Quantum Dot Quantum Computing in Si:
Lifting Degeneracies with strain & confinement

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Quantum Computing Funding

Leveraged NEMO work

This research was carried out in part at the Jet Propulsion Laboratory, California Institute of Technology under a contract with the National Aeronautics and Space Administration.

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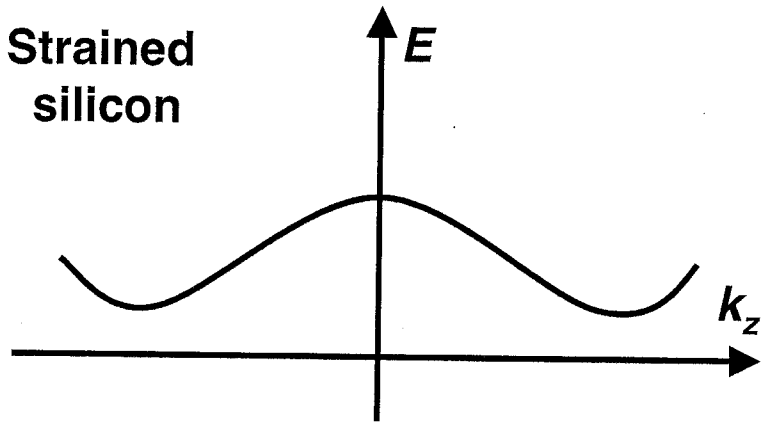
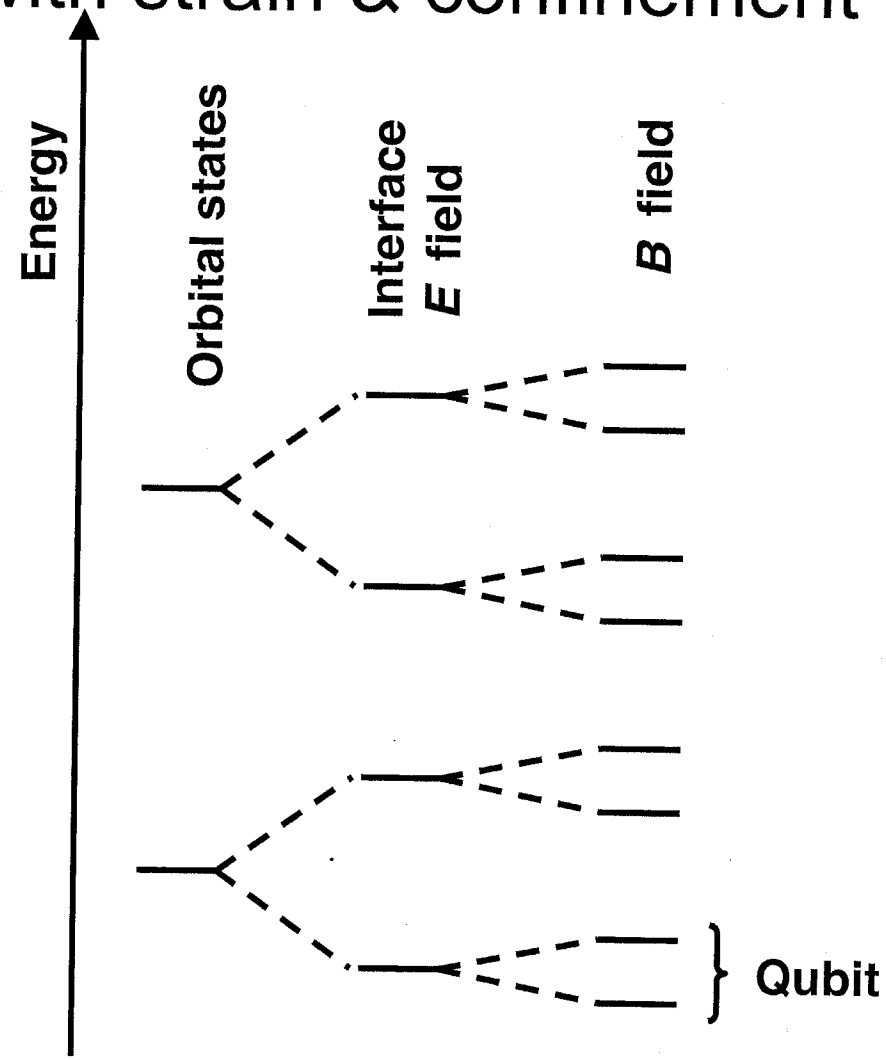


Valley degeneracy in X direction is broken by interface and electric field

Are the qubit states separated enough from higher energy states?



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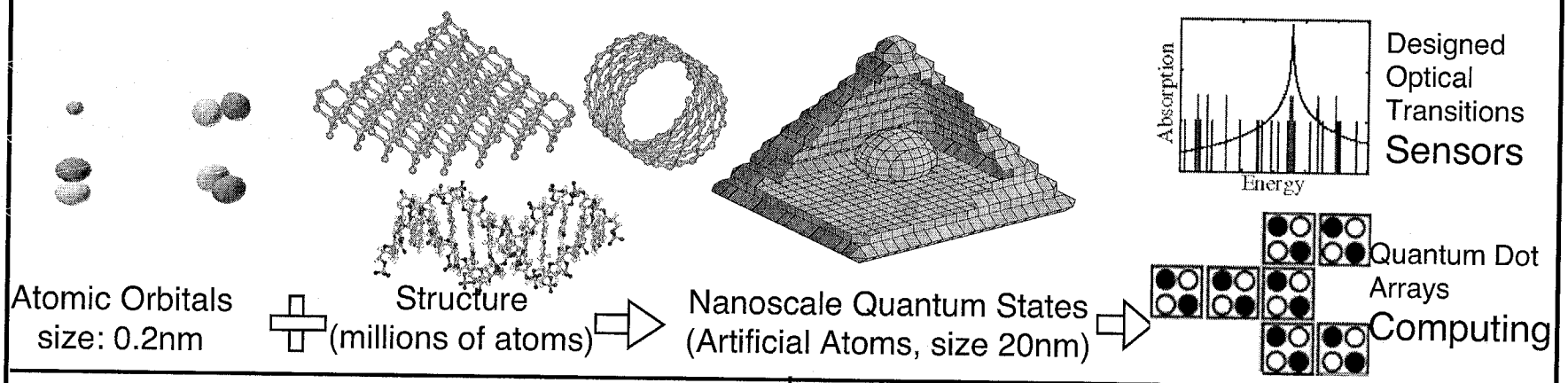
NEMO: Nanoelectronic Modeling Agenda



Problem:

Nanoscale device simulation requirements:

- Cannot use bulk / jellium descriptions, need description of the material atom by atom => use pseudo-potential or local orbitals
- Consider finite extent, not infinitely periodic => local orbital approach
- Need at minimum one million atoms. => need massively parallel computers
- The design space is huge: choice of materials, compositions, doping, size, shape. => **need a design tool**

Approach:

- Leverage NEMO 1-D:
  - 25 person years at TI / Raytheon
  - 250,000 lines of code.
- Use local orbital description for individual atoms in arbitrary crystal / bonding conf.
  - Use s, p, and d orbitals
  - Use genetic algorithm for fitting
- Compute mechanical strain in the system.
- Develop parallel algorithms to generate eigenvalues/vectors of very large matrices ($N=3.2\times10^8$ for a 16 million atom system).
- Develop prototype GUI for (NEMO-3D)

Outline

- **Bi-axial strain on Si.** Lifting 4 of the 6 degenerate valleys $\Delta E>100meV$

- **Confinement in 1D:** Valley Splitting $\Delta E\sim1meV$

- **Confinement in 3D:** (1D heterostr. & 2D lat gates & mag. field) $\Delta E\sim0.1meV$

