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
  - ...

This work: 3-D Device simulator

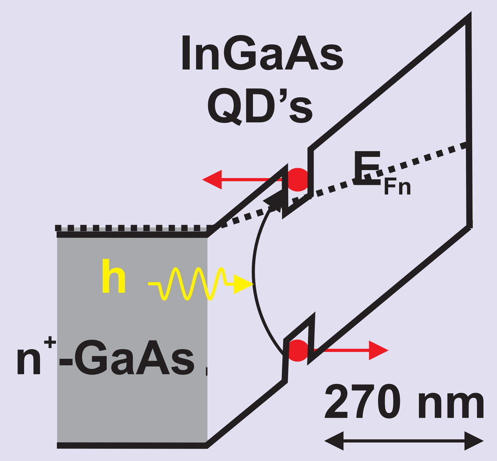
- State-of-the-art electronic structure calculation from nm to m scale for any 3-D geometry/composition and applied bias
- Calculation of carrier transport limited to situations near equilibrium

Method

- 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



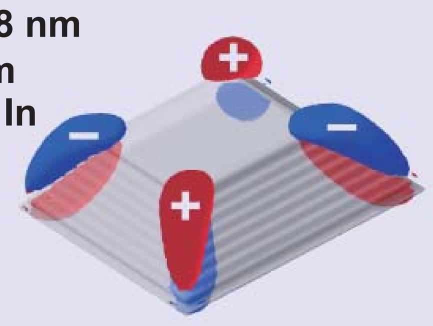
- Comparison with experimental* photocurrent data as a function of applied bias

*) Findeis et al, APL 78, 2958 (01)

Results: Relation between shape and piezo-charges in InGaAs quantum dots

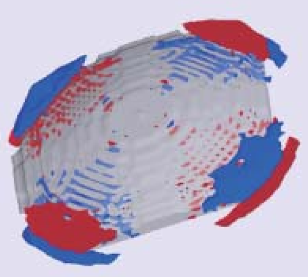
Strain-induced piezoelectric charges are large for pyramidal shapes and small for lens shapes

Height: 8 nm
: 30 nm
Av. 22% In



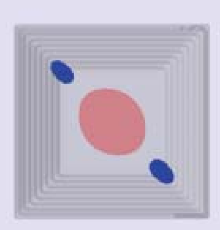
Truncated pyramid

Height: 8 nm
: 40 nm
Av. 22% In



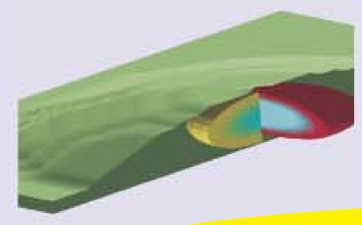
Lens shape

Localization of electrons and holes



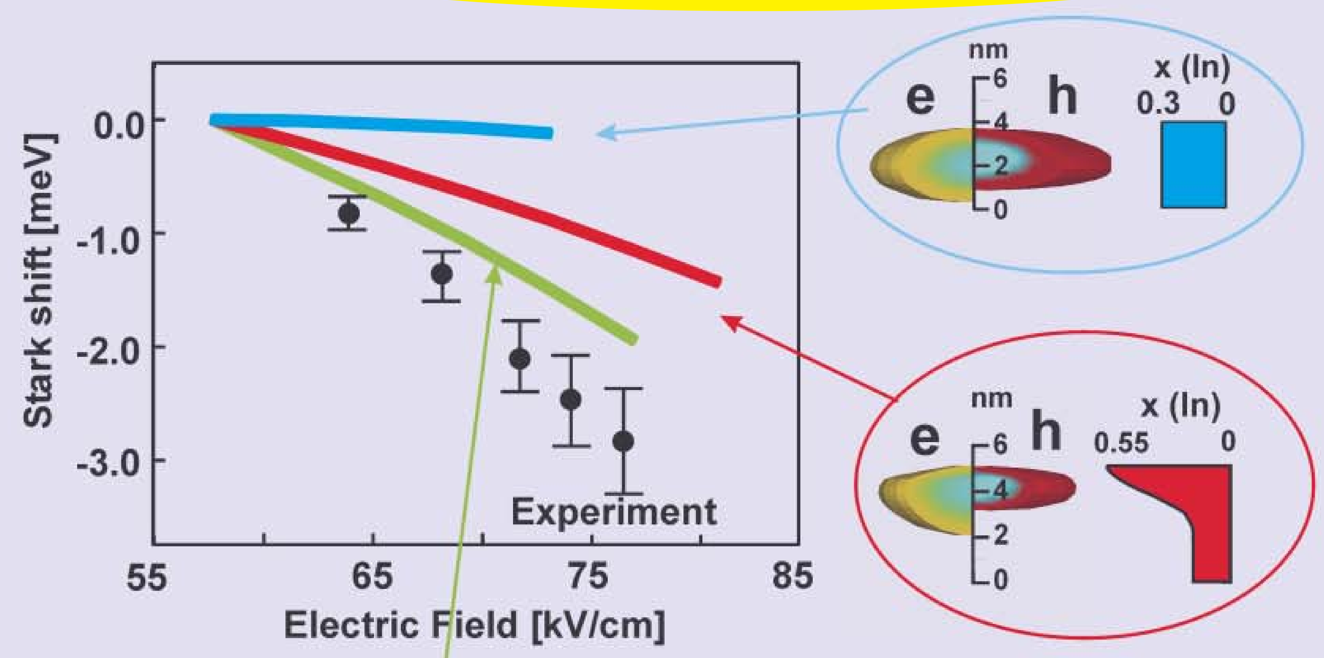
Efficient optical generation only for lens-shaped dots

