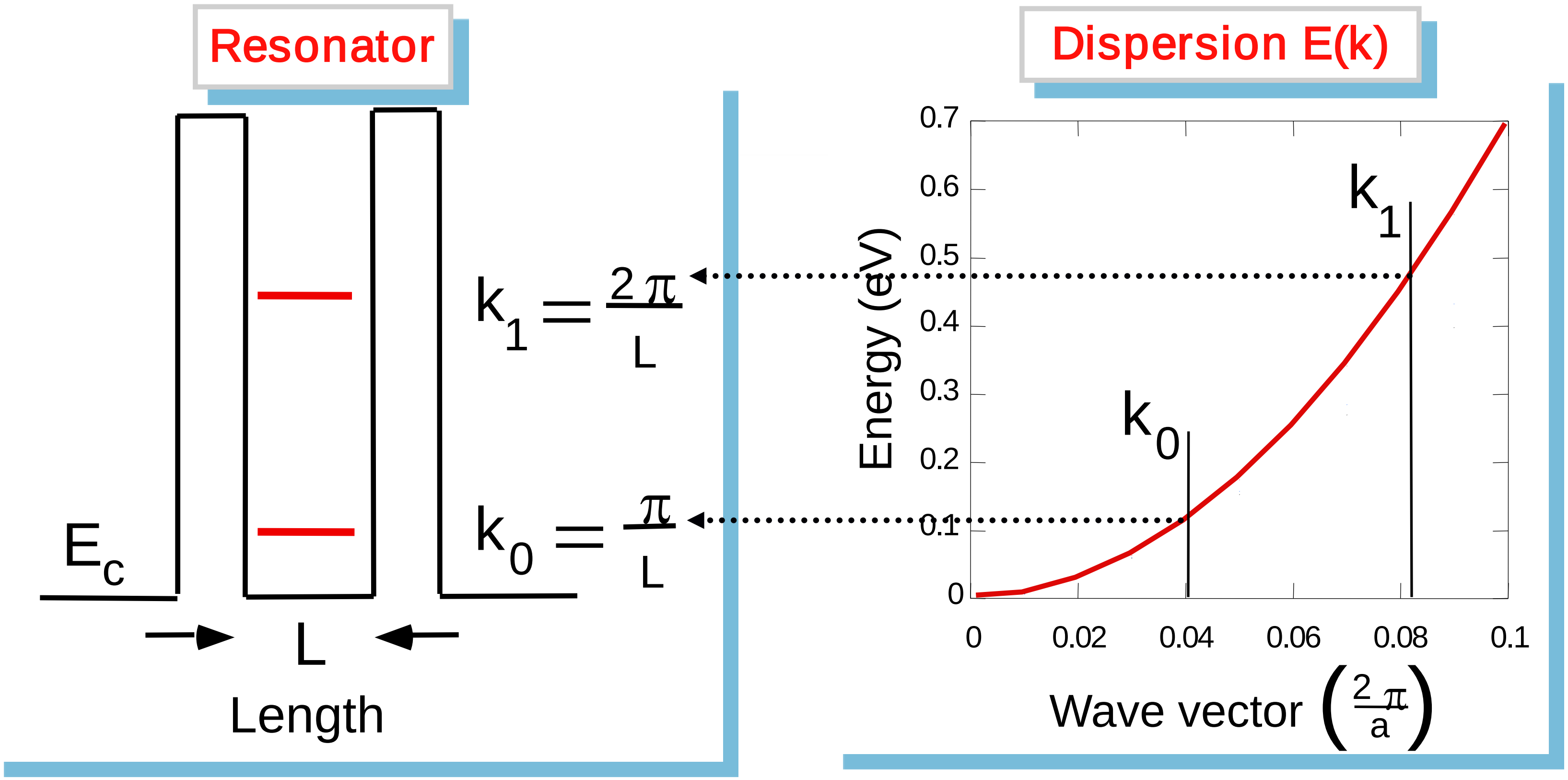
Usually considered a device
This is also a new material!

Empirical Tight Binding
makes the connection between
materials and devices!

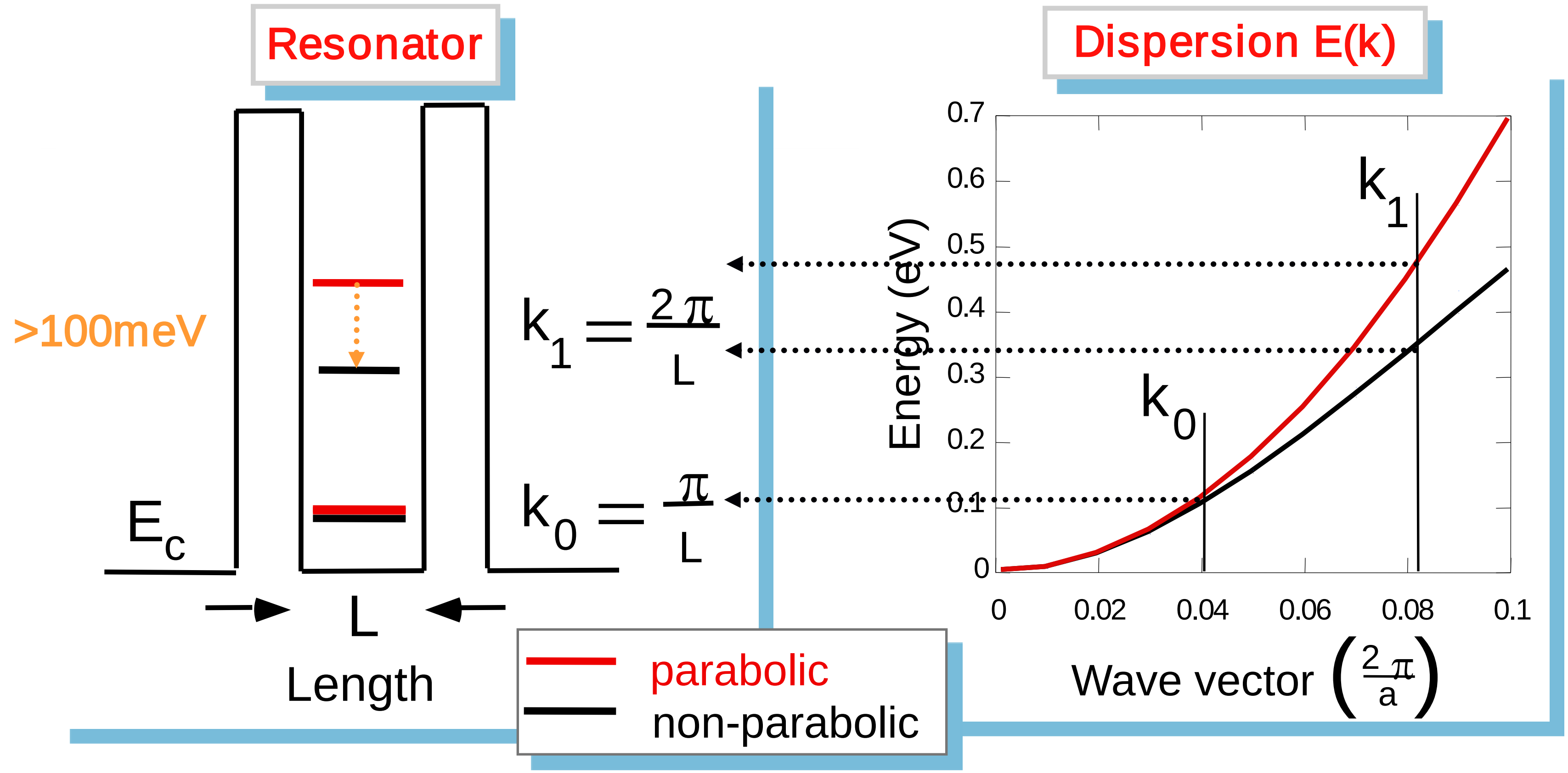
Quantitative Engineering:
Design, Analysis, Synthesis



