# Nanoelectronic Modeling at JPL

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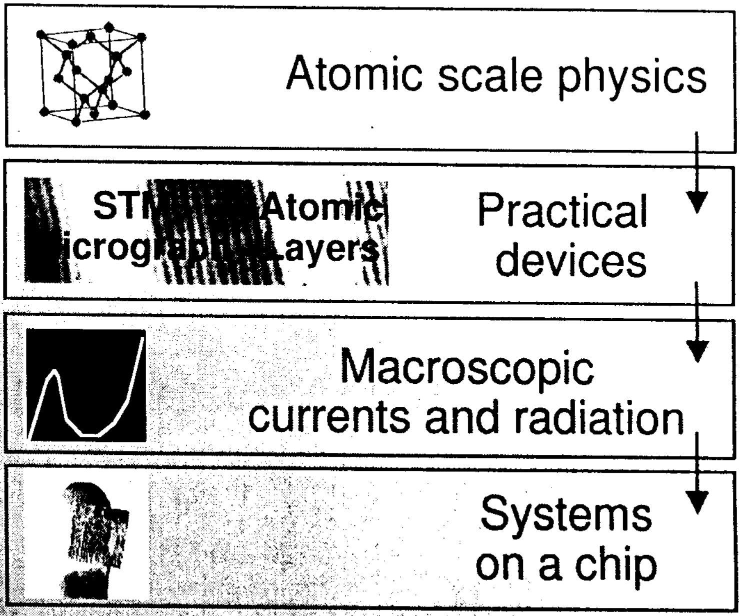
The NASA/JPL goal to reduce payload in future space missions while increasing mission capability demands miniaturization of measurement, analytical and communication systems. Currently, typical system requirements include the detection of particular spectral lines, associated data processing, and communication of the acquired data to other subsystems. While silicon device technology dominates the commercial microprocessor and memory market, semiconductor heterostructure devices maintain their niche for light detection, light emission, and high-speed data transmission. The production of these heterostructure devices is enabled by the advancement of material growth techniques, which opened up a vast design space. The full experimental exploration of this design space is unfeasible and a reliable design tool is needed.

Material variations on an atomic scale enable the quantum mechanical functionality of devices such as resonant tunneling diodes (RTDs), quantum well infrared photodetectors (QWIPs), quantum well lasers, and heterostructure field effect transistors (HFETs). The design and optimization of such heterostructure devices requires a detailed understanding of quantum mechanical electron transport. NEMO is a general-purpose quantum device design and analysis tool that addresses this problem. This presentation highlights the nanolelectronic development plans of the High Performance Computing Group and two recent NEMO developments: 1) genetic algorithm based parameter optimization and 2) full band hole transport simulation.

# Engineering Tools for Advanced Devices and Concepts

Objective:

- **Provide engineering design tools for electronic and photonic dev.**
- **Near Term:**
  - **1-D and 2-D structures: RTDs, QUIPs, HFETs, HBTs, Lasers (far IR, near IR).**
- **Long Term:**
  - **3-D structures: Quantum dots, quantum dot arrays, automata, nanotubes.**



Atomic scale physics

Practical devices

Macroscopic currents and radiation

Systems on a chip

Approach:

- **Bring in advanced modeling tools from research institutions (NEMO, MINILASE, ...)**
- **Build new models if necessary.**
- **Co-integration of the tools into ONE common WEB-based worksurface.**

Impact:

- **Enable device optimization for microelectronic-based missions.**
- **Near Term:**
  - **Optimize devices.**
- **Long Term:**
  - **Provide vision and modeling for new architectures beyond the SIA roadmap.**

# Genetically Engineered NanoElectronic Structures: GENES

## Objective:

- Automated device synthesis and analysis using genetic algorithms.
- Material spectroscopy through genetic algorithms analysis.

