Atomistic Modeling of a Tunable Single-Electron Quantum Dot in Silicon using NEMO3D-peta

Junzhe Geng[1], Sunhee Lee[1,2], Hoon Ryu[1,3] and Gerhard Klimeck[1]
1. Network for Computational Nanotechnology, Purdue University USA
2. Samsung Advanced Institute of Technology, Republic of Korea.
3. Supercomputing Center, Korea Institute of Science and Technology Information, Republic of Korea.

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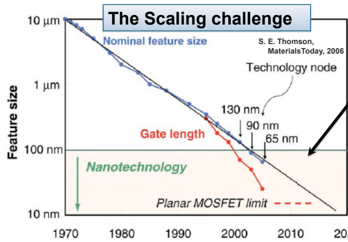
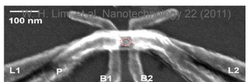
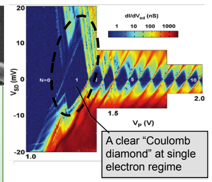
I. Introduction



If the trend continues, device will reach atomic scale by 2030

→Quantum Computing could be next!





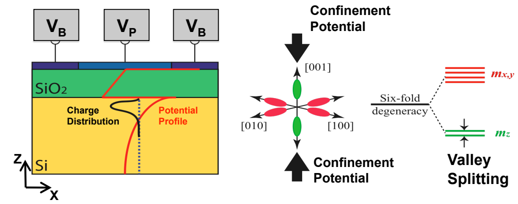
Si MOS Quantum Dot
Confinement created by electric field from gate bias
▪**Advantage**: State-of-the-art Si MOS fabrication technology and Industrial compatibility
▪**Challenge**: Si/SiO_2 interface disorder impedes single electron occupancy

▪**Recent breakthrough**: Experimental realization of Si MOS QD with low Si/SiO_2 interface disorder → operates in the **single electron regime**

A promising candidate for "Spin Qubit"?

II. Objective

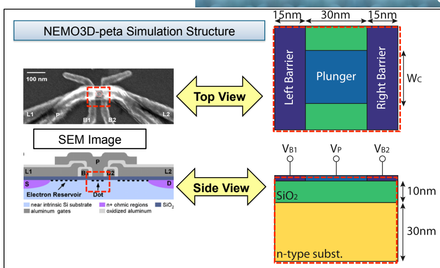
Valley splitting (VS) — The energy seperation between the lowest two confined states
➢Large VS → prevent loss of spin information → good for spin qubit



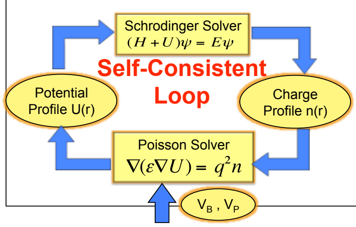
Project Goal:
a)Explore VS behavior in Si MOS QD:
- What is the range of VS?
- What factors determines VS and how?

b)Guide experimental design of VS for Si MOS QD

III. Methodology

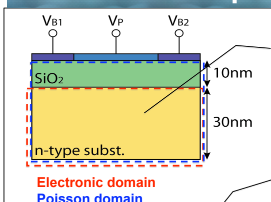


Key assumptions:
▪Only the QD region included in calculating VS
▪Equilibrium throughout the entire device, E_F set by source and drain
▪Low temperature ~ 100mK
▪QD size varies:
➢30 x 60 x W_C nm^3
➢W_C= (30, 40, 50, 60) nm



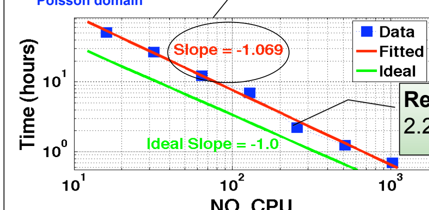
Self-Consistent Simulation
▪Convergence check: Compare U(r) after each iteration
▪Single electron in the QD:
➢E_F must cross exactly the ground state
▪VS value changes little when simulation is close to convergence

IV. NEMO3D-peta Scaling Performance



Huge problem Size:
▪8 million atoms
▪$sp^3d^5s^*$ tight-binding model
➔Matrix size of 80 million

Almost perfect scaling!

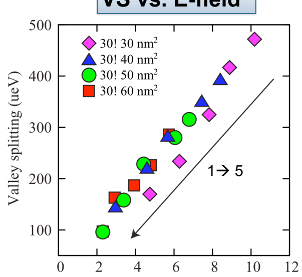


Reasonable cost: 2.2 hours @ 256 cpu

NEMO3D-peta is capable of simulating atomistic structure of realistic size !

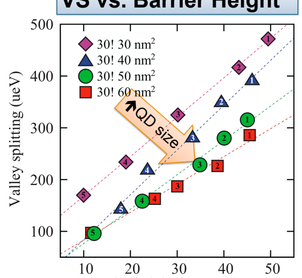
V. Results and Conslusion

VS vs. E-field



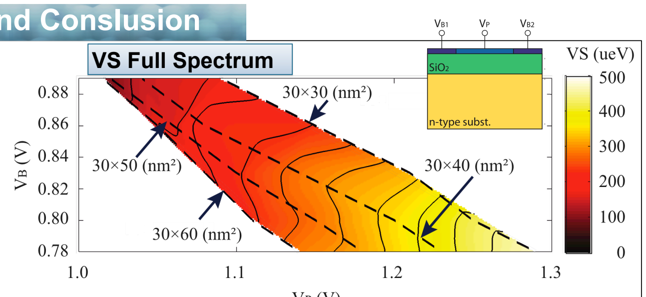
Regardless of QD size:
▪Larger electric field → Larger VS

VS vs. Barrier Height



▪Higher barrier → Larger VS
▪Same barrier height:
Smaller gate → Stronger confinement → Larger VS

VS Full Spectrum



VS range:
▪ This work: 95~470µeV; Experimental measurement: ~100µeV

Electron Conservation: V_B and V_P must "balance"
▪ Larger V_P pushes QD deeper → More electrons
▪ Smaller V_B raises barrier height → Less electron

Conclusion
▪Simulated VS results matches well with experiment
▪Small QD is preferred since it has larger VS
▪A high potential barrier is preferred for large VS but hampers electron tunneling

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