Resonator State Quantization

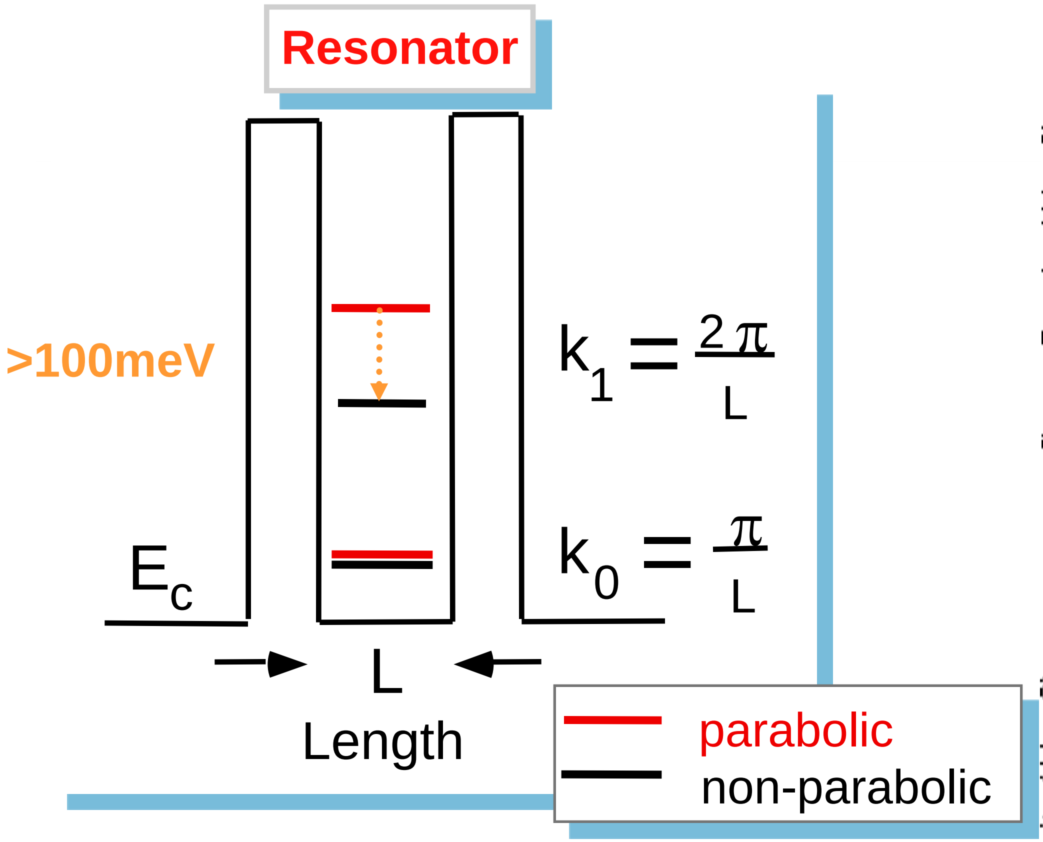


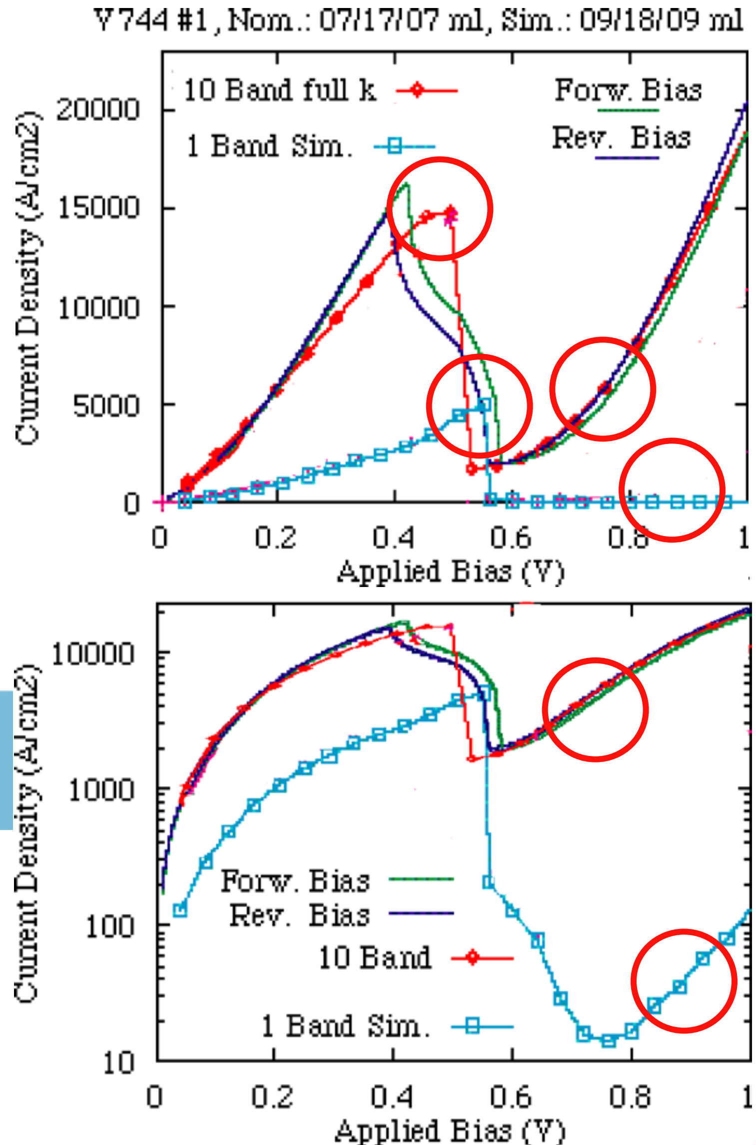
Resonator State Quantization
Effects of Band Non-Parabolicity



- Second state lowered by >100mev ~ 4kT

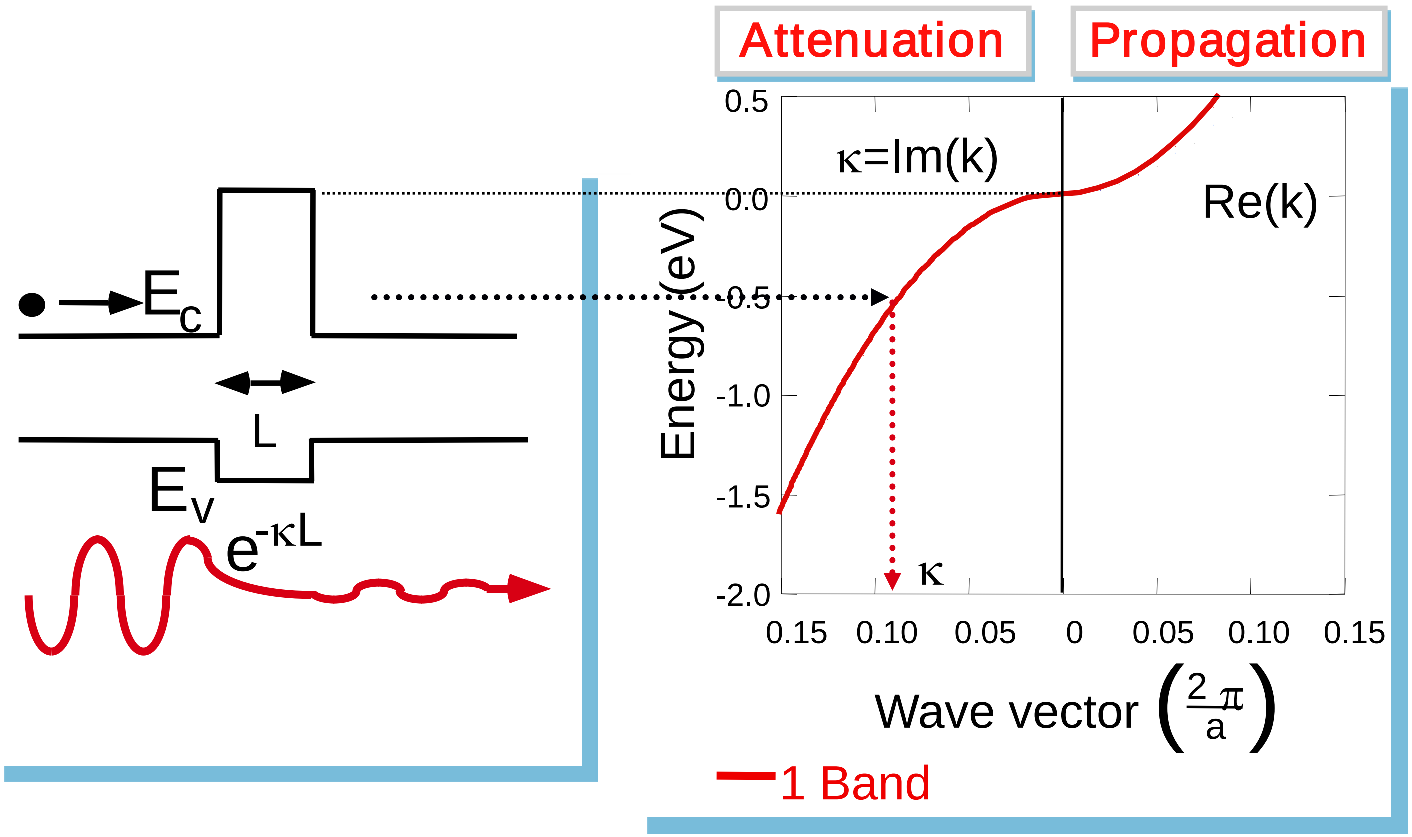
Effects of Band Non-Parabolicity on I-V Characteristics



