Nonequilibrium Band Structure of Nano-devices
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Motivation
- Realistic prediction of fully three-dimensional nano-devices:
  - Single-quantum-dot photodiodes
  - Cleaved-edge overgrowth wire and dot structures
- State-of-the-art electronic structure calculation from nm to m scale for any 3-D geometry/composition and applied bias
- Calculation of carrier transport limited to situations near equilibrium

This work: 3-D Device simulator
- Electronic structure:
  - 8-band k·p method
  - Charge self-consistency, including piezo-effect
  - Fully strain relaxed
  - Strain dependent band shifts
- Current calculation:
  - Assume carriers to be in local equilibrium, determined by spatially varying quasi-Fermi levels
  - Current calculated semiclassically with quantum mechanical density and self-consistently determined quasi-Fermi levels

Application:
Study of single-quantum-dot photodiodes
- Self-assembled InGaAs quantum dots embedded in Schottky diode
- Nominally 50\% InAs -> Exciton energy of 1.3 eV
- Comparison with experimental* photocurrent data as a function of applied bias
  *) Findeis et al, APL 78, 2958 (01)

Results:
Relation between shape and piezo-charges in InGaAs quantum dots
- Strain-induced piezoelectric charges are large for pyramidal shapes and small for lens shapes
- Hole tunnels faster than electron because of lower barrier
- For F = 50 kV/cm:
  - Decay time for holes ~ ns
  - Decay time for electrons ~ s
- Summary
  - Novel method to calculate 3-D electronic structure and current density of nano-structures
  - Self-assembled InGaAs quantum dots possess highly non-uniform alloy composition and can lead to
    - reversed electron-hole alignment
    - large Stark shifts and corresponding changes in optical transition rates
    - higher tunneling rate for holes than for electrons

Lens shape
- Stark shift reflects alloy profile and resulting electron and hole localization
- Electron and hole localization shows up in luminescence:
- Optical matrix element $<p|^2$
- **Strong localization of holes at top of dot**
- **Dot height**
- **Large Stark shift**

InGaAs QD’s
In n-GaAs
n-GaAs
Lens-shaped dots
- Stark shift
- Electric Field [kV/cm]
- 0.0
- 2.0
- 4.0
- 6.0
- 8.0
- 10.0
- Growth axis [nm]
- 0
- 2
- 4
- 6
- 8
- 10
- Electron tunneling
- Hole tunneling
- Energy [eV]
- 0.0
- 0.2
- 0.4
- 0.6
- 0.8
- 1.0
- 1.2
- 1.4
- Growth axis [nm]
- 0
- 2
- 4
- 6
- 8
- 10
- 12
- 14
- Energy [eV]
- 0.0
- 0.2
- 0.4
- 0.6
- 0.8
- 1.0
- 1.2
- 1.4
- Growth axis [nm]
- 0
- 2
- 4
- 6
- 8
- 10
- 12
- 14
- 16
- Growth axis [nm]
- 0
- 2
- 4
- 6
- 8
- 10
- 12
- 14
- 16
- Growth axis [nm]