- **Conclusions**

Tight Binding Material Parameterization

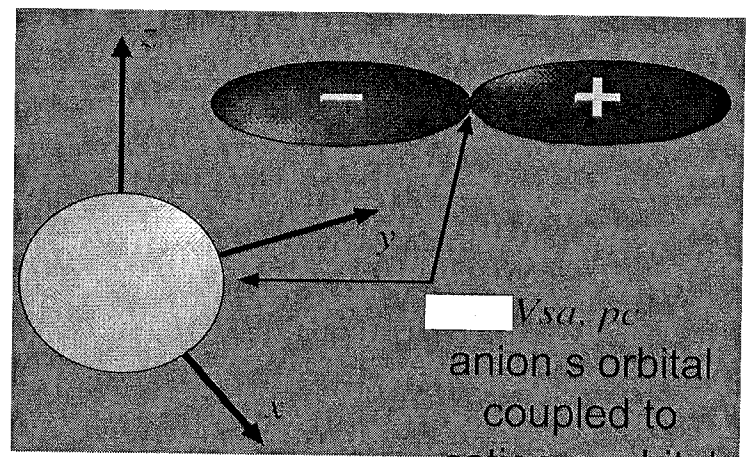
Bulk Semiconductors are described by:
- Conduction and valence bands, bandgaps (direct, indirect), effective masses
- 10-30 physically measurable quantities

Tight Binding Models are described by:
- Orbital interaction energies.
- 15-30 theoretical parameters

Analytical approach:
- Exact diagonalization at Γ for $sp^3d^5s^*$
- Formulas developed by Tim Boykin at UAH for effective masses and bandgaps from interaction energies

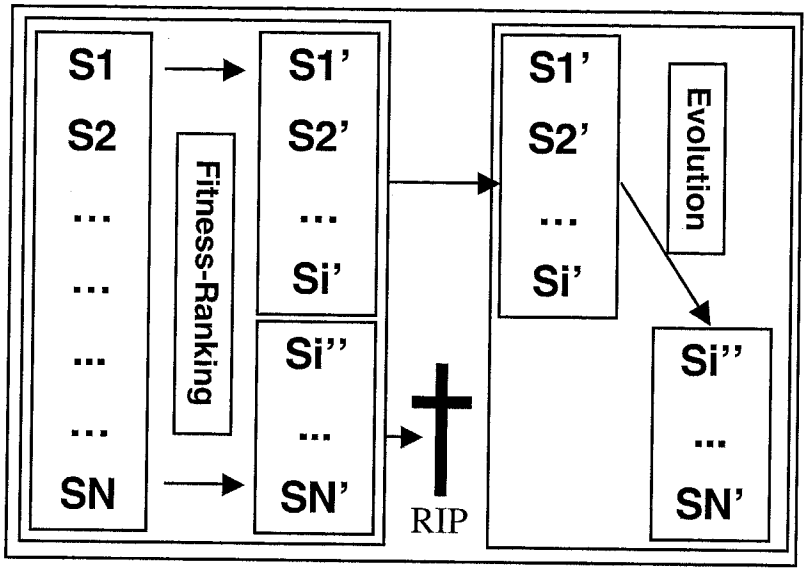
Numerical approach:
- Use a genetic algorithm to do fitting.

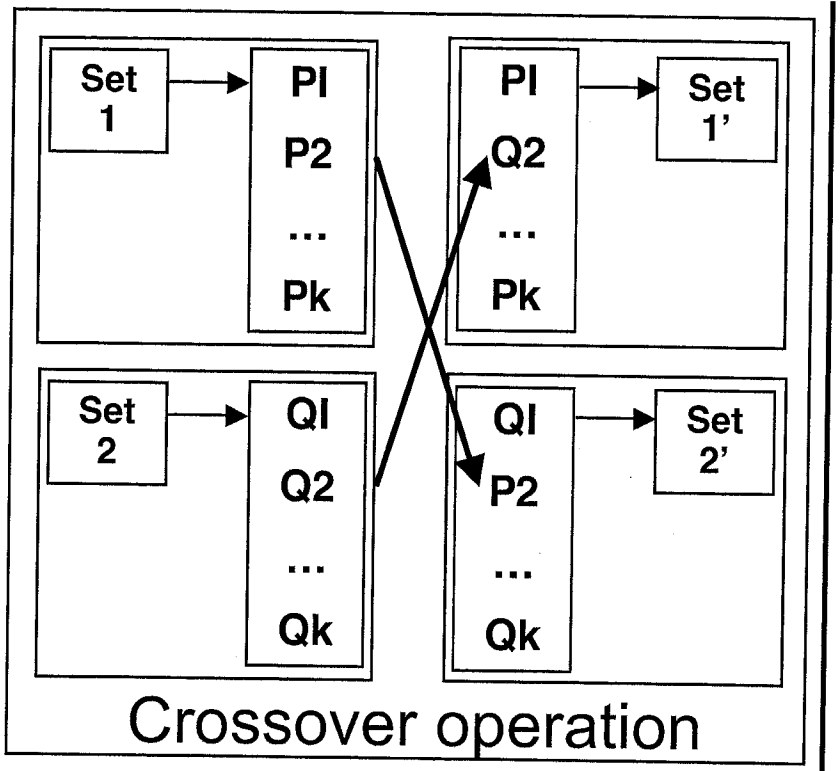
- Match experimental data in various electron transport areas of the Brillouin zone:
  - Effective masses of electrons at Γ, X and L
  - Effective masses of holes at Γ
  - Band edges at Γ, X and L