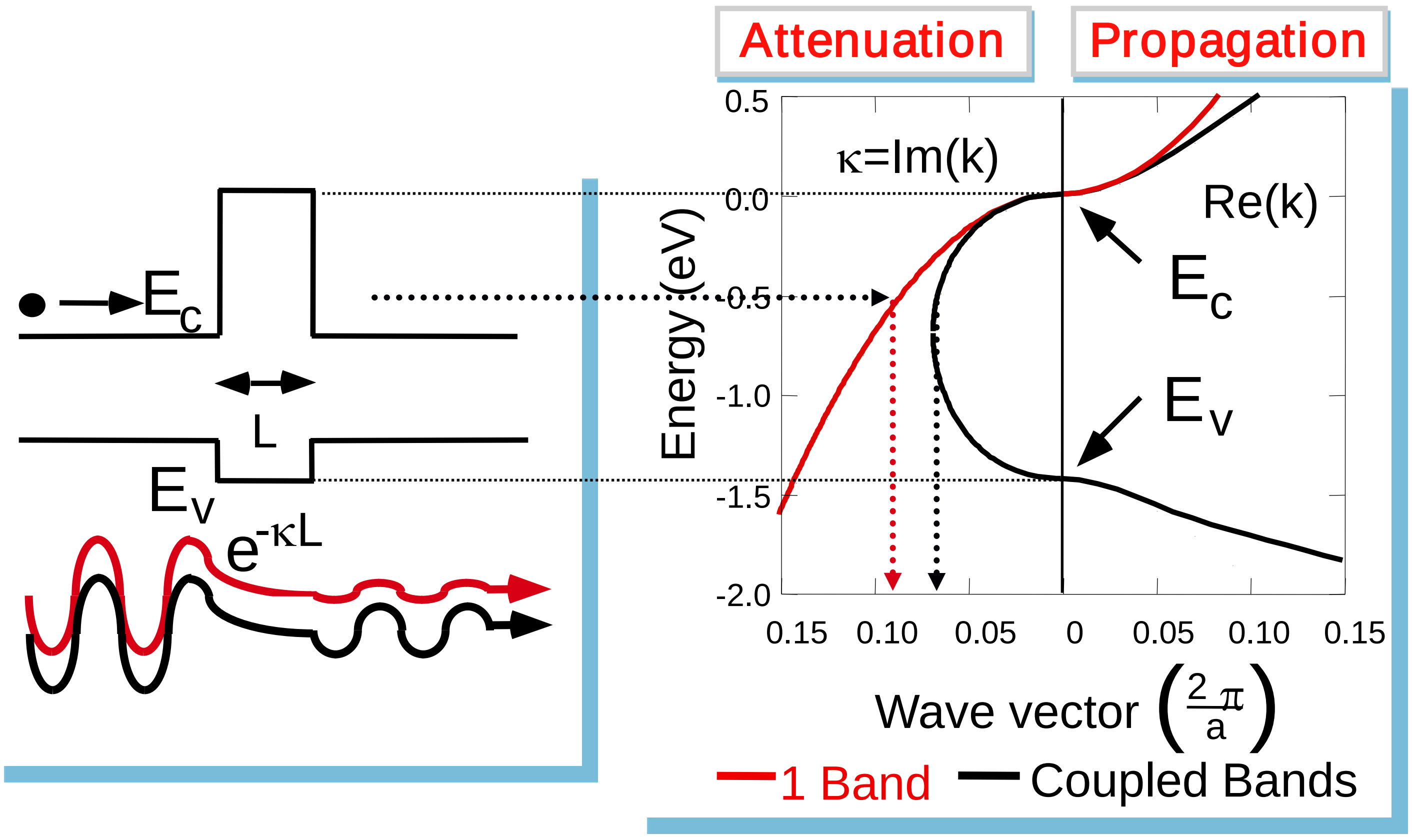


- Second state lowered by >100mev ~ 4kT
- Second diode turn-on at lower voltages
- Valley current mostly due to thermal excitations
- k_0 about equal - Why is peak current different?

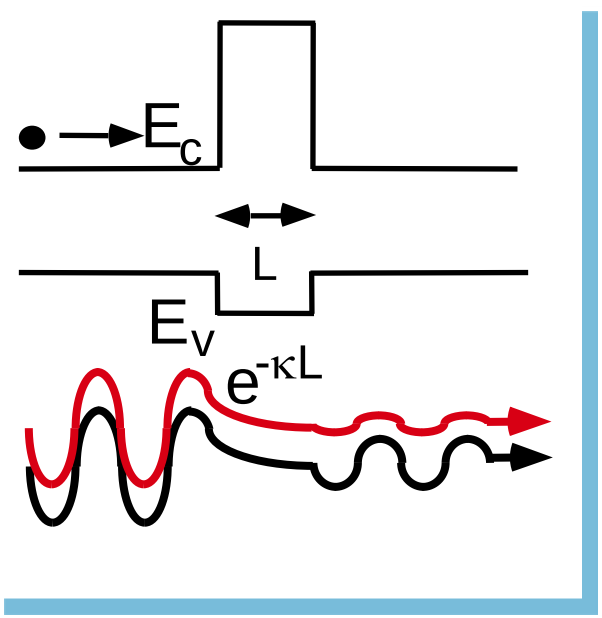
Wave Attenuation in Barriers
Single Parabolic Band

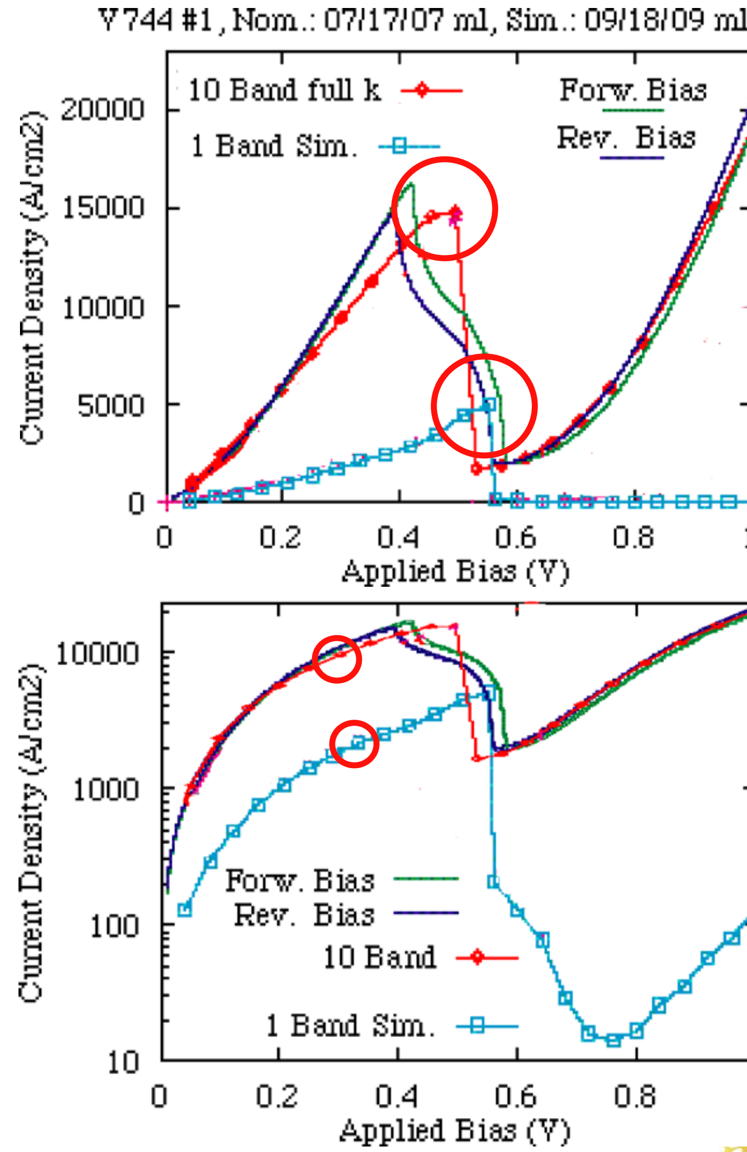


Wave Attenuation in Barriers Coupled Bands



Band Warping in Barriers
Impact on I-V Characteristics





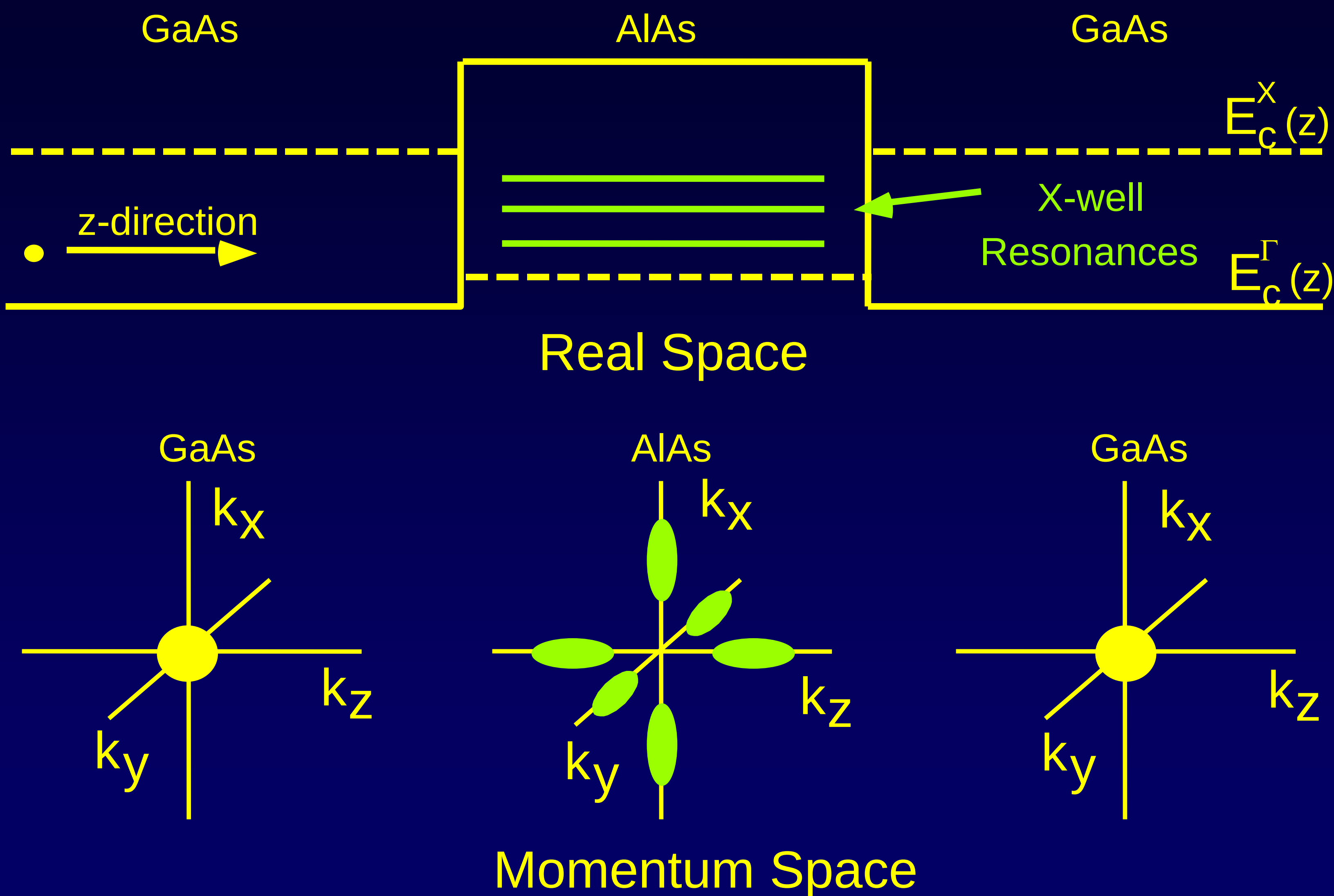
Non-Parabolicity:

- Second state lowered by >100mev ~ 4kT
- Second diode turn-on at lower voltages
- Valley current mostly due to thermal excitations

Complex Band Coupling:

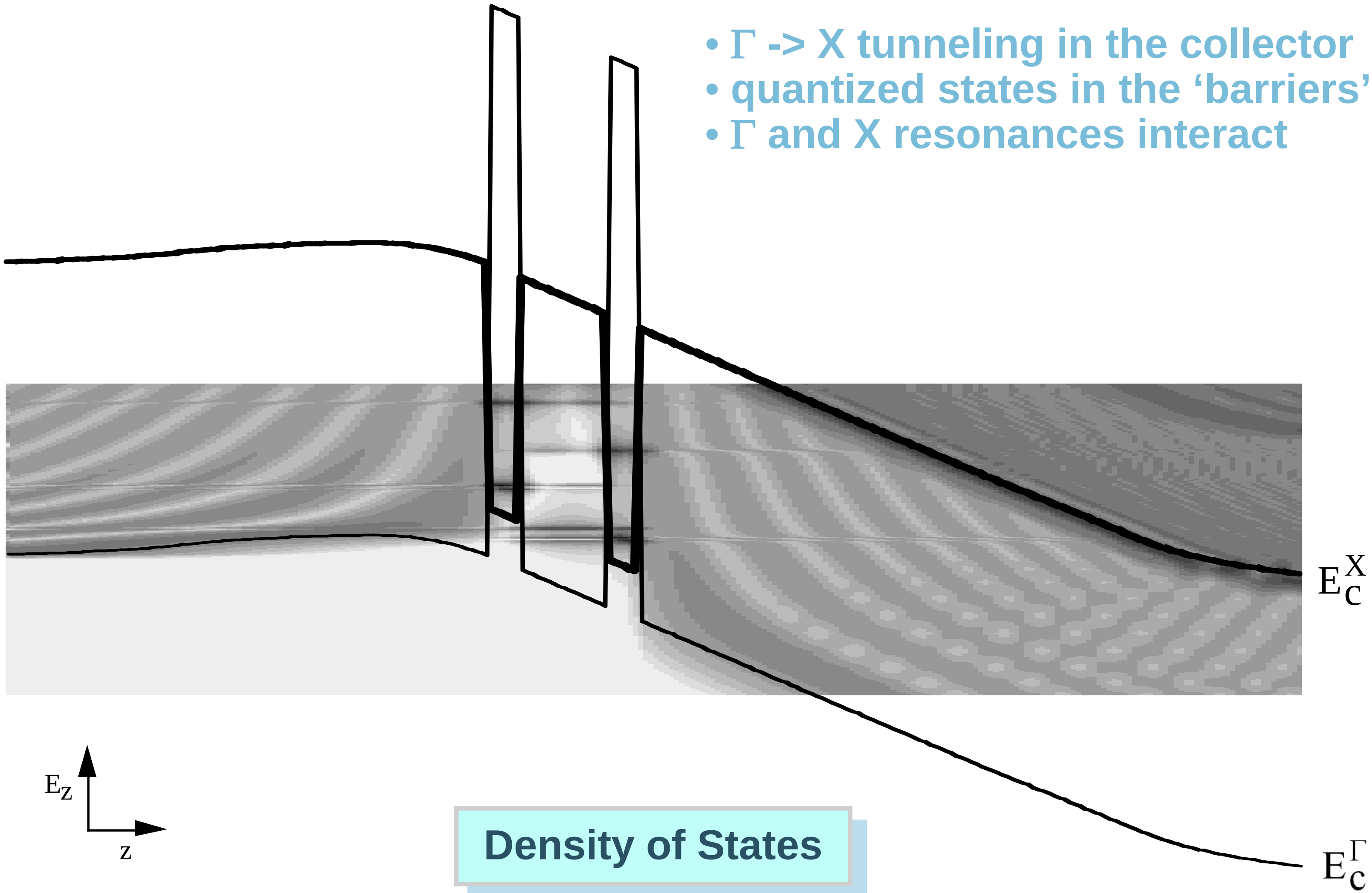
- RTD more transparent - correct peak current

Transport in Indirect Gap Barriers



Multiband Effects in GaAs/AlAs RTD's

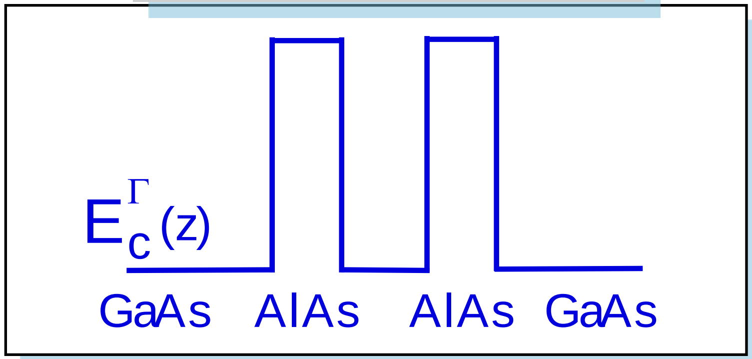
- Γ -> X tunneling in the collector
- quantized states in the 'barriers'
- Γ and X resonances interact



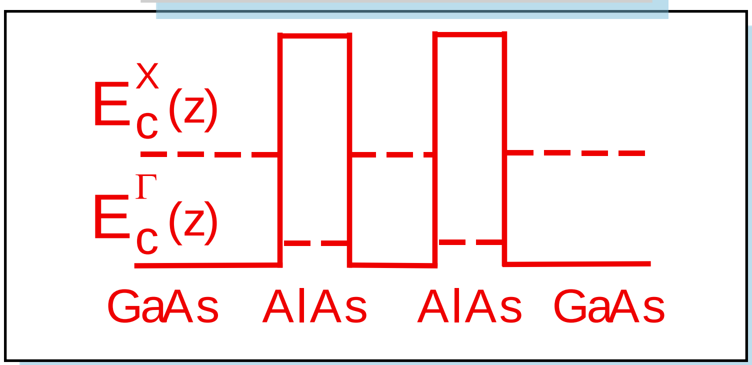
Essential Bandstructure consequences

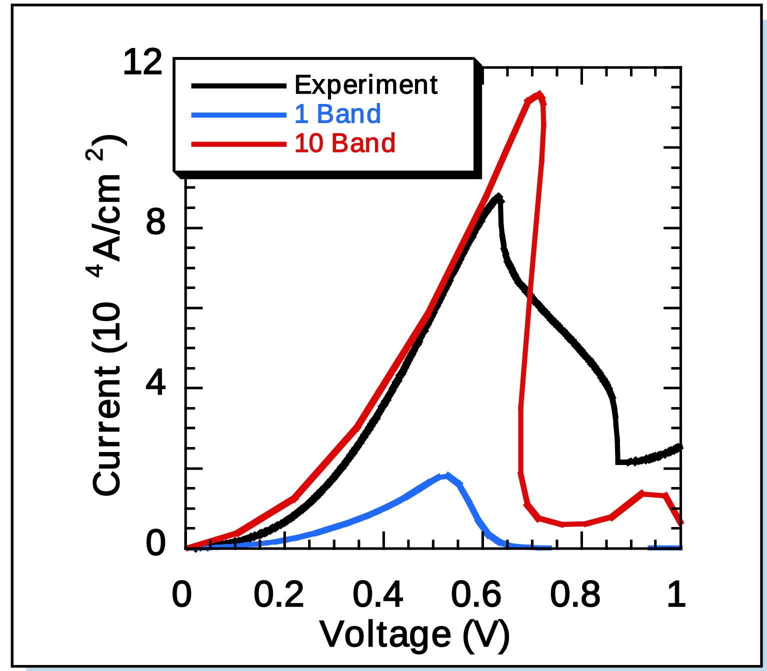
Addition of essential band structure effects