## Justification:

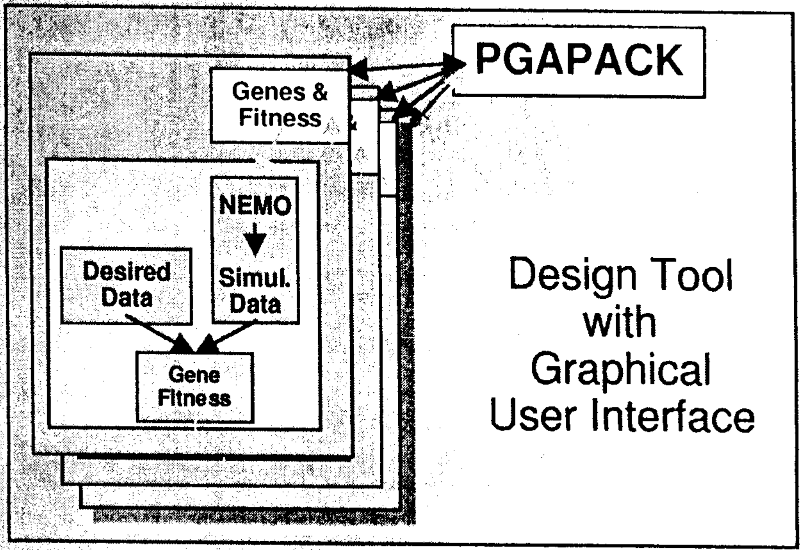
- Empirical Design (usual process) is sub-optimal. Complete design space search is unfeasible.
  => Develop automated design tools.

## Impact:

- Rapid nanotechnology device synthesis and development.
- Prototype development for a general purpose optimization tool, that can be expanded towards other scientific problems:
  - Electromagnetic modeling
  - Laser modeling
  - Evolvable hardware

## Approach:

- Adept NEMO to analyze individual structures in parallel.
- Adept parallel genetic algorithm package (PGApack) to optimize and select desired structures in NEMO.
- Explore other optimization methods such as simulated annealing and directive approaches.
- Develop graphical user interface.



PGAPACK

Genes & Fitness

NEMO

Simul. Data

Desired Data

Gene Fitness

Design Tool with Graphical User Interface

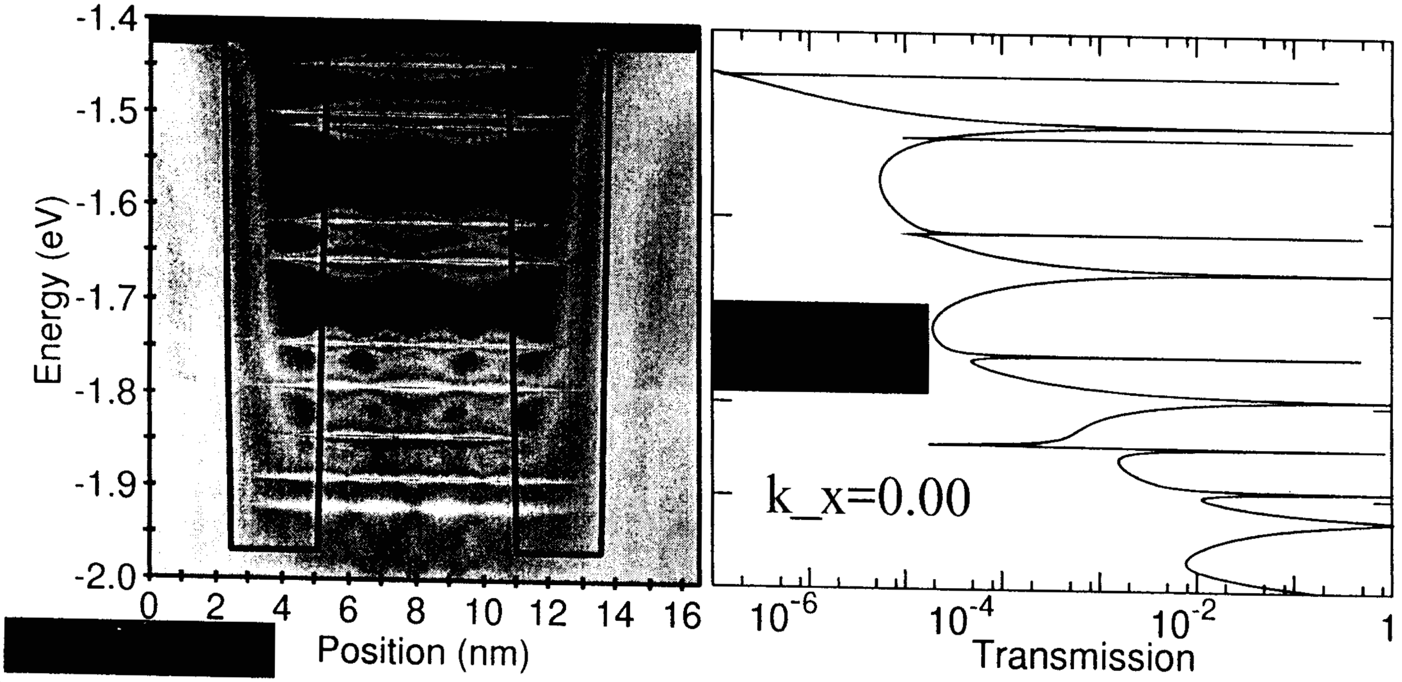
# Steps towards Laser Modeling: Heterostructure Hole Transport

**Objective:**

- Long Term: Develop ability to model electron and hole interactions in a semiconductor laser including transport.
- Short Term: Analyze transport in a hole resonant tunneling diode.

