Atomistic modeling of silicon quantum dots for solid-state qubits

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1. Motivation

Silicon Quantum Dots

- Ideal host for spin qubits because of long spin coherence time.
- Various properties and behavior are highly sensitive to atomic scale details of interface.
- Effect of Interface roughness is not yet fully understood.

Motivation for atomistic modeling

- Accurately model realistic interface with miscuts, step roughness, alloy disorder.
- Thus capture interactions on atomic scale.

2. Atomistic modeling strategy

Atomistic Tight-binding Method
- Atomic scale roughness
- Inhomogeneous strain
- Alloys beyond VCA
- Defects/donors
- Full band structure

Electrostatics
- Device geometry & potential
- Semiclassical: Fermi-Dirac
- Quantum: Effective mass/tight-binding
- FEM Poisson
- Self-consistency

Spin/Charge Relaxation
- Electron-phonon interaction
- Atomistic deformation potential
- Spin-orbit
- Valley effects

Configuration Interaction
- Electron-electron interaction
- Exchange & Correlation
- Multi-electron spectrum

4. Spin relaxation in Si QD with interface roughness

Motivation

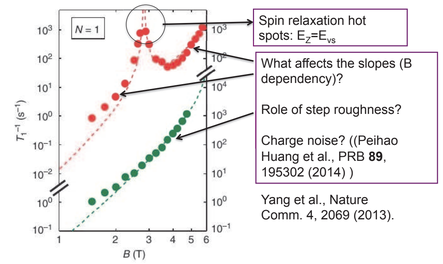
- Recent experimental measurement of spin relaxation in Si QD shows evidence of spin-valley coupling (Yang et al., Nature Comm. 4, 2069 (2013)).
- Spin-Orbit coupling + Valley-Orbit coupling (Interface roughness)=Spin-Valley Coupling.
- Previous models considered fitting parameters for valley-orbit coupling.
- Experimental data shows a deviation from analytical model at low B-fields
- Use atomistic method without any adhoc fitting parameters to investigate the effect of interface roughness on spin relaxation rates.

Technique

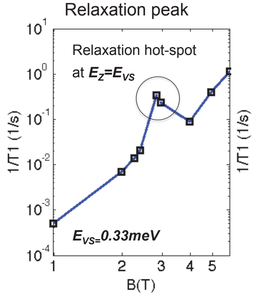
- Interface roughness modeled with tilted quantum well.
- Deformation potential computed atomistically using strain dependent tight-binding Hamiltonian.
- Relaxation times calculated using Fermi's Golden rule with atomistic wavefunctions.

Results

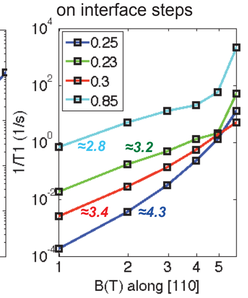
- Ideal QDs show a B^7 dependency of the relaxation rate, and a relaxation hotspot at E_Z=E_{VS}.
- With interface roughness the B-field dependency changes to B^5 or less. Exact dependency depends on the size of steps relative to the QD wavefunctions, as reflected in miscut angle.



Relaxation peak



Relaxation rate depends on interface steps



5. Valley relaxation in a Si QD

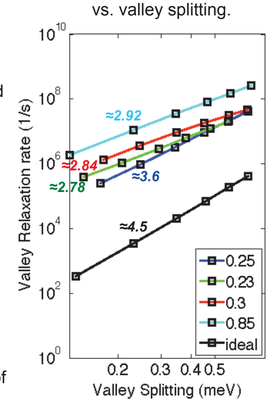
Motivation

- In the presence of spin-valley coupling, valley relaxation controls spin relaxation times.
- How are valley relaxation rates affected by interface steps?

Results

- Relaxation rates between valley states were computed using the atomistic treatment of electron-phonon interaction described earlier.
- Valley relaxation rate increases with valley splitting, but the slope of the curves depend on interface steps.
- Interface steps cause valley-orbit hybridization, and affects both valley and spin relaxation rates.

Valley relaxation rate vs. valley splitting.



Slope of valley relaxation rate depends on tilt angle.