Single Band Model



Multi-Band Model





Transport via Transmission Coefficients

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

Cylindrical Coordinates

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

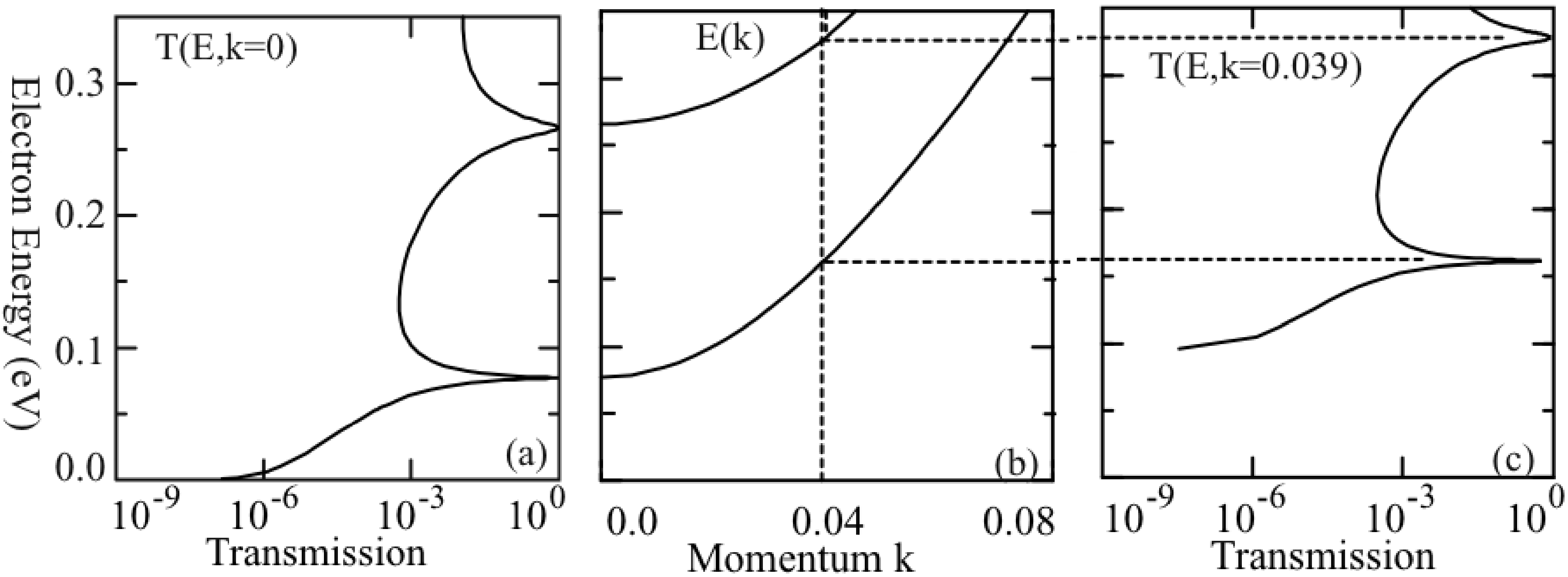
Throw out angular dependence

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

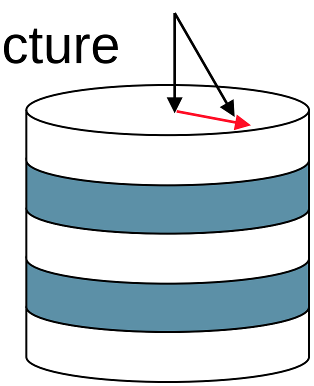
Parabolic transverse subbands

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

Electron Transmission and Dispersion

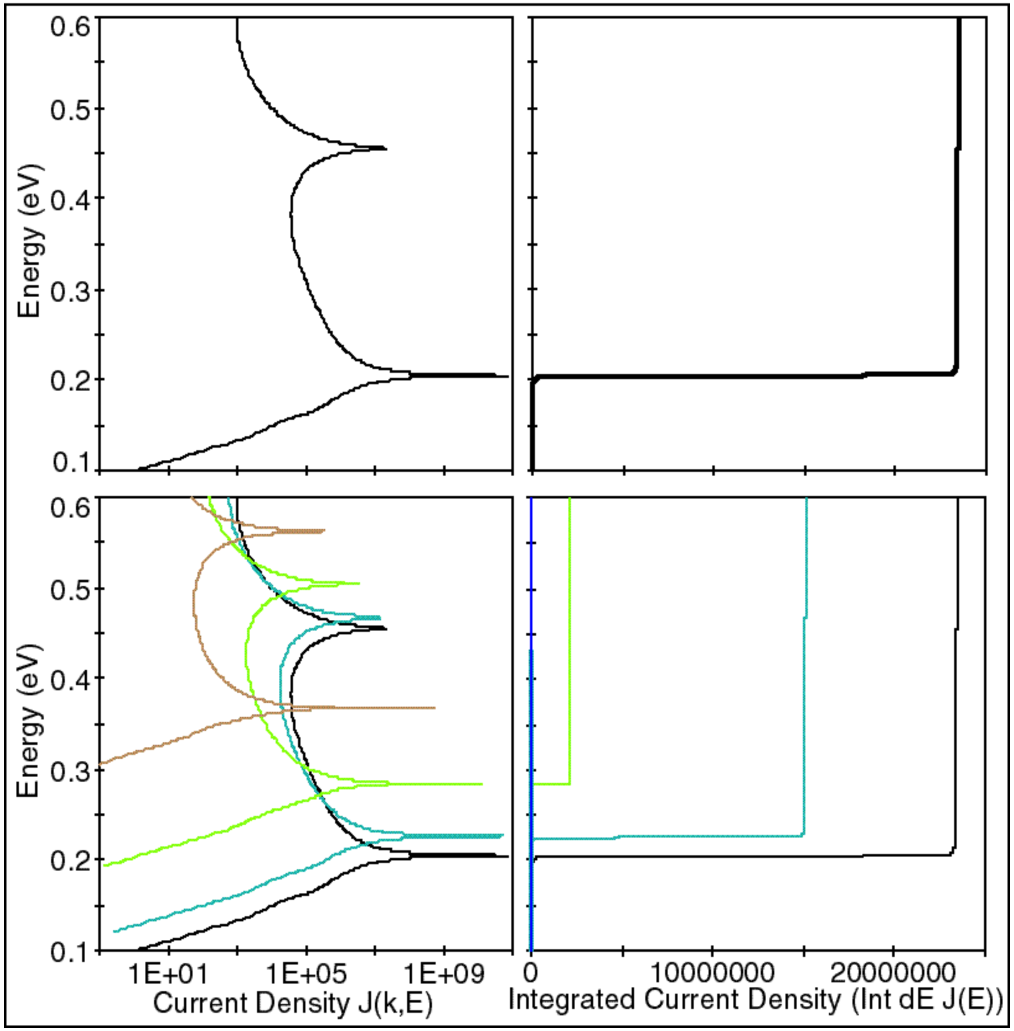


- Electron transmission coefficients are typically simple in structure
- Electron transmission is often quite parabolic
  => transmission at k>0 often
  a simple translation from k=0 transmisison



Mechanics of 2D Integration

- Transmission coefficient is masked by Fermi distribution in injecting lead.
- Running sum integral points out where in energy space significant current contributions occur.
- Multiple instead of a single transmission coefficient are evaluated and summed up.



