nextnano³ - A powerful tool for the simulation of 3D nanometer semiconductor structures

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SFB 348 Project A4

Capabilities Overview

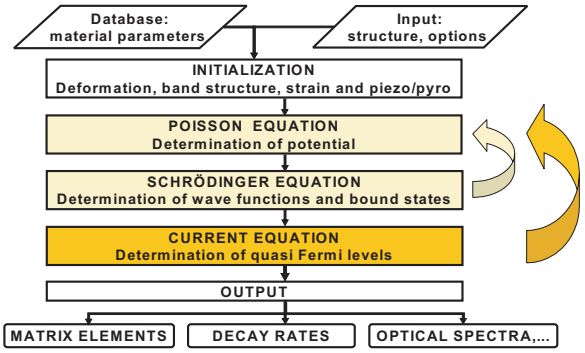
Simulation software for 3D semiconductor nano-structures

- Si/Ge and III-V materials
- Flexible structures and geometries
- Fully quantum mechanics simulation
- Equilibrium and nonequilibrium systems
- Convenient graphical device editor
- Approx. 50 regular users worldwide

❑ **Calculation of electronic structure**
- 8-band k.p-Schrödinger and Poisson equation
- Global strain minimization
- Piezoelectric and pyroelectric charges
- Exciton energies and optical matrix elements
- Magnetic fields and spin effects

❑ **Calculation of current**
- Drift-diffusion current using quantum densities
- Ballistic current through scattering theory

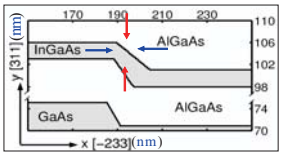
Program Flow

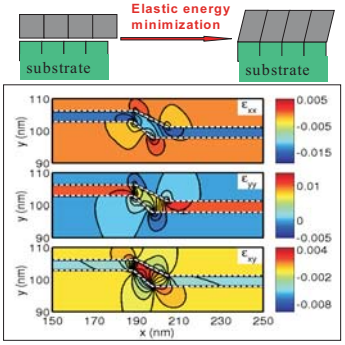


Elastic deformations – Quantum wire

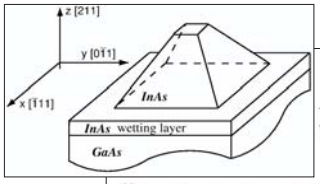
M.Povolotskyi *et al.*
University "Tor Vergata"
Rome, Italy

$In_{0.2}Ga_{0.8}As/Al_{0.5}Ga_{0.5}As$ quantum wire, grown on a patterned (311)-GaAs substrate





Elastic deformations – Quantum dot



Self-assembled InAs/GaAs quantum dot, grown on (211)-GaAs substrate

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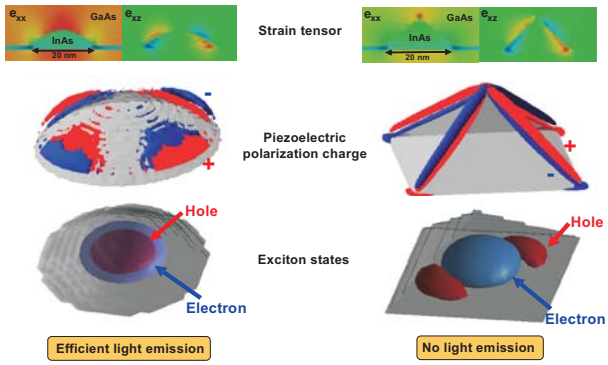
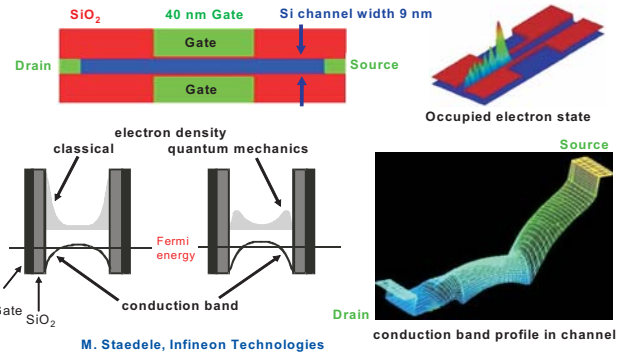
Piezoelectric charges and excitons in quantum dots



Efficient light emission

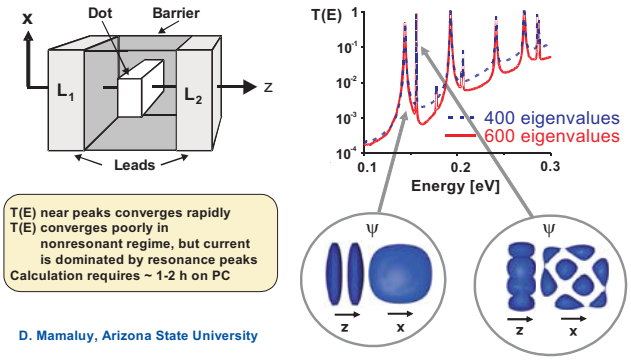
No light emission

Double-Gate MOSFET – Electronic States



M. Staedele, Infineon Technologies

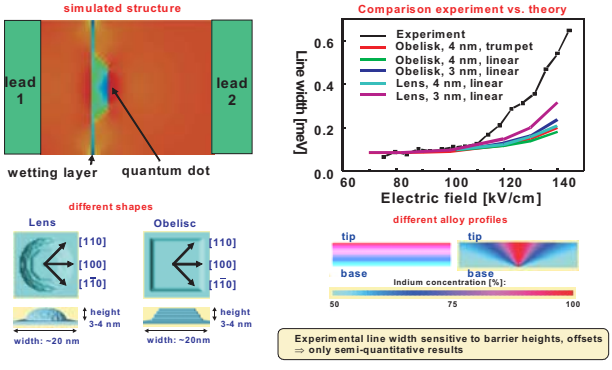
Ballistic current through a model resonant tunneling diode



T(E) near peaks converges rapidly
T(E) converges poorly in nonresonant regime, but current is dominated by resonance peaks
Calculation requires ~ 1-2 h on PC

D. Mamaluy, Arizona State University

Electron tunneling from quantum dots



Experimental line width sensitive to barrier heights, offsets
⇒ only semi-quantitative results