Multi-Scale Nonequilibrium Green’s Function Method for LEDs: Balance of Thermalization and Tunneling

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Key Challenges in LED Development

- Efficiency droop
  - Auger effect at high carrier density
  - Band-to-band recombination
- Uneven carrier distribution
  - Carrier pile-up causes ‘deep’ drops
- Current density distribution
  - Carrier profile leads to ‘short’ drops

Device Physics

- Quantum Effects Too Important to Ignore
  - Quantum interference everywhere
  - Distinct classical and quantum regions
  - Coupling between continua and discrete states
  - Strong scattering introduces broadening
- Current transport behavior
  - Classical transport often ignored
- Carrier density
  - Impact on efficiency, recombination, and calculated efficiency

Simulation on a realistic LED

- Atomic resolution with sophisticated bandstructure
- Potential energy band diagram
- Results
  - IQE, QM emission matches experimental observations
- Results
  - Long range tunneling
    - Efficient transport in the model
    - Long range tunneling impacts device operation

Results: IQE, QM emission matches experimental observations

Results: Long range Tunneling + Hot Electron Formation

- Quantum transport
  - Carrier density
  - Turn on voltage

Modeling Challenges

- Classical Models Missing Key Information
- Multi-charge self-consistent transport
- Electrons and holes
- State injection
- Quantum transport
- Tunneling and thermionic emission

Modeling Challenges — Full NEGF Transport Solution Too Expensive

- Easy solution
  - No quantum transport tool available for LED industry
- NEGF throughout device
  - Quantum mechanics are “exact” everywhere
- Model must provide
  - Carrier transport behavior, carrier density, and turn-on voltage
  - Current and hole transport through extended structure
  - Accurate treatment of tunneling and thermionic emission
  - Physical, radiative recombination model
  - Numerical efficiency, low level engineering

Multi-Domain, Multi-Physics Model

- Charge self-consistent + quantum transport + detailed balance
- Atomistic 20 band tight binding
- MQW: GaN/InGaN
- Structure: GaN(3.1/4.6)/InGaN(3.1/4.6)/GaN
- Simulation on a realistic LED
  - Rate equations coupling electron/hole transport
  - Multiple Domains / Physics
    - Barriers:
      - High carrier density, strong scattering
    - Coherent transport (s-mobile, e-ballistic)
    - Scattering can be included
  - NEGF throughout device
  - Quantum mechanics are “exact” everywhere

Status and Future Plan

- Needs for other applications
  - Auger emission spectroscopy
  - Auger model
  - Quantum transport tool
  - Quantum mechanics are “exact” everywhere

Footnotes:

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