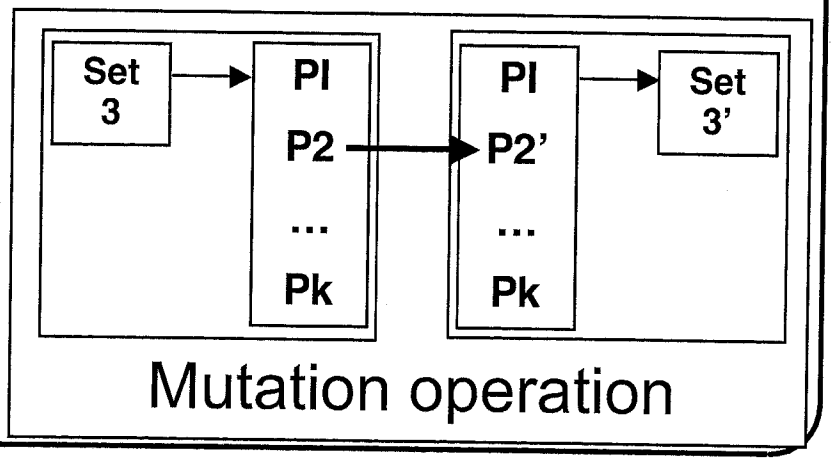


15-30 theoretical interaction energies

Genetic Algorithm





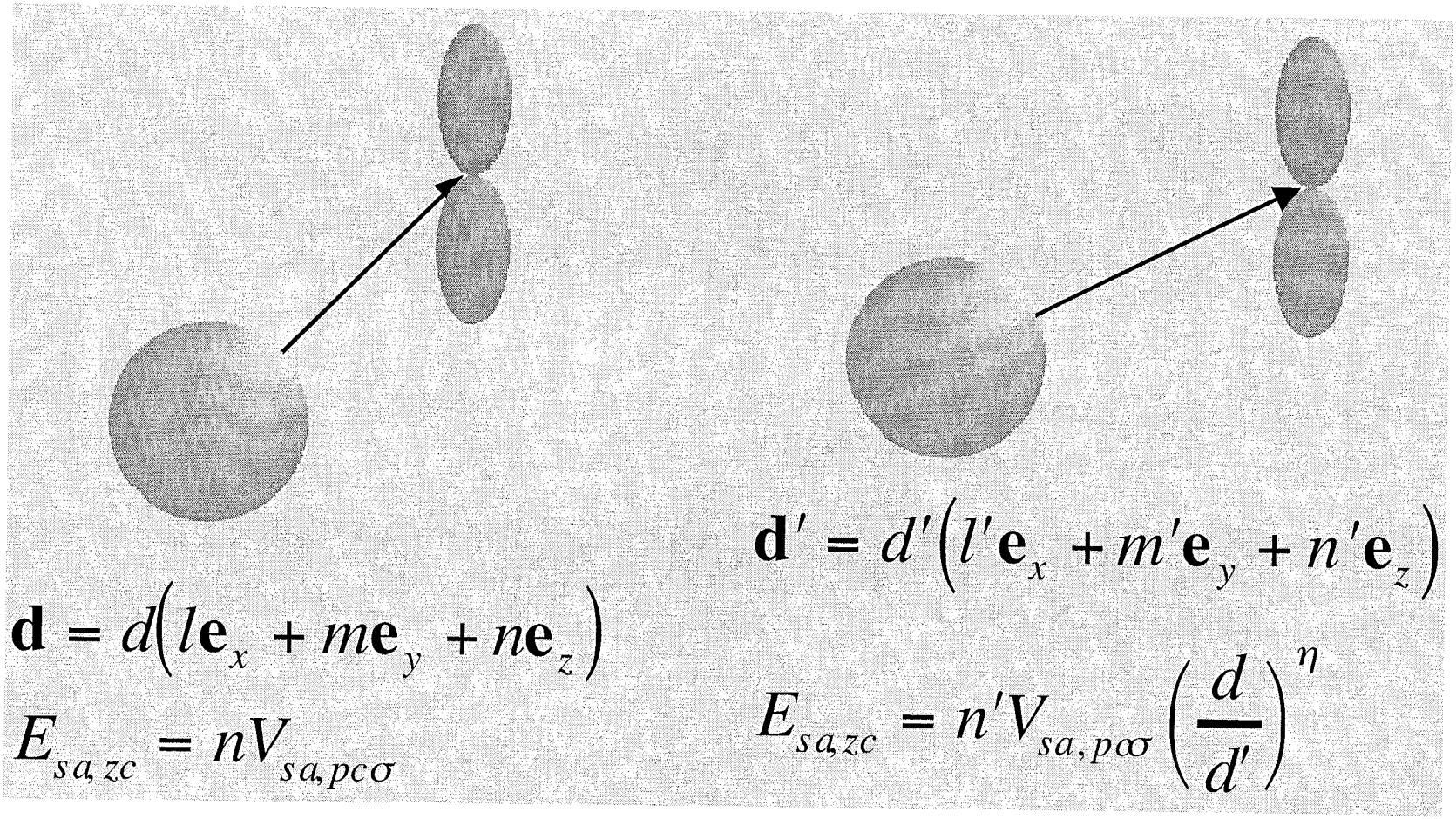


- Genetic algorithm parameter optimization is based on:
  - Survival of good parameter sets
  - Evolution of new parameter sets
  - Persistence of diversity (ensures global exploration)

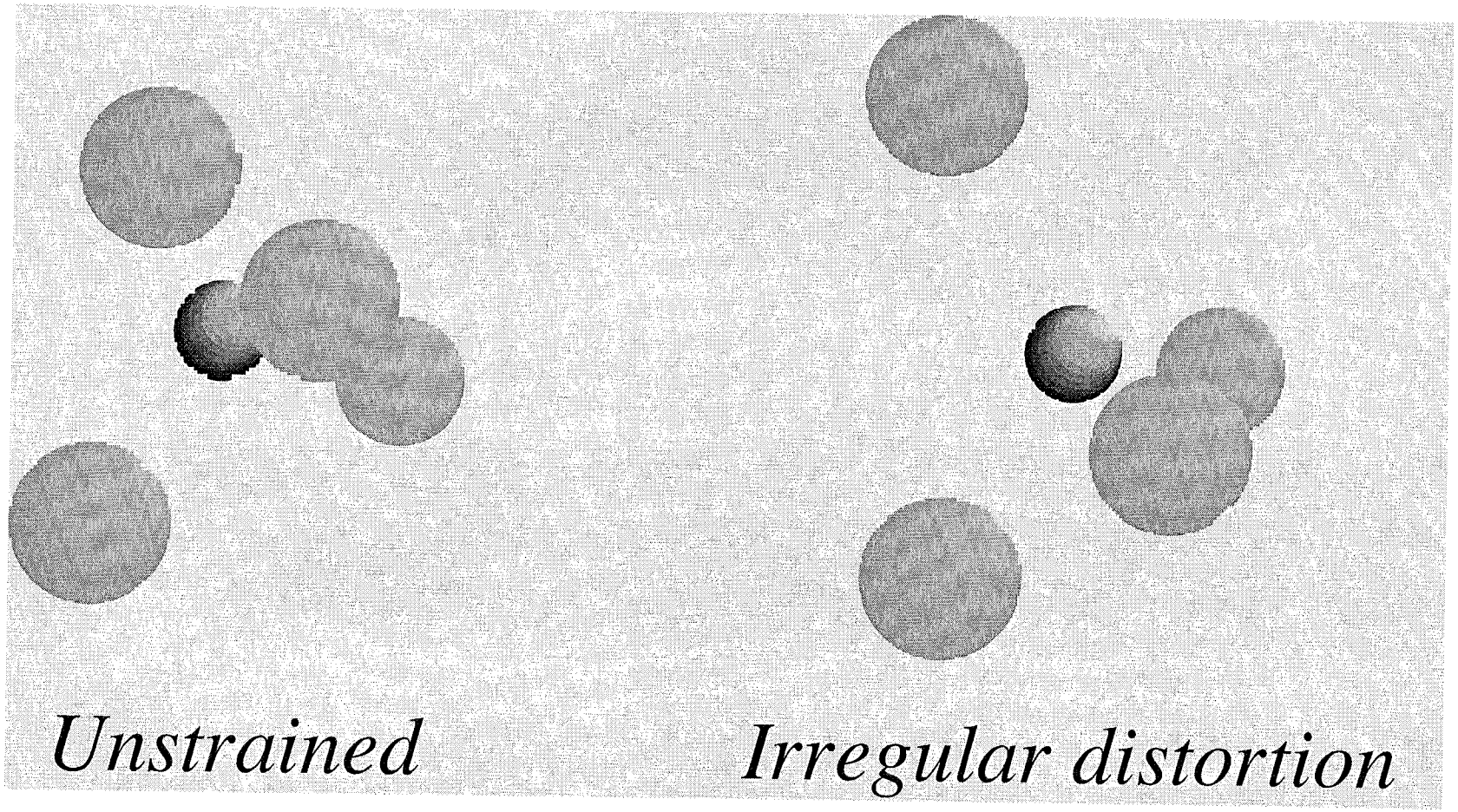
- Basic Operations:
  - Crossover – gross exploration
  - Mutation – fine tuning

Modeling Strain

Bond Lengths and Angles Change



Distortions: Regular and Irregular



On-site Parameters Change

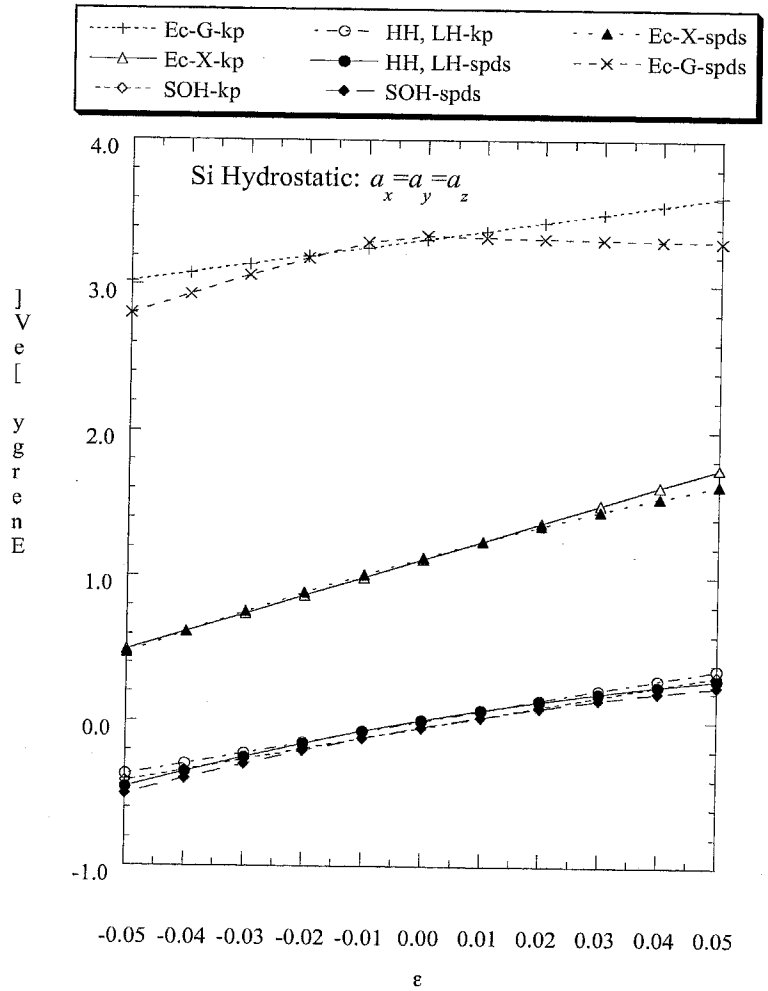
- Overlaps of true atomic orbitals change due to altered bond angles, lengths
- Must compute new orthonormal basis – use Lowdin procedure
- Need new overlaps – use Harrison's form