**Approach:**

- Use real space tight binding bandstructure representation to resolve finite size of heterostructures. (nearest and second nearest neighbor sp3s*)
- Examine dependence on transverse momentum and resonance broadening.



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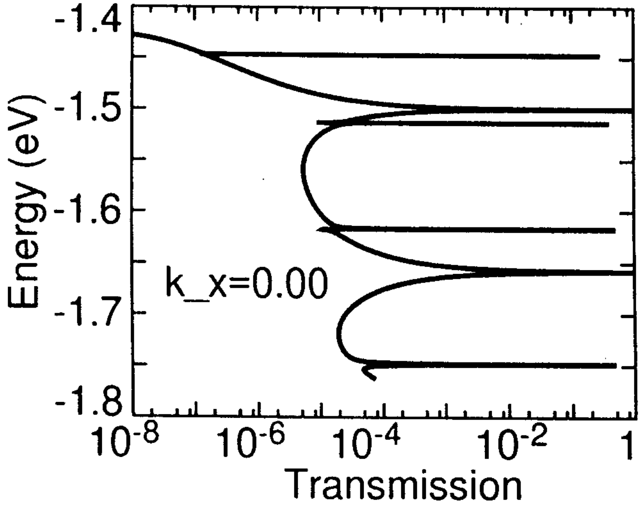
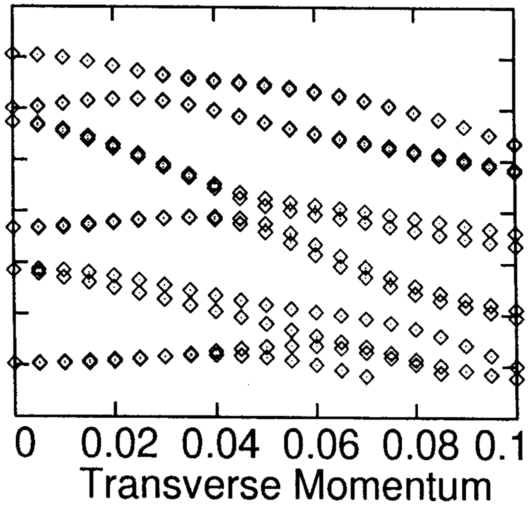
# Transverse Hole Subbands in GaAs/AlAs RTD

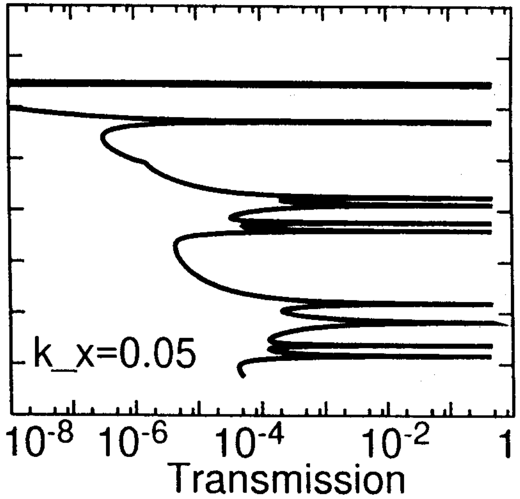
- Transmission coefficient at $k_x$=0



- Resonance states as a function of transverse momentum:
  -> transverse subbands