3. Valley-orbit hybridization in Si quantum dot

Motivation

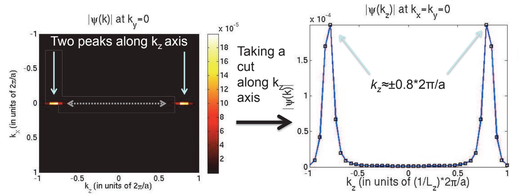
- Analytical theories predict valley-orbit hybridization (VOH) in the presence of interface roughness. (John Gamble et. al., PRB **88**, 035310 (2013)).
- Should come out automatically from atomistic analysis.

Methods

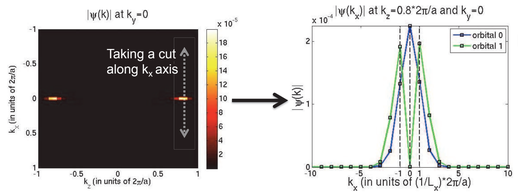
- Modeled interface roughness with ideal miscut (tilted) quantum well.
- Computed atomistic tight-binding wavefunctions from NEMO3D.
- Fourier transformed real space wavefunctions to k-space wavefunction.

Results

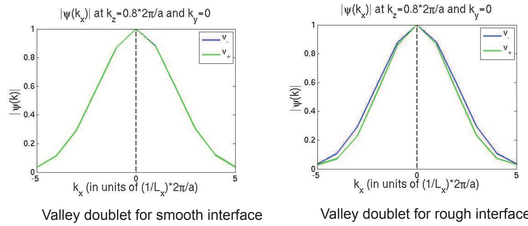
- *k*-space wavefunctions peak near k_z≈±0.8*2π/a, the two valley minima along k_z.
- Along k_x or k_y axis, at a valley minima, we can identify different orbital and valley states.
- Wavefunctions of opposite valley eigenstates exactly match for smooth interface, but not for a disordered one.
- The difference comes from mixing from other orbital states : valley-orbit hybridization.



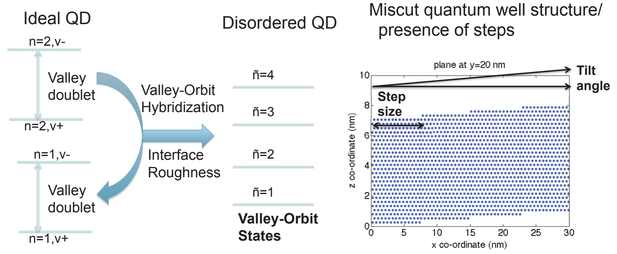
Fourier transformed wavefunction shows superposition of ±k_z valleys



Looking along k_x or k_y axis, at a valley minima we can identify different Orbital and Valley states



Opposite valley eigenstates exactly match for smooth interface but not for a disordered ione.



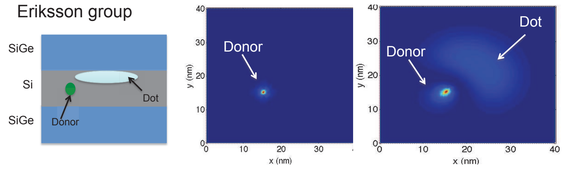
Miscut quantum well structure/ presence of steps

6. Simulation of gated donor-dot in strained Si

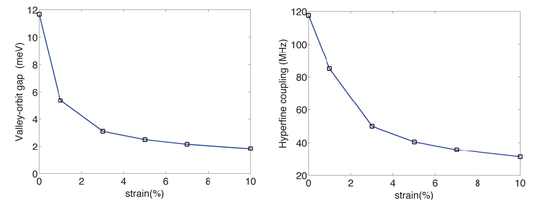
Donor-Dot in SiGe/Si:

In collaboration with the Eriksson group

Wave functions of the Donor-Dot system

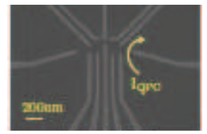


Valley-orbit gap and hyperfine frequency in a P donor with strain



TCAD: Modeling of realistic gate potential

- Semi-classical TCAD tool Sentaurus has been interfaced with NEMO.
- Development of a TCAD module in NEMO5 has been underway.
- In-house TCAD needed to customize simulation capability for semiconductor QDs as qubits.



Gate geometry from Xian Wu et. al. (arXiv: 1403.0019)

Device structure from Sentaurus

7. Conclusion

- Established from atomistic theory that valley quantum numbers are not good quantum in silicon QDs in the presence of interface steps.
- Spin relaxation rates are strongly affected by interface steps in silicon QDs with valley-orbit hybridization.
- Development under-way to incorporate TCAD in the atomistic modeling framework to simulate gated donor-dot devices.