$$J(E,k) \qquad \int_{-\infty}^{E} dE\, J(E,k)$$

Mechanics of 2D Integration

- Transmission coefficient is masked by Fermi distribution in injecting lead.
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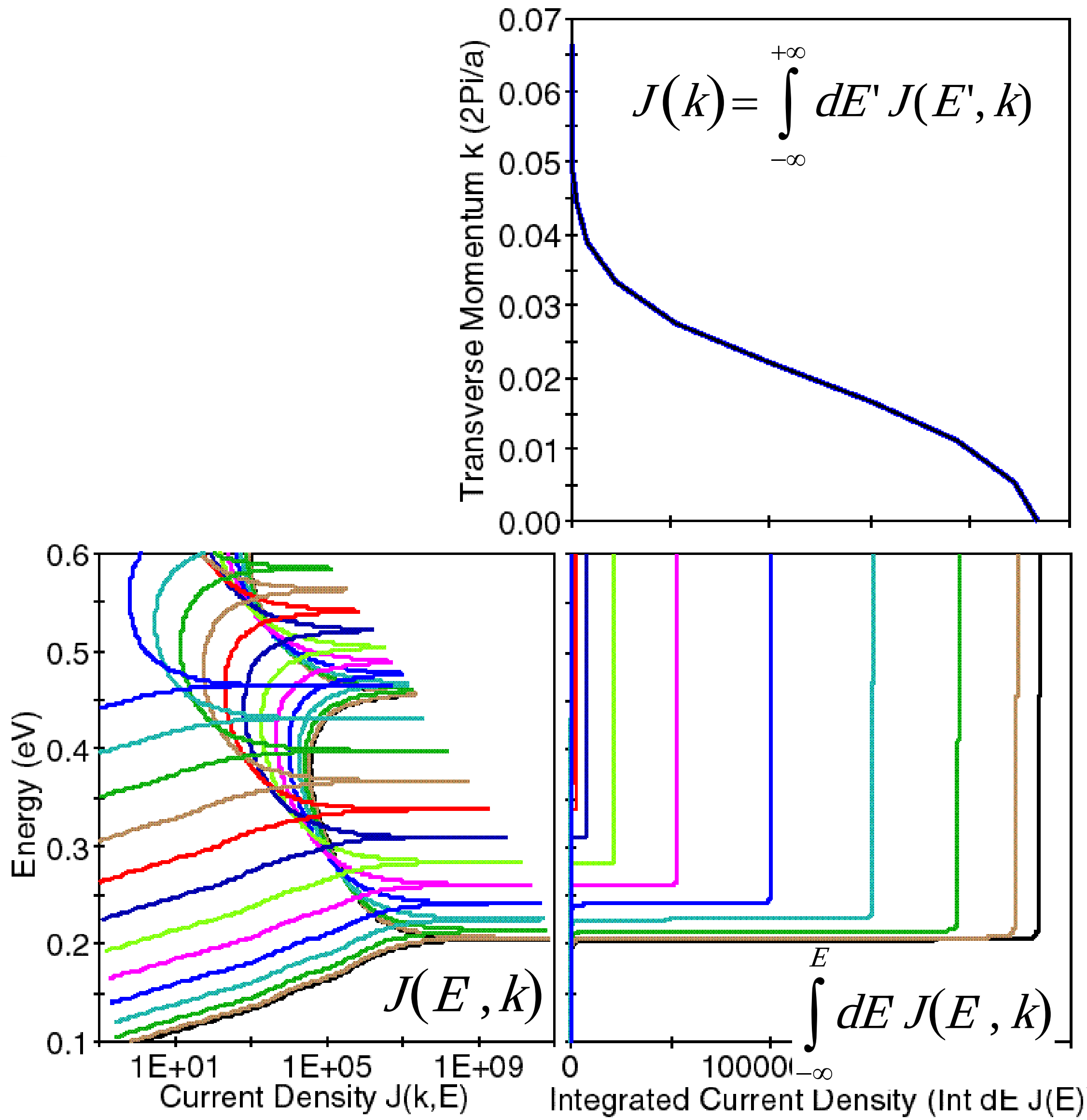
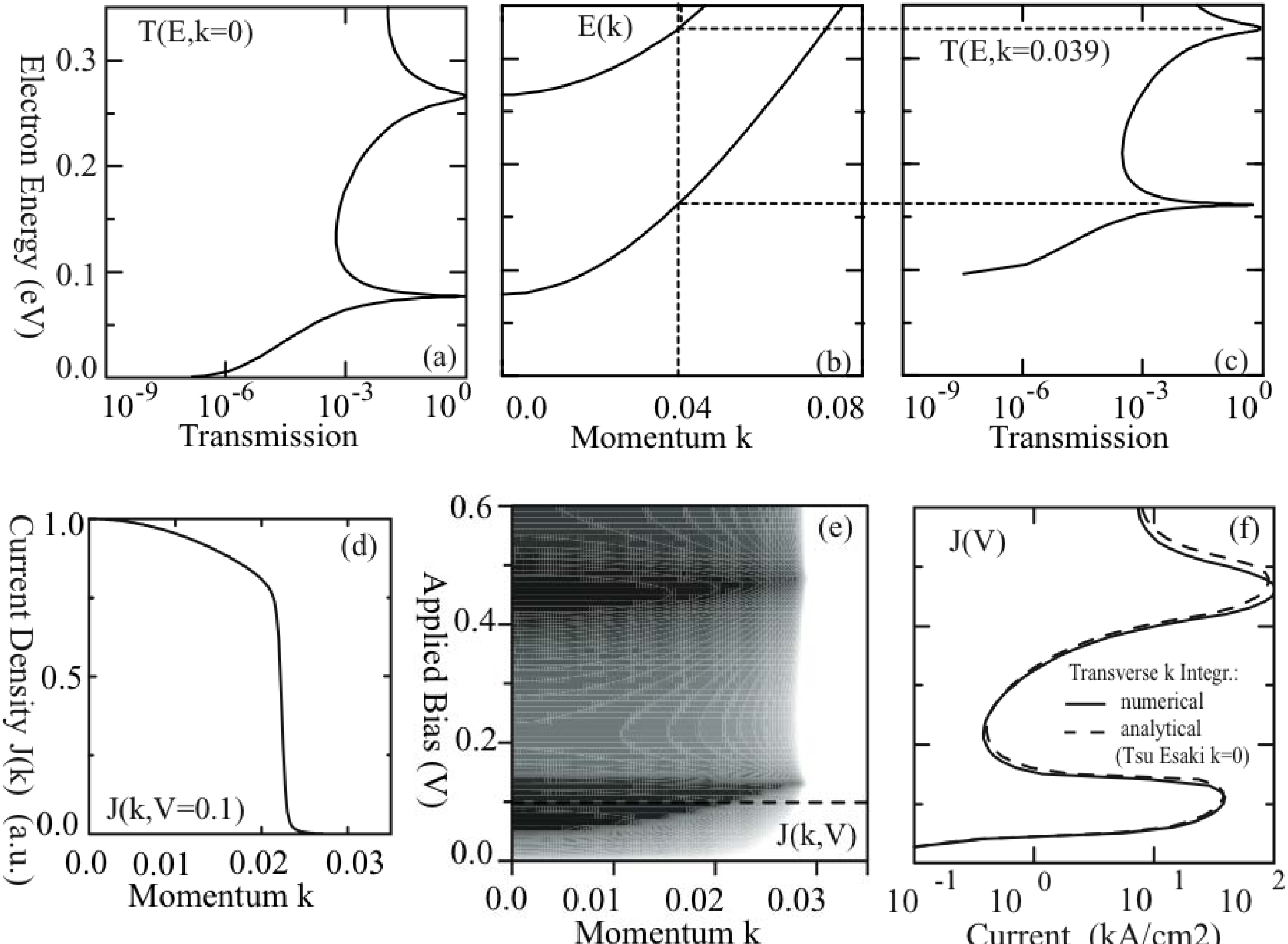
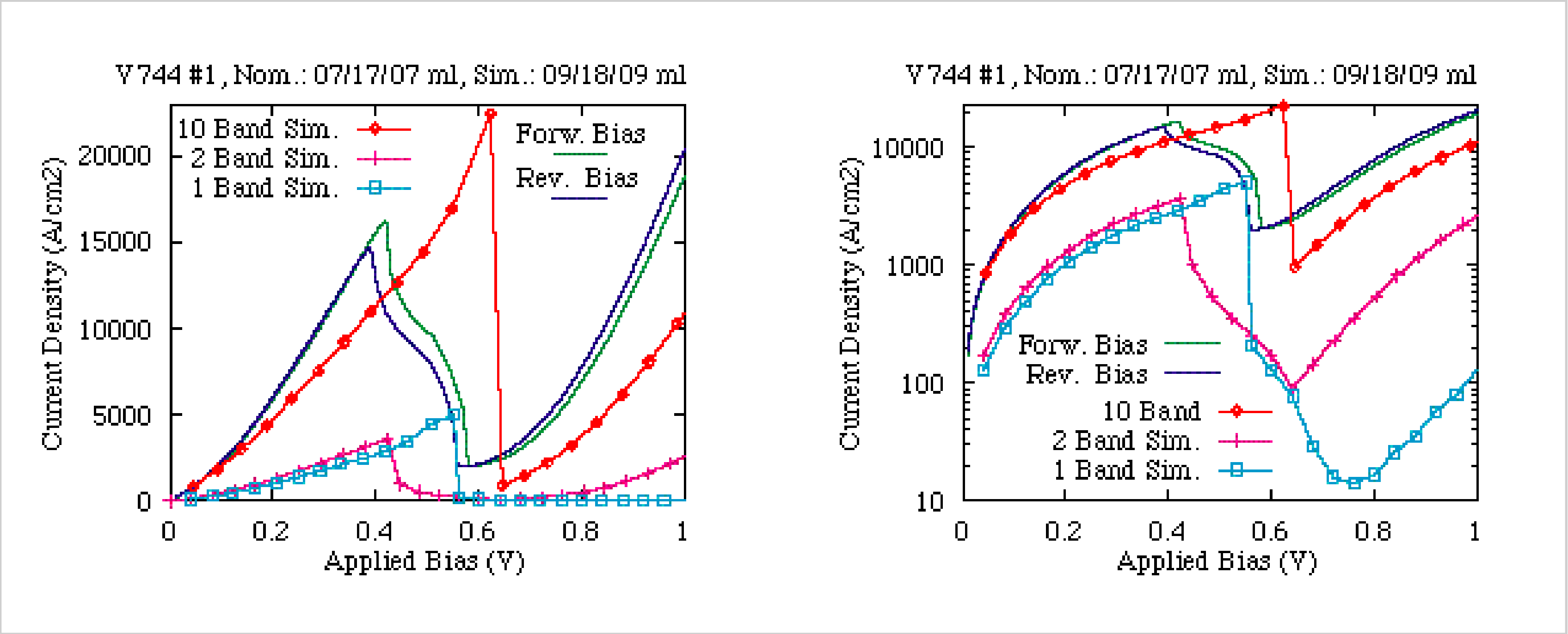


Electron Transmission and Dispersion for almost parabolic systems (GaAs)



I-V Calculations: 1 band, 2 band, 10 band



1 band uses k.p corrected effective mass in the the AlAs barriers
1 band and 2 band results do not predict the turn-on correctly.
10 band looks much better, but still does not get the turn-on right.

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

Transport via Transmission Coefficients

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

Cylindrical Coordinates

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

Throw out angular dependence

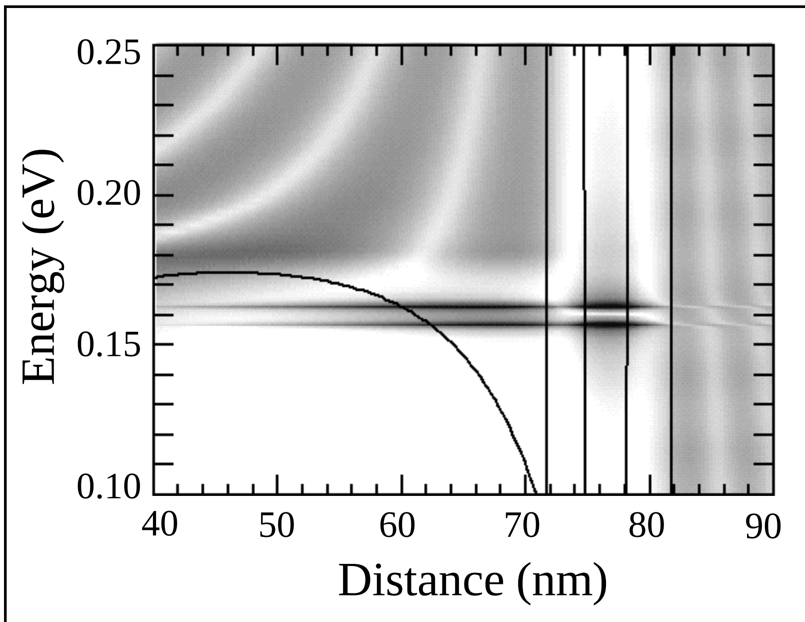
$$I \propto 2\pi \int k dk \int dE\, T(E, k)\left(f_L(E) - f_R(E)\right)$$

Parabolic transverse subbands

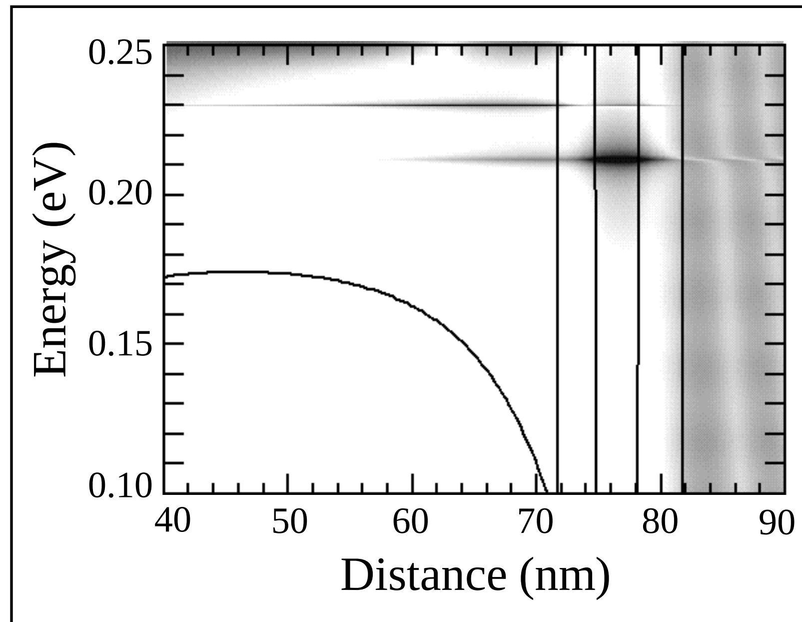
$$I \propto \rho_{2D} \int T(E)\left(f_L(E) - f_R(E)\right)$$

Resonance Coupling vs. Transverse Momentum

Density of States (k_x=0.00)