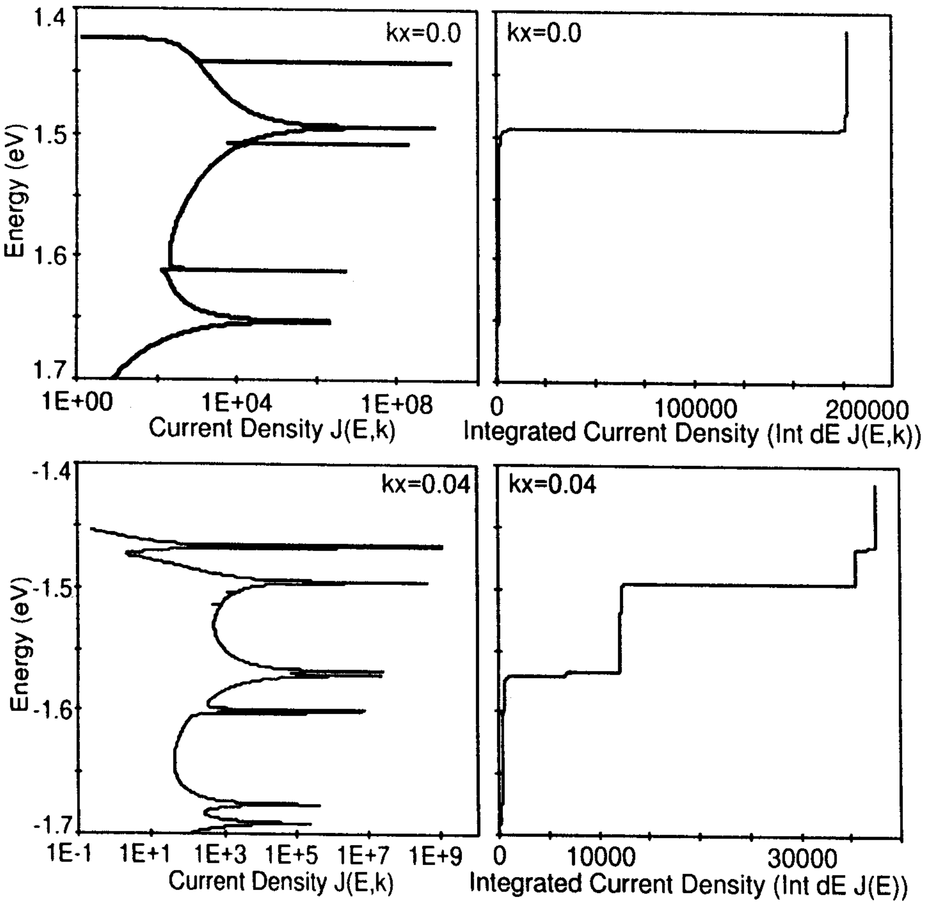


- Transmission coefficient at $k_x$=0.05



- Transverse subbands exhibit:
  - complex structure of anti-crossings
  - Strong mixing of light and heavy electron states
  - non-monotonic behavior - some subbands are electron-like.
- Transmission coefficient is strongly dependent on transverse momentum