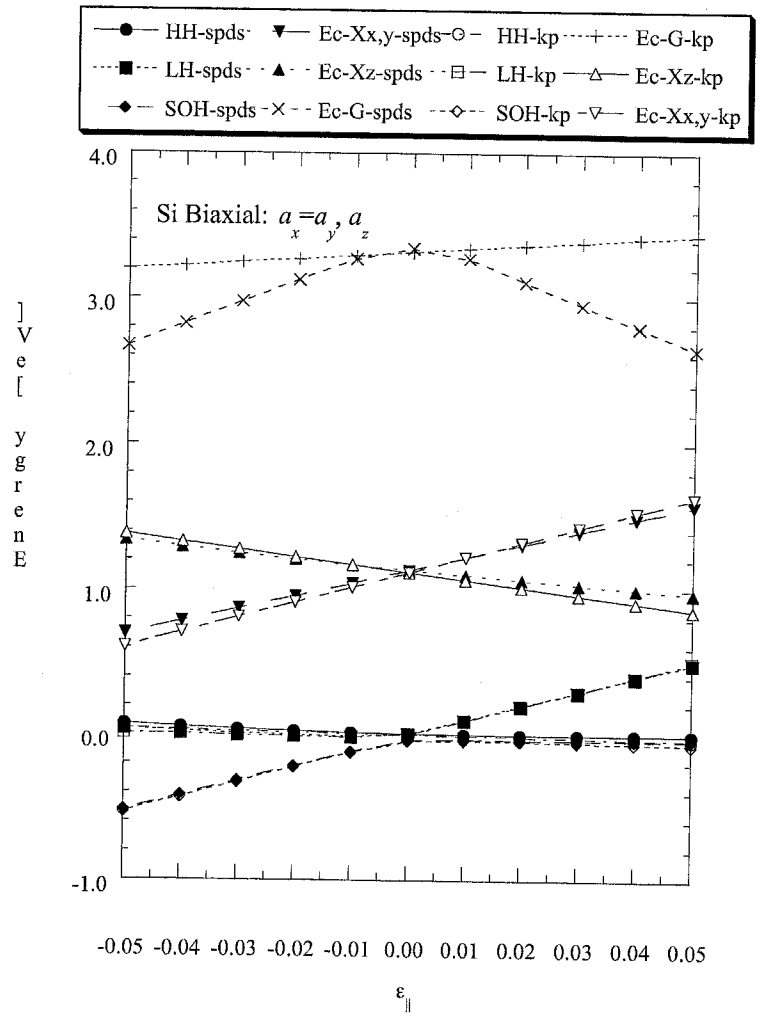
$$S_{(n',\mu'),(n,\mu)} = K_{(n',\mu'),(n,\mu)} \frac{v_{(n',\mu'),(n,\mu)}}{\varepsilon^{(0)}_{(n',\mu')} + \varepsilon^{(0)}_{(n,\mu)}}$$

- Gives new nearest-neighbor parameters
- ALSO give new On-Site parameters
- New fitting parameters, *C*, which characterize changed overlaps
- Procedure valid for arbitrary displacements
- End result is…

$$\varepsilon'_{i,\alpha} = \varepsilon_{i,\alpha} + \sum_{\substack{j,\beta \\ j \in NN-i}} C_{(j,\beta),(i,\alpha)} \frac{v^2_{(j,\beta),(i,\alpha)} - v'^2_{(j,\beta),(i,\alpha)}}{\varepsilon_{j,\beta} + \varepsilon_{i,\alpha}}$$

Si: Strain Behavior





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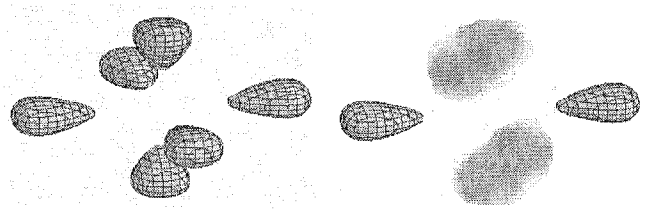
Outline

- **Bi-axial strain on Si.** **Lifting 4 of the 6 degenerate valleys ΔE>100meV**

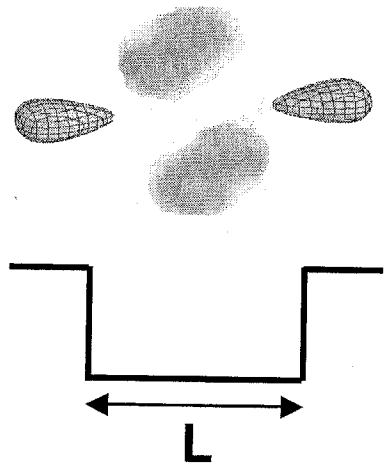


- **Confinement in 1D:**

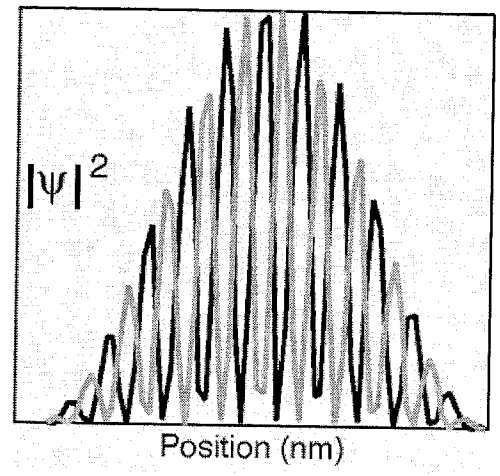
- **Confinement in 3D:**

- **Conclusions**

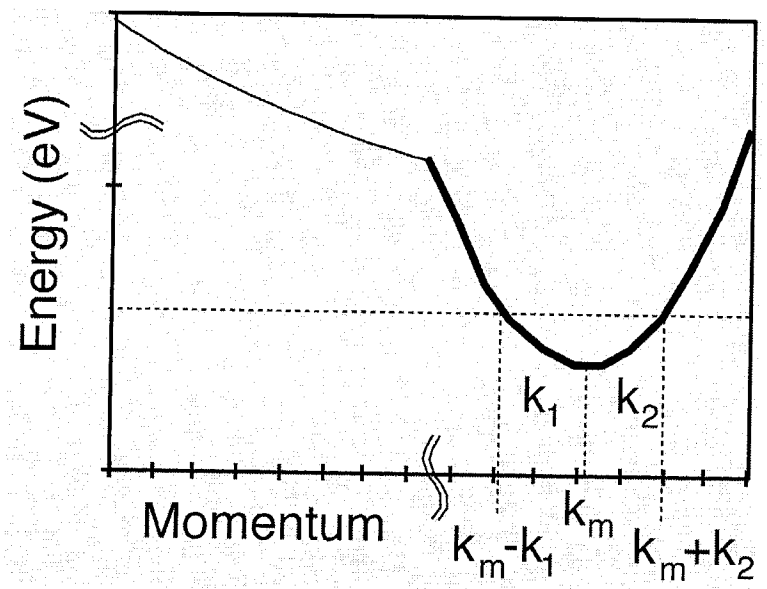
1D Confinement Creates Valley Splitting:



$k=\pi/L$



Valley Splitting ΔE~1meV



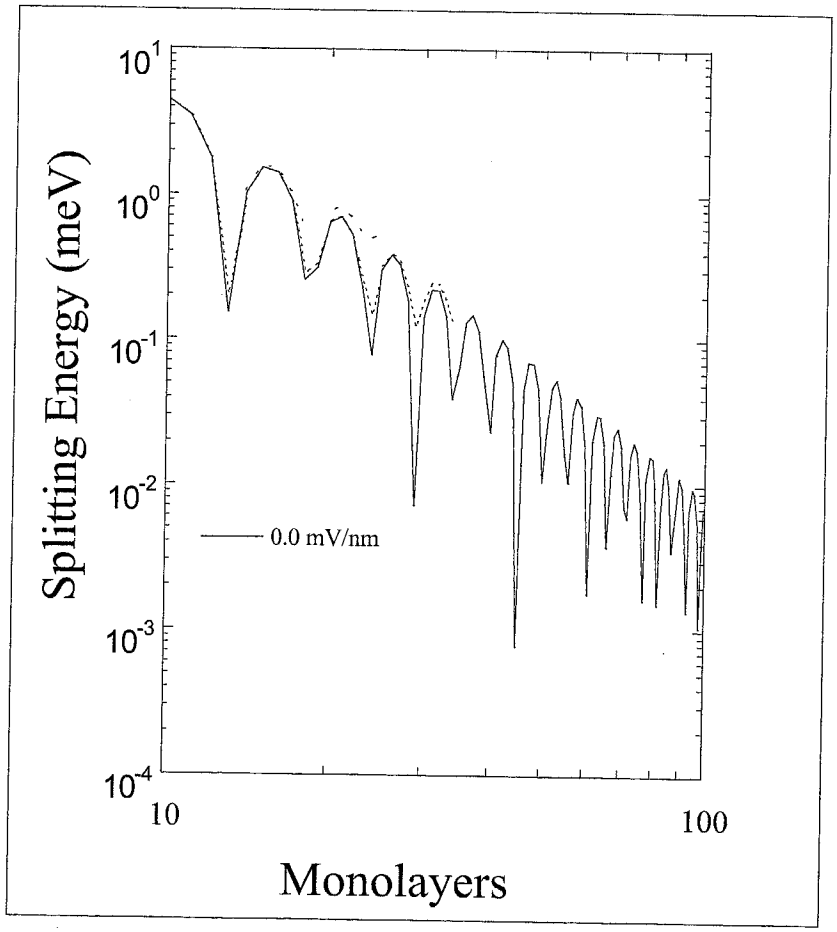
4 propagating states

↓

2 bound states
$k_{1,2}$ envelope
k_m fast oscillations

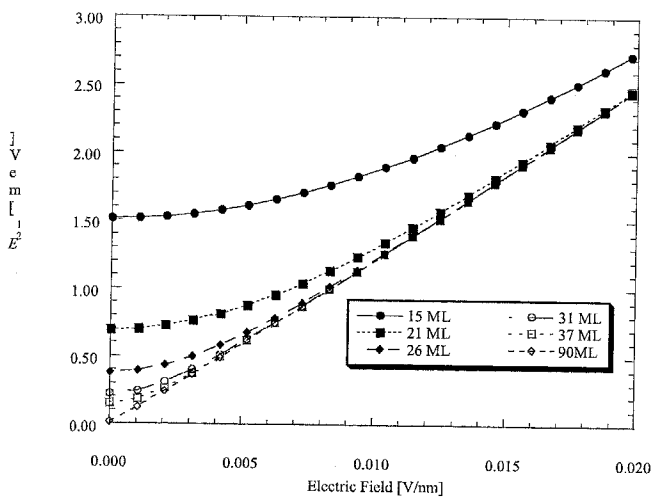
Splitting Behavior With Quantum Well Width

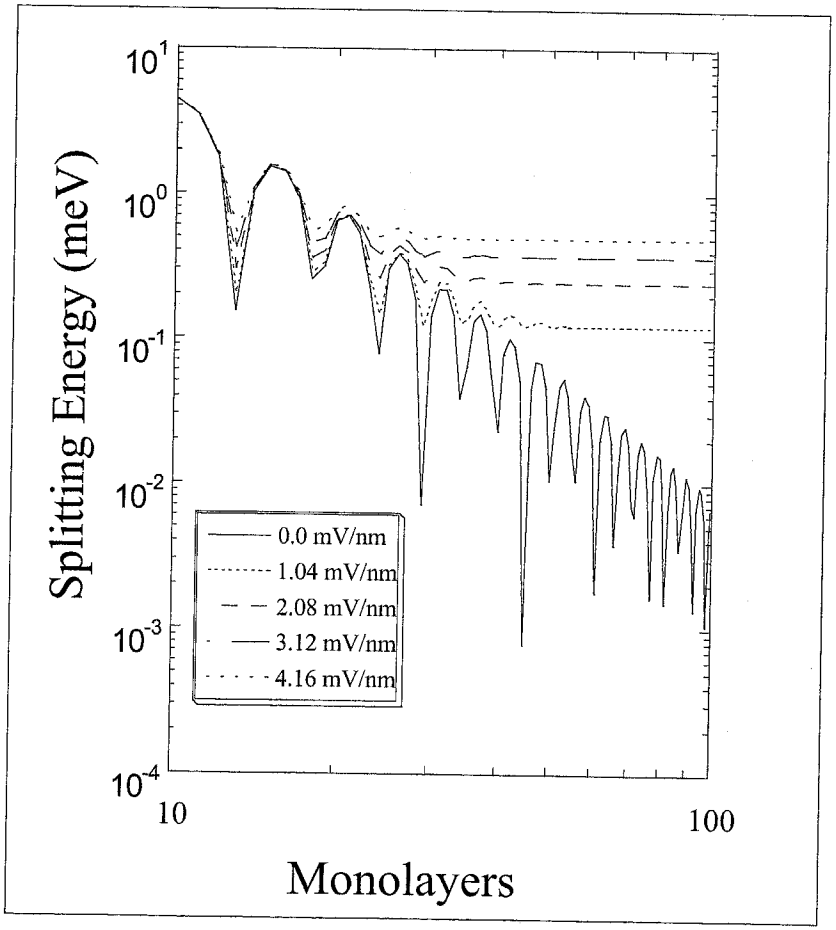
- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers (decay as ML^{-3})



Splitting Behavior With Quantum Well Width and Electric Field

- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting
- For fixed *L*, splitting linear at high field, nonlinear at low field





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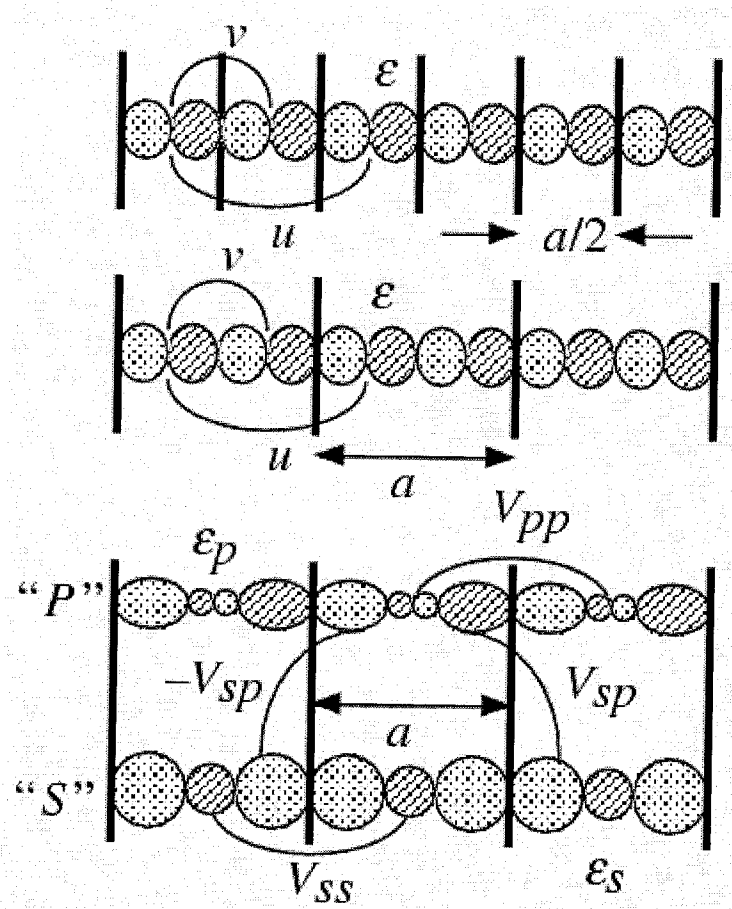
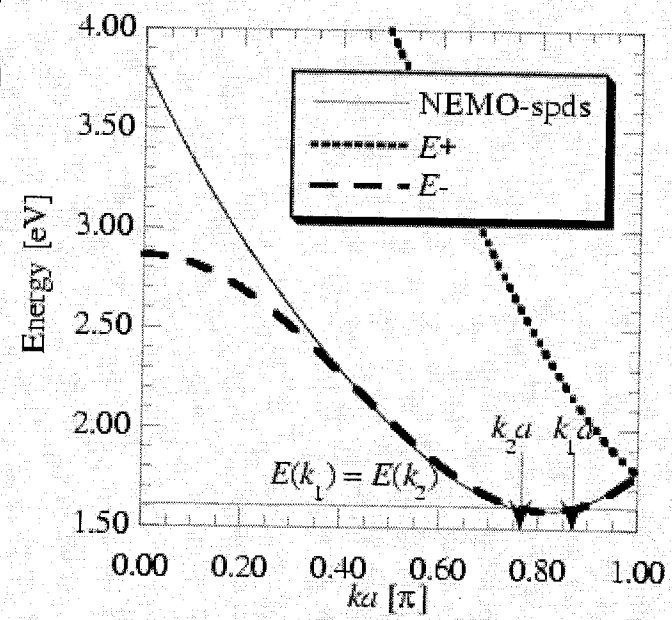
Analytical Model: 1-band and 2-band tight binding