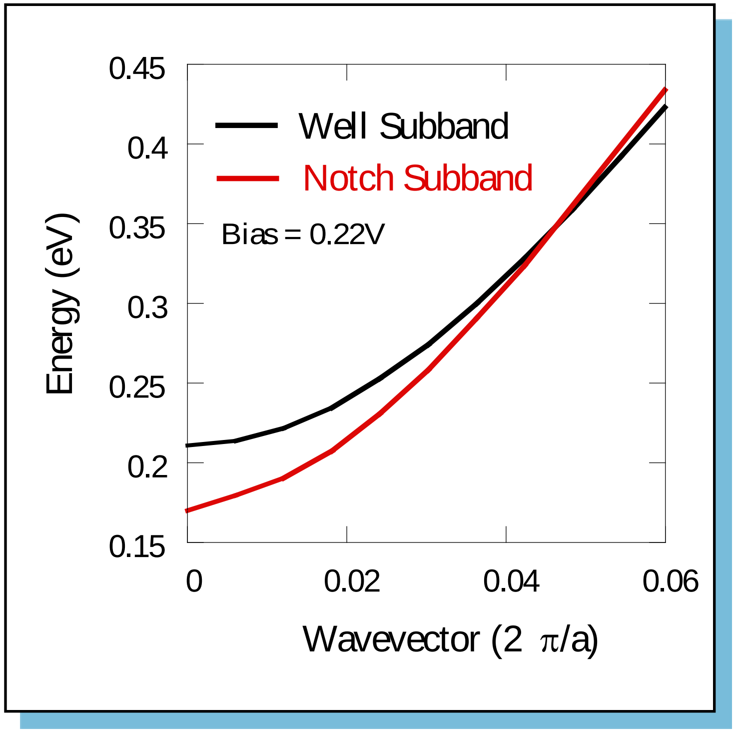


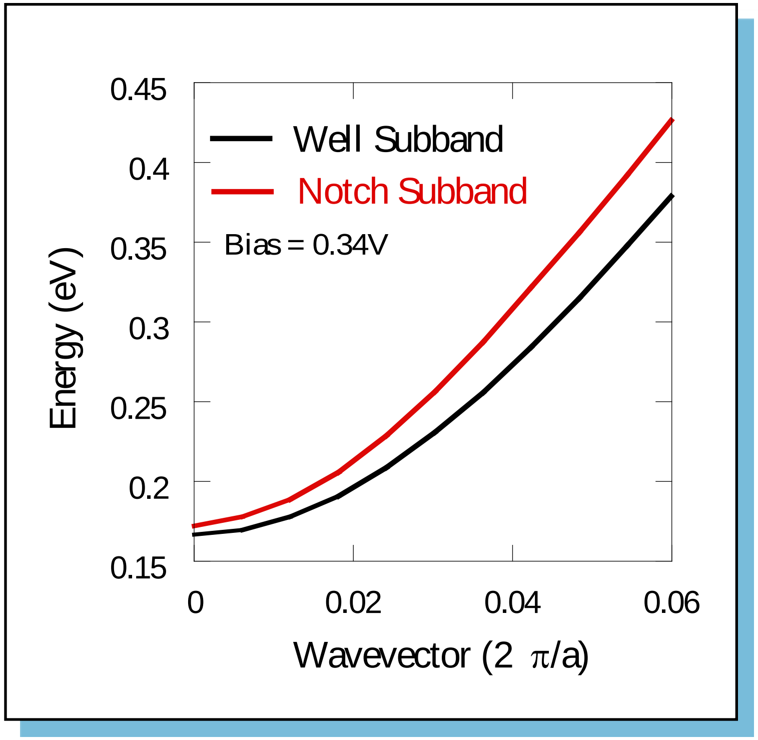
Density of States (k_x=0.03)



Resonance coupling depends on the transverse momentum

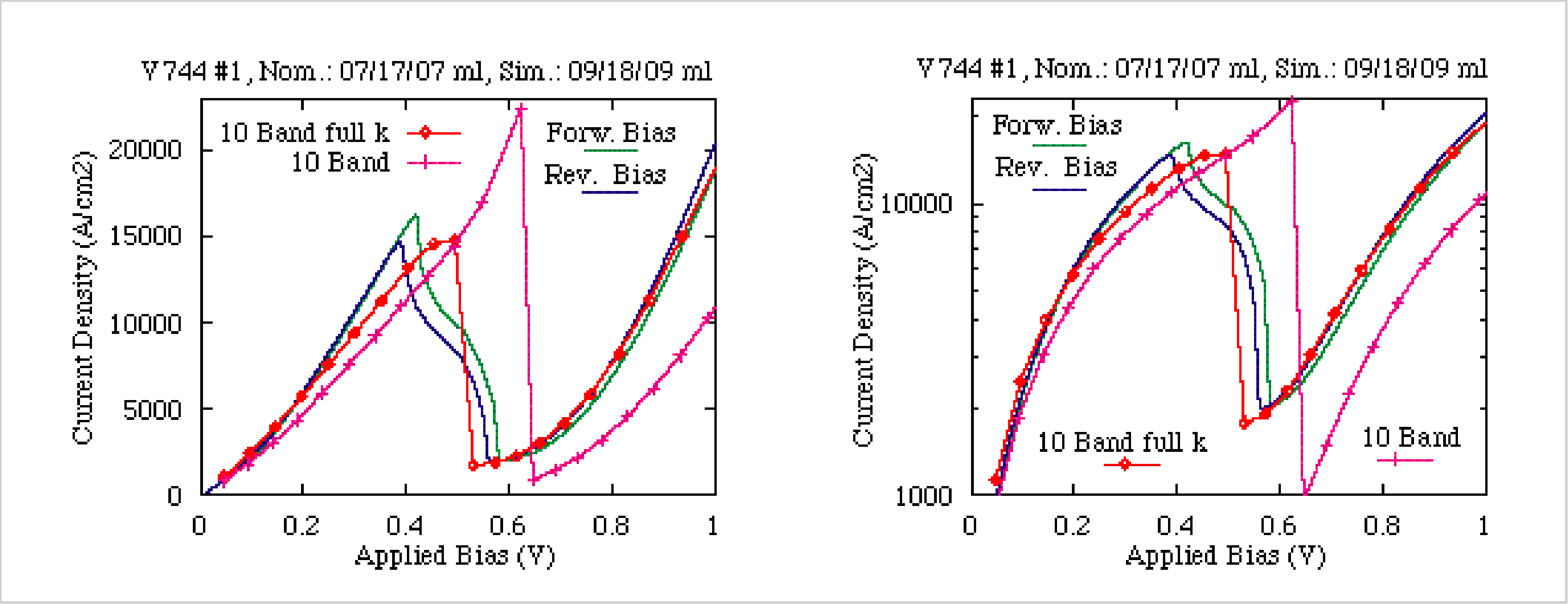
Quantum Well and Notch Subbands





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

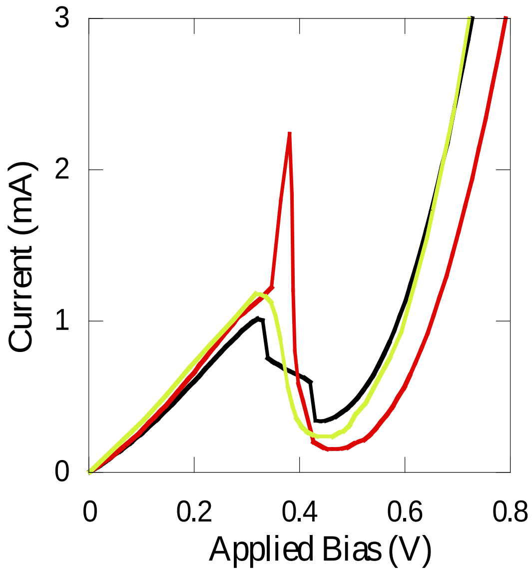
I-V Calculations: Analytic Transverse Momentum (ρ_{2D}) vs. Full Band

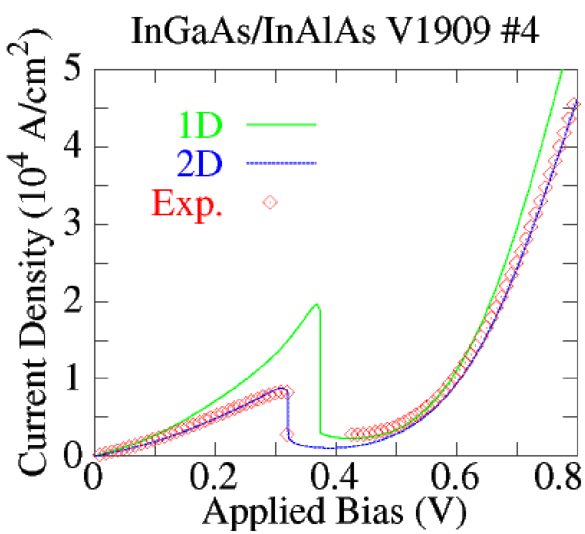


Need full band integration to get the peak and the turn-on right.

