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Parameterization:
- TB parameters determined from genetic algorithm to match experimentally measured band edges and masses.

Mechanical Strain:
- CG-based minimization of mechanical strain to determine atomic positions

Electronic Structure:
- Custom Lanczos eigenvalue solver

Numerical Simulation:
- Problem size is large: 100 GB is typical storage requirement for Hamiltonian
- Parallel implementation of both strain and electronic structure calculation is necessary!
- 1D data decomposition
• Divide Simulation domain into slices.
• Communication only from one slice to the next (nearest neighbor)
• Communication overhead across the surfaces of the slices.
• Limiting operation: sparse matrix-vector multiplication
• Enable Hamiltonian storage or re-computation on the fly.
• Eigenvalue computation ranging from 1/4 to 16 million atoms
• Large problems are too big for a single CPU (memory requirements)
• sp3s* basis set, Matrix sizes up to $1.6 \times 10^8 \times 1.6 \times 10^8$
• Recompute Hamiltonian matrix on the fly.
• Measure time for 30 Lanczos iterations, Full problem 1000-5000 iterations
• 1 million atoms 5000 iteration 1 CPU: ~48 hours  20 CPUs: ~3.4 hours
• Computation time linear in system size.
Problem (1 million atoms):
- Serial strain computation: ~43 min.
- Serial electronic structure calculation (1000 iterations): ~ 9.6 hours
- Parallel electronic structure computation on 20 CPUs: ~41 min.

Solution:
- Parallelize strain calculation as well

Result:
- Reduce time to 2-5 minutes on a parallel machine.
- See difference between a fast 2Gbps and a 100Mbps network.
- Do not see that difference in the electronic structure calculation.
- Parallel strain computation is more communication dependent than the electronic structure calculation.
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 \( \Gamma \) for \( \text{sp}^3\text{d}^5\text{s}^1 \)
- Formulas developed by Tim Boykin at UAH (subcontract) 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 \( \Gamma \), X and L
  - Effective masses of holes at \( \Gamma \)
  - Band edges at \( \Gamma \), X and L

15-30 theoretical interaction energies
- Total strain energy (computed from Keating model) is minimized through CG-based algorithm
- Periodic boundary conditions require relaxation of the period
- InGaAs bond length distribution:
  - VCA on the bond length is incorrect
  - Locally, InAs and GaAs (mostly) maintain their bond length character
Problem:

- VCA provides generally a linear bandgap if interpolated from the binaries GaAs, AlAs, and InAs.

Approach:

- sp3s* tight binding model
- Perform 3-D alloy simulation of the bandedges.
- Represent each individual atom in the chunk of material
- 3-D random alloy simulation matches experimental data well.

AlGaAs:

- VCA derived from pure GaAs and AlAs results in an wrong bandgap.
- 3-D simulation gives the correct bowing.

InGaAs:

- Improved bowing versus the VCA.
- Still a problem with over estimating the band gap
  -> parameterization dependent
• Concentration may vary stochastically as well.
• Concentration noise is larger than configuration noise.
• For a system containing 1000 atoms, the variation is about 10-15 meV
  • Conduction band noise shows a significant feature at the Γ-X transition (Al~0.45)
  • Valence band dependence is much smoother.
- Cutaway of simulation domain
- Coupled InAs QDs: Diameter = 18 nm; QD separation = 5 nm
Unstrained system:

- Slight variation in the geometry of the two QDs breaks degeneracy.

- Compressive strain on the QD effectively raises $E_c$ within QD. Without strain, potential well confining electrons is deeper and essentially decouples the two QDs.
**Strained Coupled QD:**
- In absence of electron-electron interaction, ground state is bonding state; first excited state is anti-bonding state.
- Energy split (17 meV) is dependent on wave function overlap.
- Proper inclusion of strain is necessary to obtain correct eigenstates!
• Examine strain along major symmetry axis (z) for primitive cells centered about As atoms

• Tensile bi-axial strain outside QD ($\varepsilon_{||}>0$) due to stretching of GaAs to match InAs. Compressive strain in QD.

• Lattice constants follows same trends.
In-As bonds compressed in x-y
   -> Ec raised from bulk value of ~0.58eV to ~1.2eV
   -> Ev HH raised from bulk value of ~0.22eV to ~0.3eV
Ga-As bonds compressed in x-y and stretched in z inside dot
   -> Ec raised from bulk value of ~1.42eV to ~1.55eV
   -> Ev raised from bulk value of 0eV to ~0.1eV
- \( E_c \text{ and } x \) weakly correlated
- \( E_c \text{ and } E_v \) strongly correlated
- Cell granularity \( \sigma = 4.5 \text{meV} \)
- Atomic granularity \( \sigma = 2.3 \text{meV} \)
Effect on ground state electron energy:

- System: Dome-shaped In$_{0.6}$Ga$_{0.4}$As QD, 15nm radius; 5.4 nm height

  \textit{BC}: no constraints on QD; strain and ground state energy are underestimated

  \textit{BC}: QD boundary pinned; strain and ground state energy are overestimated

  \textit{BC (k_{supercell}=0)}: Eigenvalues lie in between free and fixed case, but results are much closer to case of free BC.

Conclusions:

- Overall convergence is slow.

- Varying only vertical buffer size gives a good approximation.
Question: What is the contribution of alloy disorder to linewidth broadening?

- Previous PL experimental results have found large contributions due to inhomogenous broadening (~30 meV) [R. Leon et al., PRB, 60, pR8517]

- Single QD PL measurements have found narrow linewidths (~0.9 meV) [Nagamune, APL, 67, p3257]

Computation:
- Use a ‘direct sampling method’ (roughly 100-200 samples)
- Assume no correlation between location of In, Ga cations within the QD

Results:
- Convergence is slow but can place an upper bound of 0.35 meV, so the effect is small.

Caveats:
- Have not included interface interdiffusion
- Variation is larger if there is short-range order (clustering).