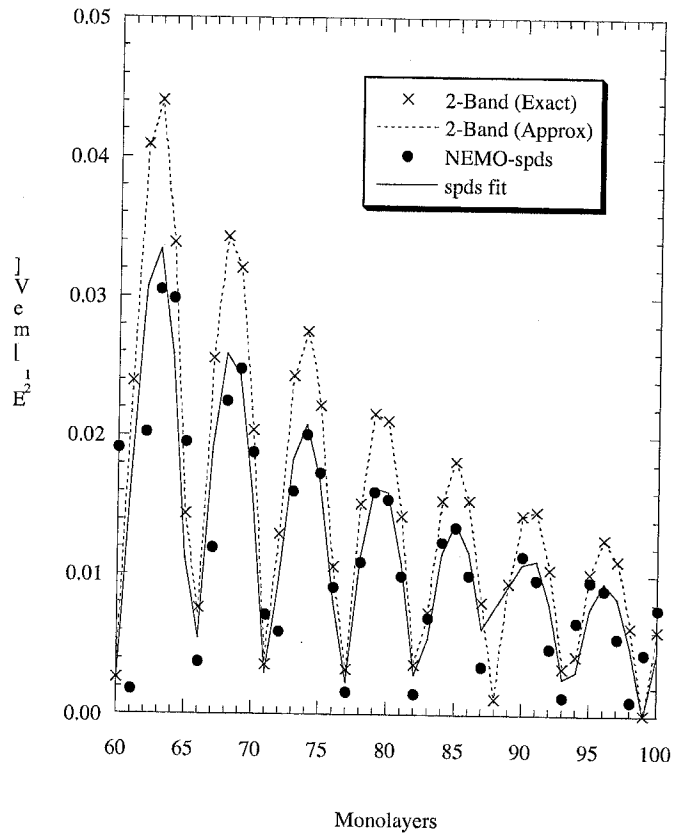




Splitting: 2-Band and spds

- Zero field splitting oscillates with *L*
- Strained Si QW, hardwall BCs
- Calculated with NEMO and 2-Band
- Minima occur when phase-matching of the 2 states are nearly the same at interfaces
- Splitting follows same functional form for both (*S* = no. atoms):

$$E_{21} \approx \frac{16\pi^2 u}{(S+2)^3}\left|\sin\left[(S+2)\phi_0\right]\right|\sin(\phi_0), \quad \sin(\phi_0) = \sqrt{1-\left(\frac{v}{4u}\right)^2}$$



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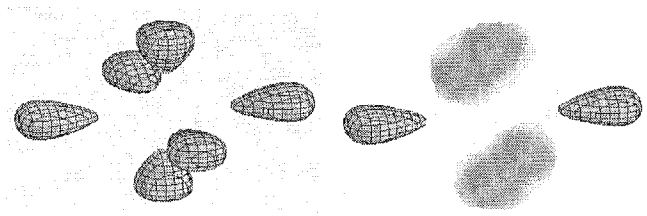

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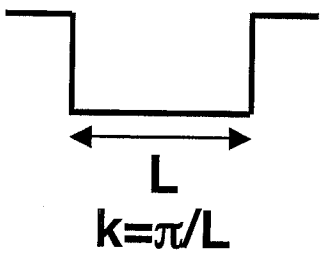

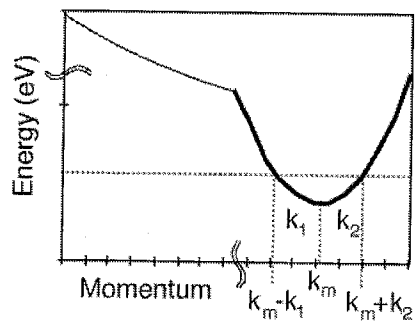

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2 bound states
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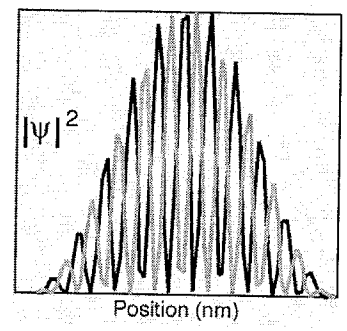
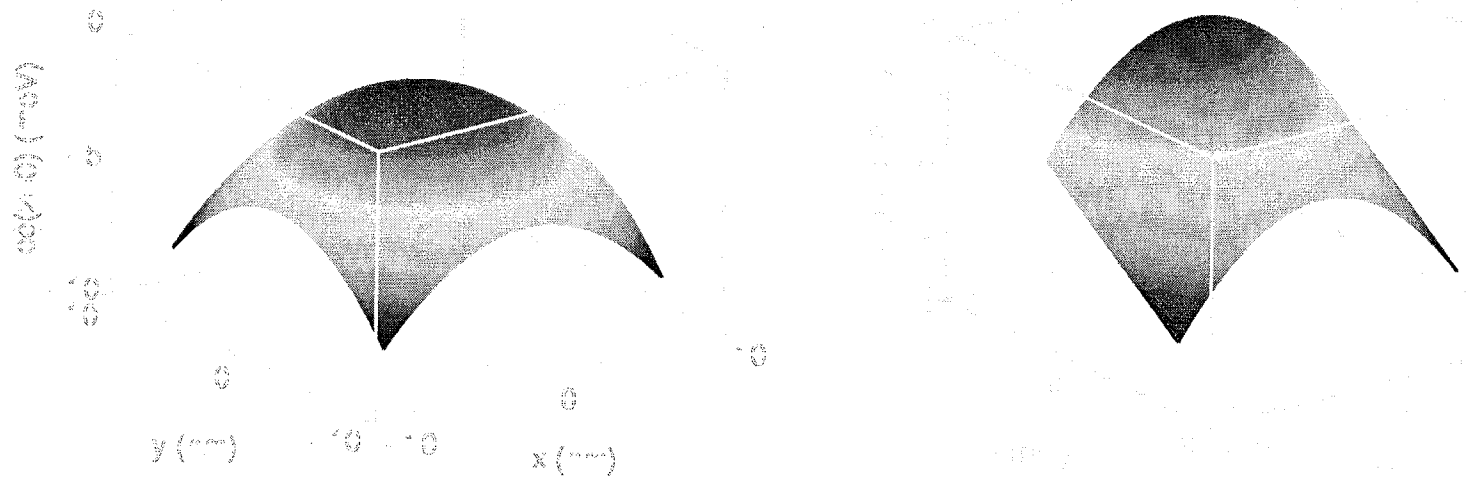