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

Full Band Simulation of Electron Transport

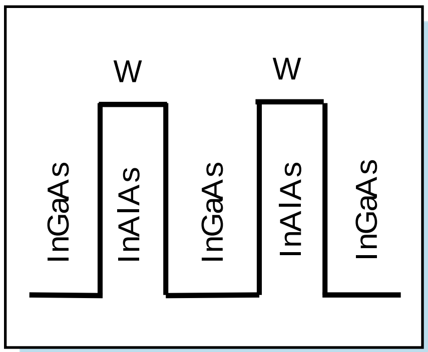




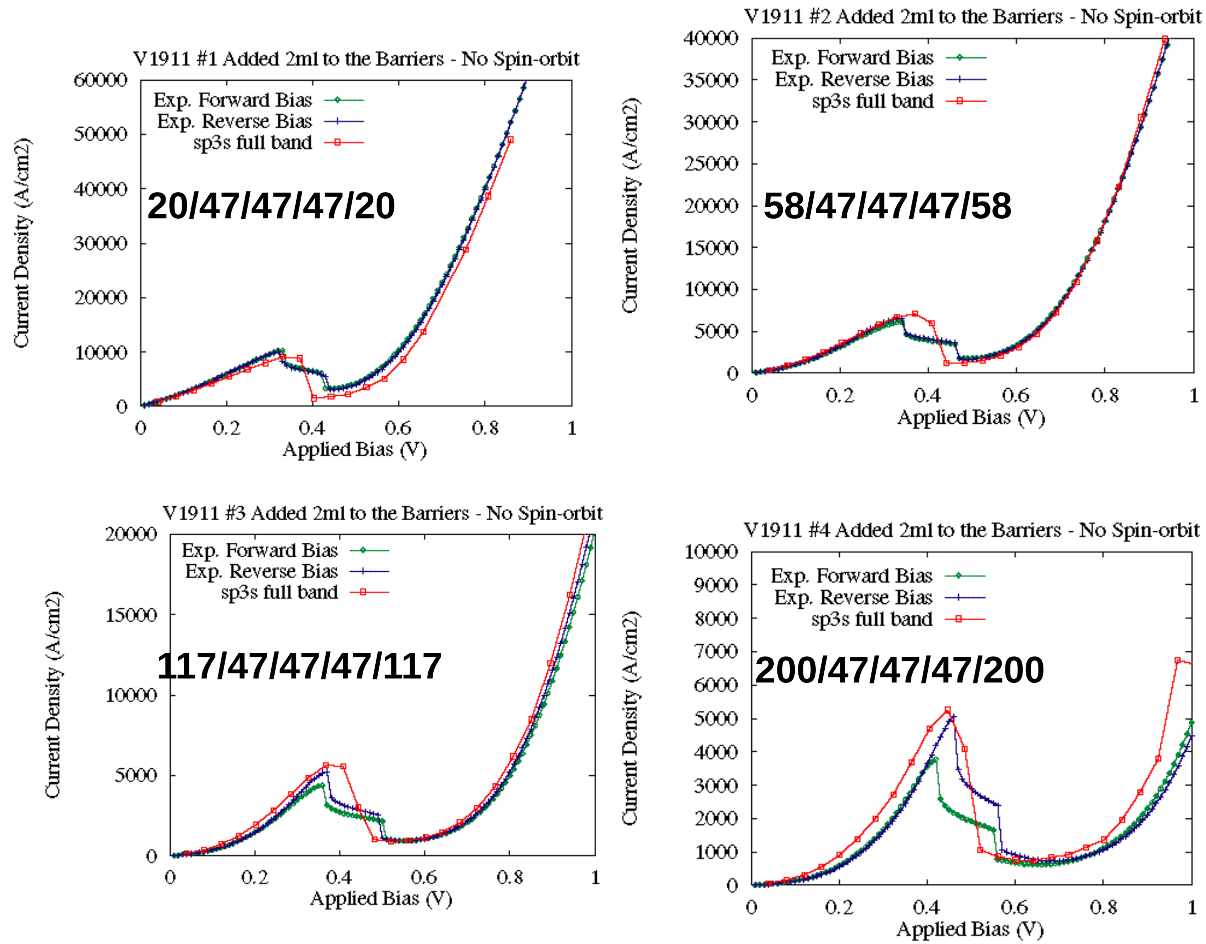
- 1D integration assuming parabolic subbands can lead to unphysical current overshoots.
- 2 Examples on InGaAs/InAlAs simulations:
  - » Sp3s* simulation with partial charge self-consistency
    -> sharp spike at turn-off
  - » Parameterized single band simulation which incorporates the band-non-parabolicity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

4 Stack RTD with Spacer Variation

Vary Spacer Length

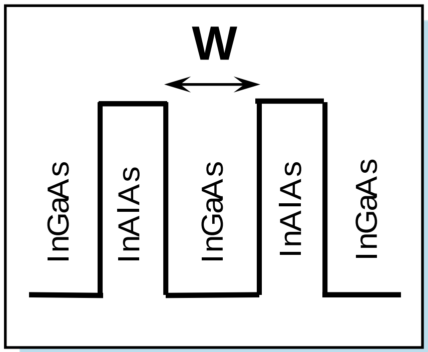


Four nominally symmetric devices:
20/47/47/47/20 A [1]
58/47/47/47/48 A [2]
117/47/47/47/117 [3]
200/47/47/47/200 [4]



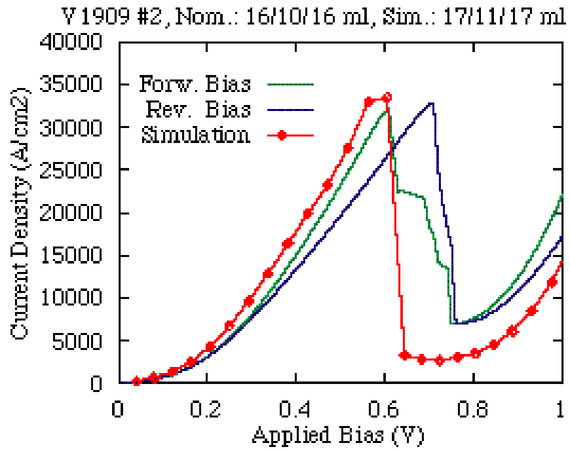
4 Stack RTD with Well Width Variation

Vary Well Width

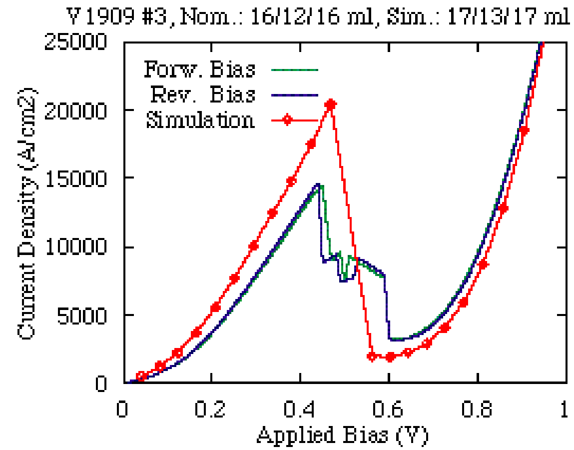


Three nominally symmetric devices:
47/29/47 A [1]
47/35/47 A [2]
47/47/47 A [3]

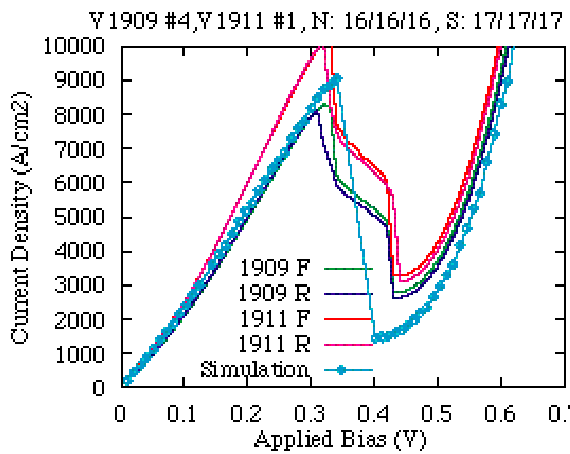
One asymmetric device:
35/47/47 A



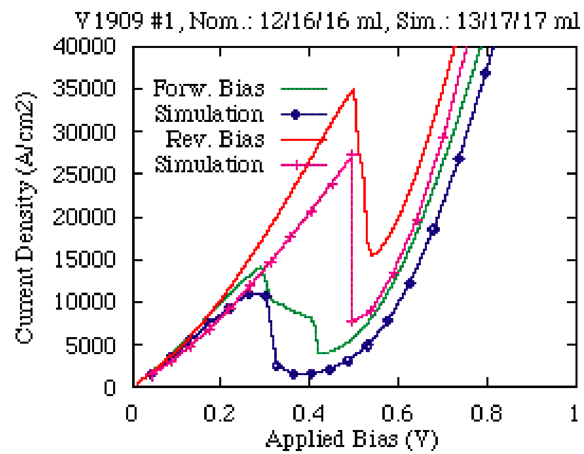
20/47/29/47/20



20/47/35/47/20

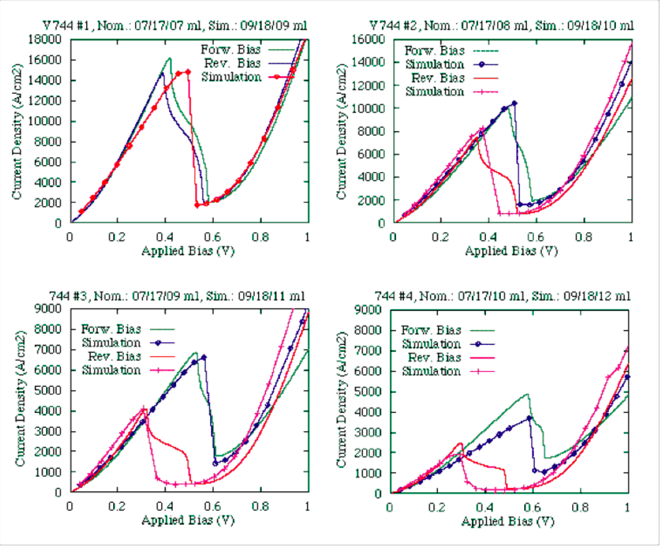


20/47/47/47/20



20/35/47/47/20

State-of-the-art RTD Modeling and Simulation Knowledge 1998



Knowledge:

- Scattering inside RTD
  - » Only important at low temperatures
  - » Not important for room temperature, high performance
- Scattering inside extended contacts
  - » Of critical importance at any temperature
- Charge self-consistency
  - » Critical everywhere, contacts and central device
- Bandstructure – atomistic device resolution
  - » Critical for understanding high temperature, high performance devices
  - » Need non-parbolicity, band wrapping
  - » Need full integration over Brillouine Zone – not a simple 1D integral
- NEGF is the baseline of an industrial strength simulator

Availability:

- An engineering modeling and design tool for 1D heterostructures
- Experimentally verified – **analysis and design**