Results: Exciton Stark shifts as a function of applied bias



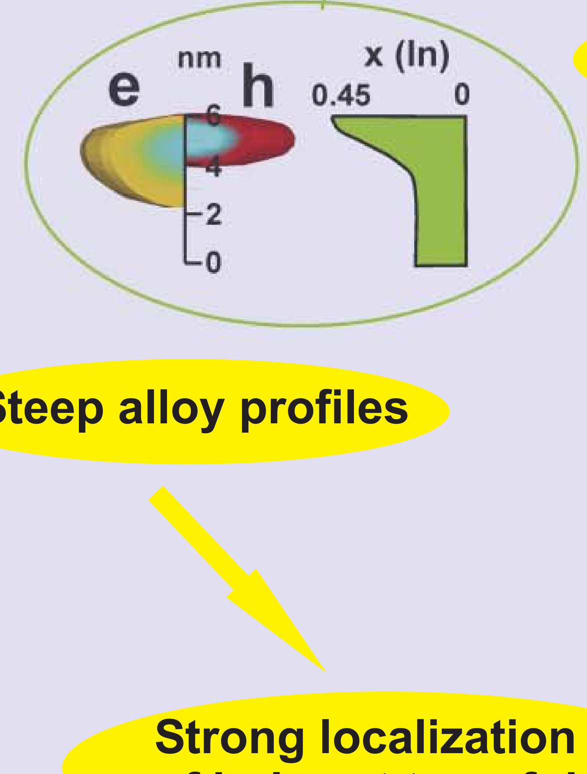
Lens-shaped dots

Stark shift reflects alloy profile and resulting electron and hole localization



Electron and hole localization shows up in luminescence:

Optical matrix element |<p>|²

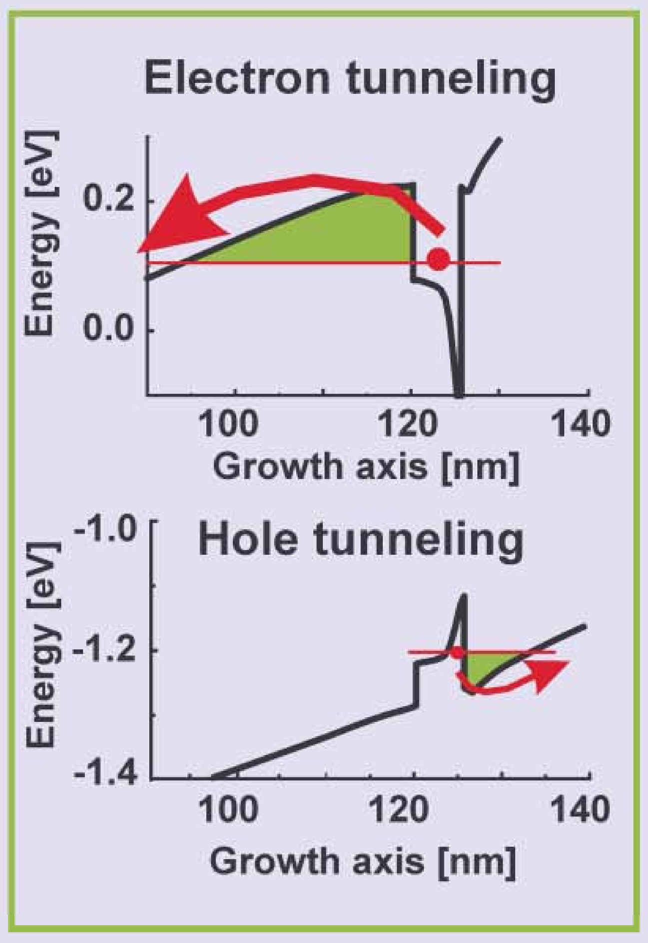


Steep alloy profiles

Strong localization of holes at top of dot

Dot height

Large Stark shift



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