- **Confinement in 3D:** **(1D heterostr. & 2D lat gates & mag. field)**

- **Conclusions**

1D Heterostructure Confinement
2D Electrostatic confinement in Si QW



- **Geometry:**
  - **5nm quantum well lattice-matched to $Si_{0.2}Ge_{0.8}$ (0.8% tensile strain)**
  - **non-zero field along z and lateral electrostatic confinement.**
  - **Rescaled problem size from ($5x10^4$ atoms) WI group**

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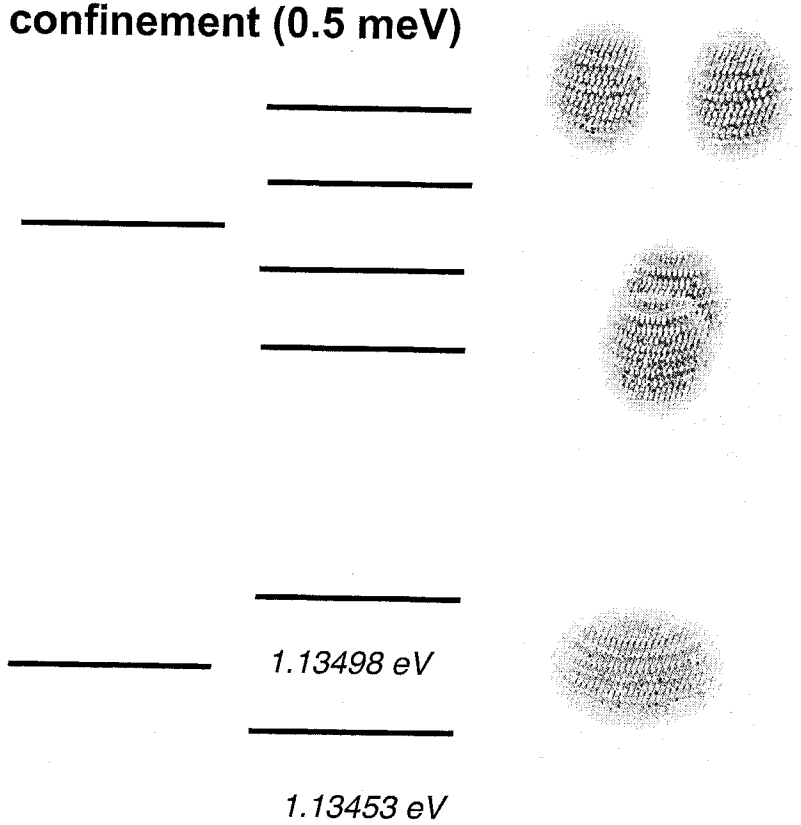
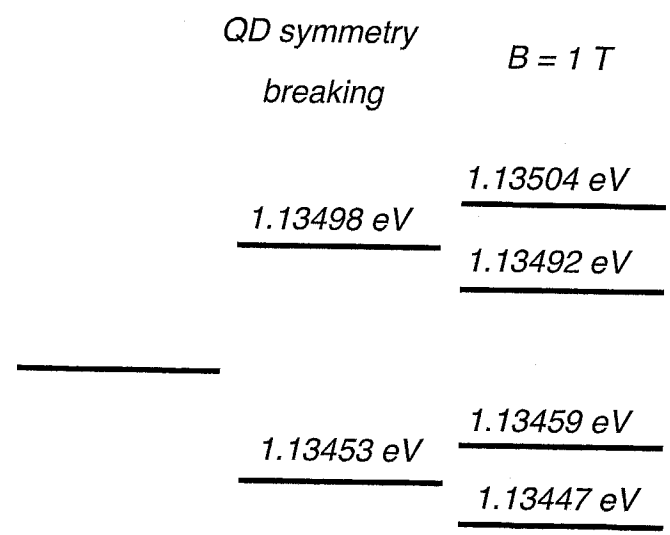
Relative Size of State Splitting
3-D Electronic structure of low-lying states

- Valley splitting due to breaking of translational invariance is typically smaller than splitting due to confinement (0.5 meV)



- Even with a large B=1T, Zeeman splitting is much smaller than valley splitting (~0.12 meV).



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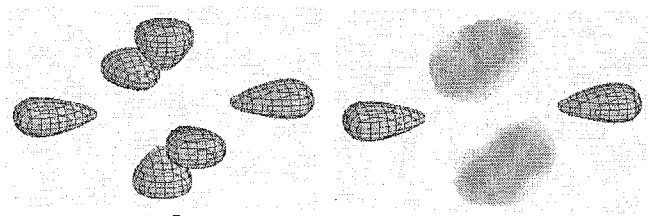

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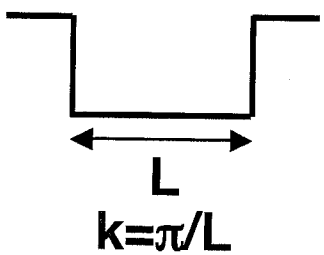

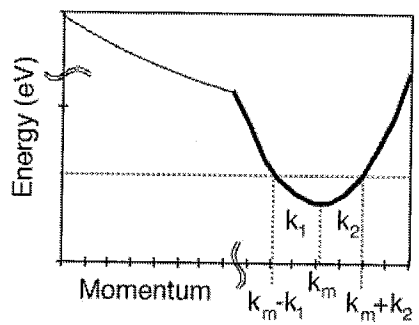

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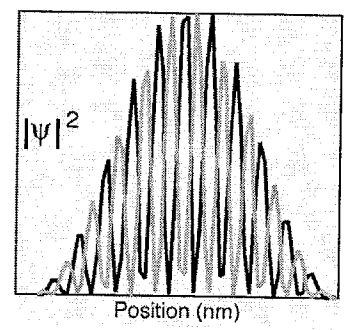


- **Confinement in 3D:** **(1D heterostr. & 2D lat gates & mag. field) ΔE~0.1meV**

- **Conclusions**

Conclusions

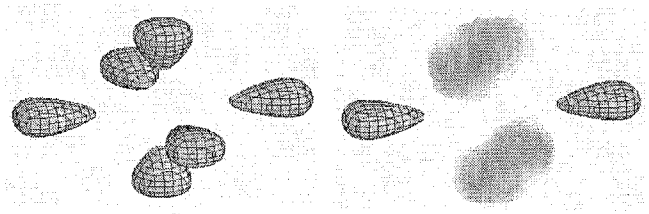
- Proper handling of distortions in Si is important
- Must adjust on-site Hamiltonian parameters to get correct behavior
- Our method works for arbitrary distortions
- Use these parameters to study splitting in QWs
- Find oscillations with well width
- Oscillations quenched by electric field
- Should see similar behavior in quantum dots

Backup

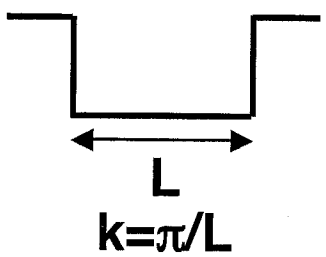
Quantum Dot Quantum Computing in Si:

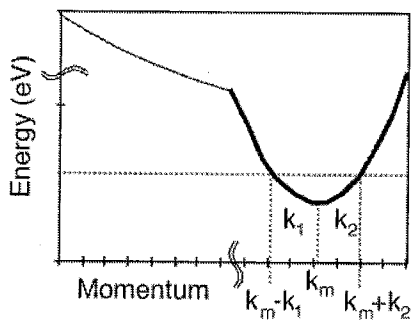
Lifting Degeneracies - strain & confinement

- **Bi-axial strain on Si. Lifting 4 of the 6 degenerate valleys ΔE>100meV**



- **Confinement in 1D: Valley Splitting ΔE~1meV**





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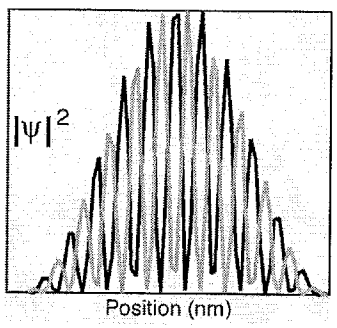