# Current Integral Varies Qualitatively with Different Transverse Momenta



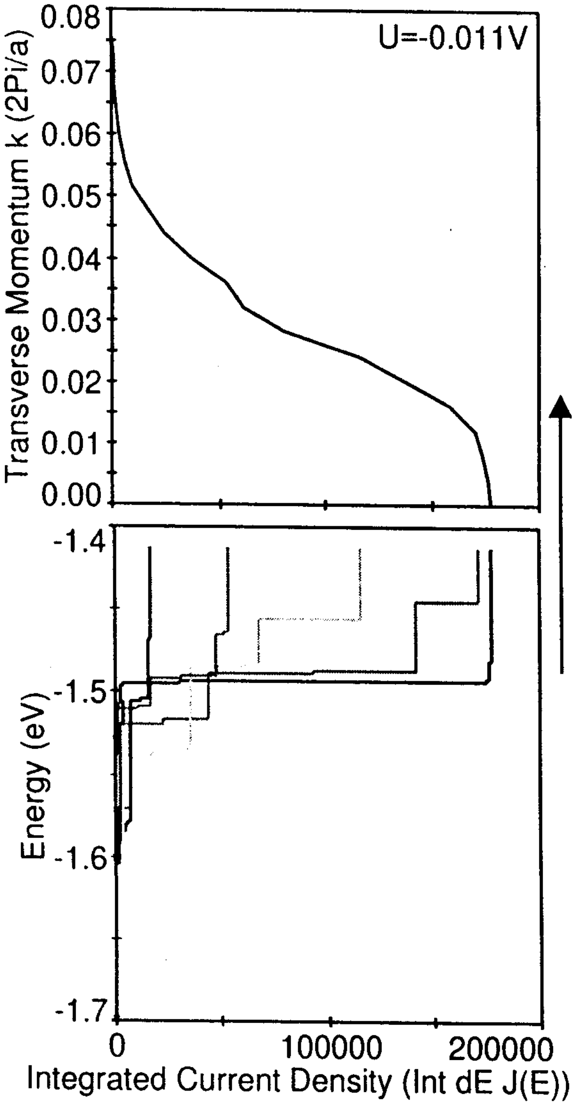
**k=0.00:**
current flows at one energy

**k=0.04:**
current flows at multiple energies

$$J(E,k)$$

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

# Current Density J(k) at low bias

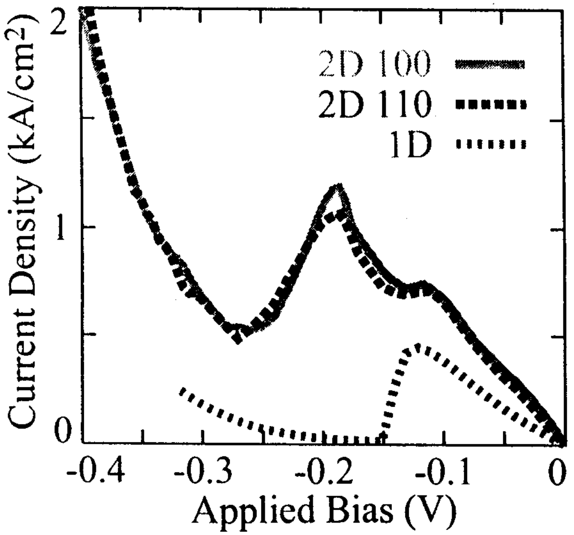


$$J(k) = \int_{-\infty}^{\infty} dE\, J(E, k)$$

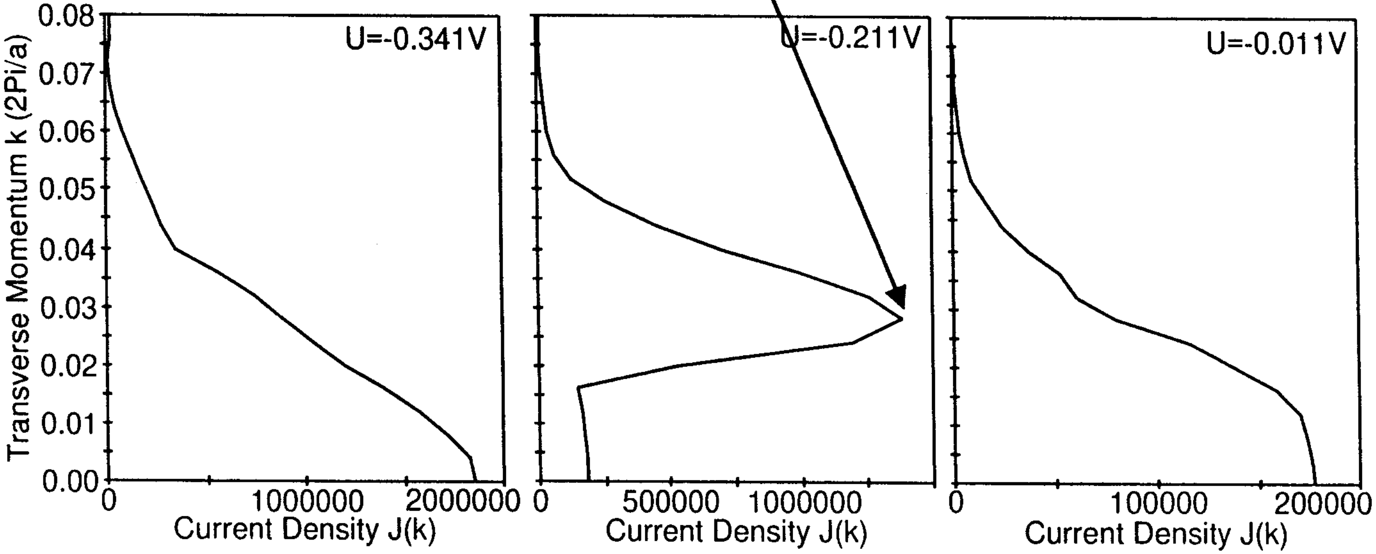
**At this bias point:**
**J(k) decreases with increasing k**
**=> hole flow at zone center**

**J(E,k) is widely distributed in energy**
**This energy distribution is strongly bias dependent!**

# Current Voltage Characteristic



- Tsu-Esaki single integral (1D) approach breaks down: Transverse integration provides qualitatively different results.
- Current dependence of $k_t$ in <100> or <110> direction is weak.
- Current may be flowing dominantly outside the zone center.



# Conclusions

- Valence band warping requires 2nd neighbor interactions to be included in the sp3s* tight-binding model

- Genetic algorithm was used to drive NEMO as a black box for structural optimization.

### Acknowledgement

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