- **Confinement in 3D: (1D heterostr. & 2D lat gates & mag. field) ΔE~0.1meV**

- **Conclusions**

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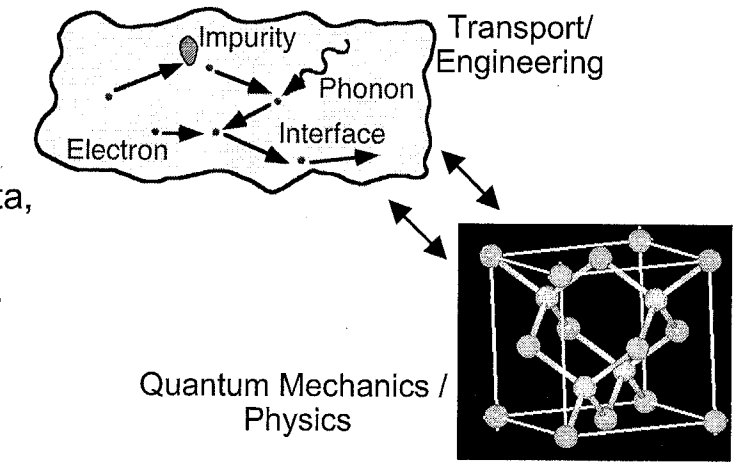
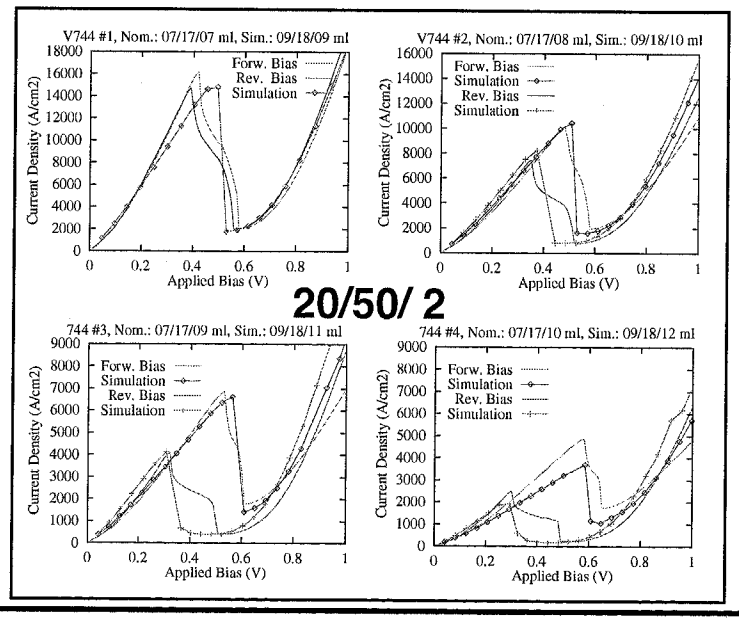
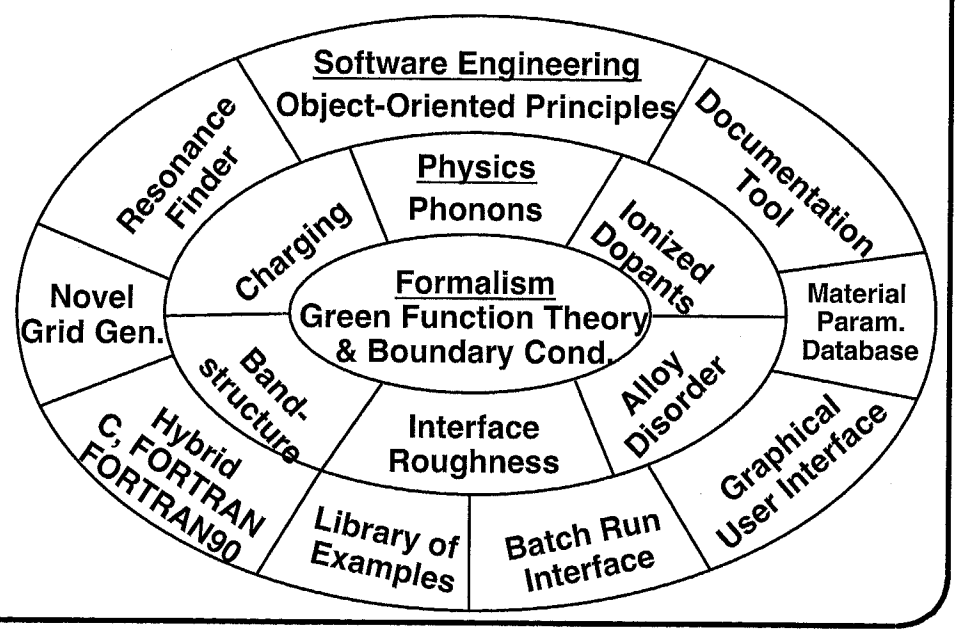
Leverage NEMO 1-D: A User-friendly Quantum Device Design Tool

- NEMO was developed under a government contract to Texas Instruments and Raytheon from 1993-97
  - >50,000 person hours of R&D
  - 250,000 lines of code in C, FORTRAN and F90
- Based on Non-Equilibrium Green function formalism (Datta, Lake, Klimeck).
- NEMO in THE state-of-the-art heterostructure design tool.
- Used at Intel, Motorola, HP, Texas Instruments, and >10 Universities.



Testmatrix



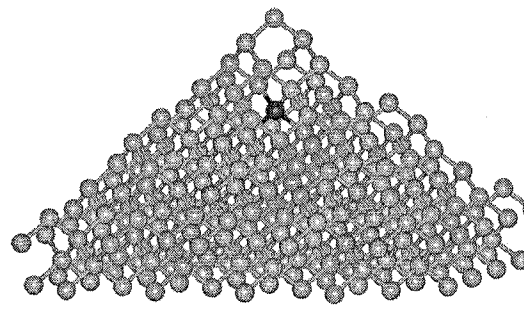


NEMO 3-D Conclusion / Future Vision

Atomistic Simulation (NEMO 3-D):
- Fitting tight binding sp3s*,sp3d5s*
- General structure input
- Several million atom solutions
- Parallel eigenvalue solvers
- Strain simulations

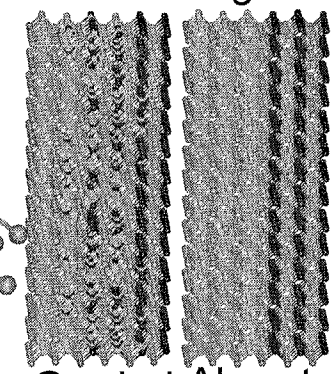
- Studied effects of alloy disorder on optical transitions and wavefunctions.

Quantum Dots



Atomistic Simulation

Grading



Graded Abrupt

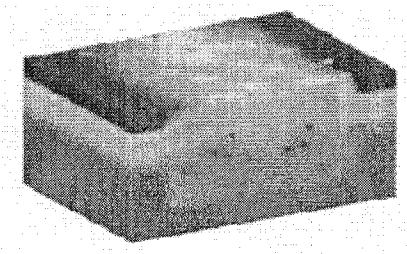
=> Quantum Computing

Extension of NEMO 3-D to Spintronics:
- Arbitrary magnetic fields
- Magnetic impurities
- Many-body interactions (electrons, phonons, photons)
- Open boundary conditions

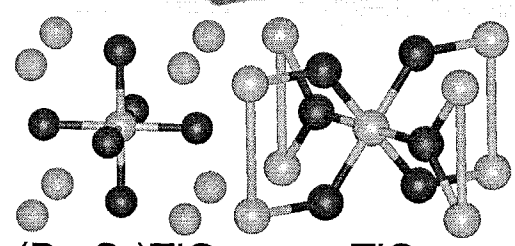
- Extension of NEMO 1-D to Spintronics:
  - DC Spin transport RTD-like structures
  - Time dependent spin - transport

End of SIA Roadmap

Dopant Fluctuations in Ultra-scaled CMOS



Electron Transport in Exotic Dielectrics



$(Ba,Sr)TiO_3$ TiO_2

Atomistic Quantum Device Simulation in the Si, Ge, and SiGe Material Systems with Realistic Bandstructure

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