SAND2015-6974C

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Materials and fabrication of Si qubits

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August 21, 2015

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

LDRD

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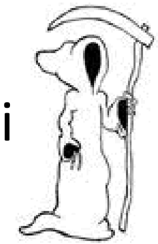
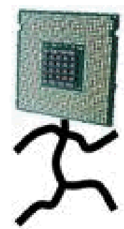
Outline

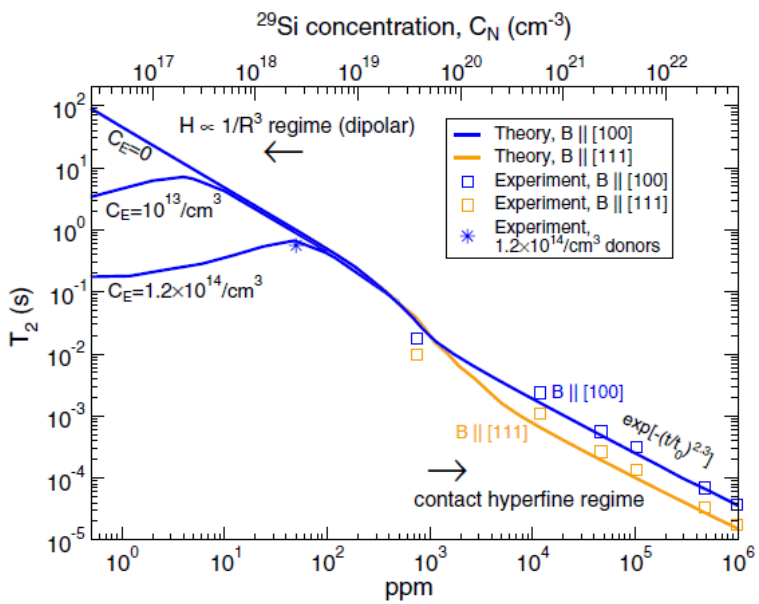
- Motivations
- MOS qubit fab and overview of performance
- Materials and modeling
- H-litho fabrication
- Summary

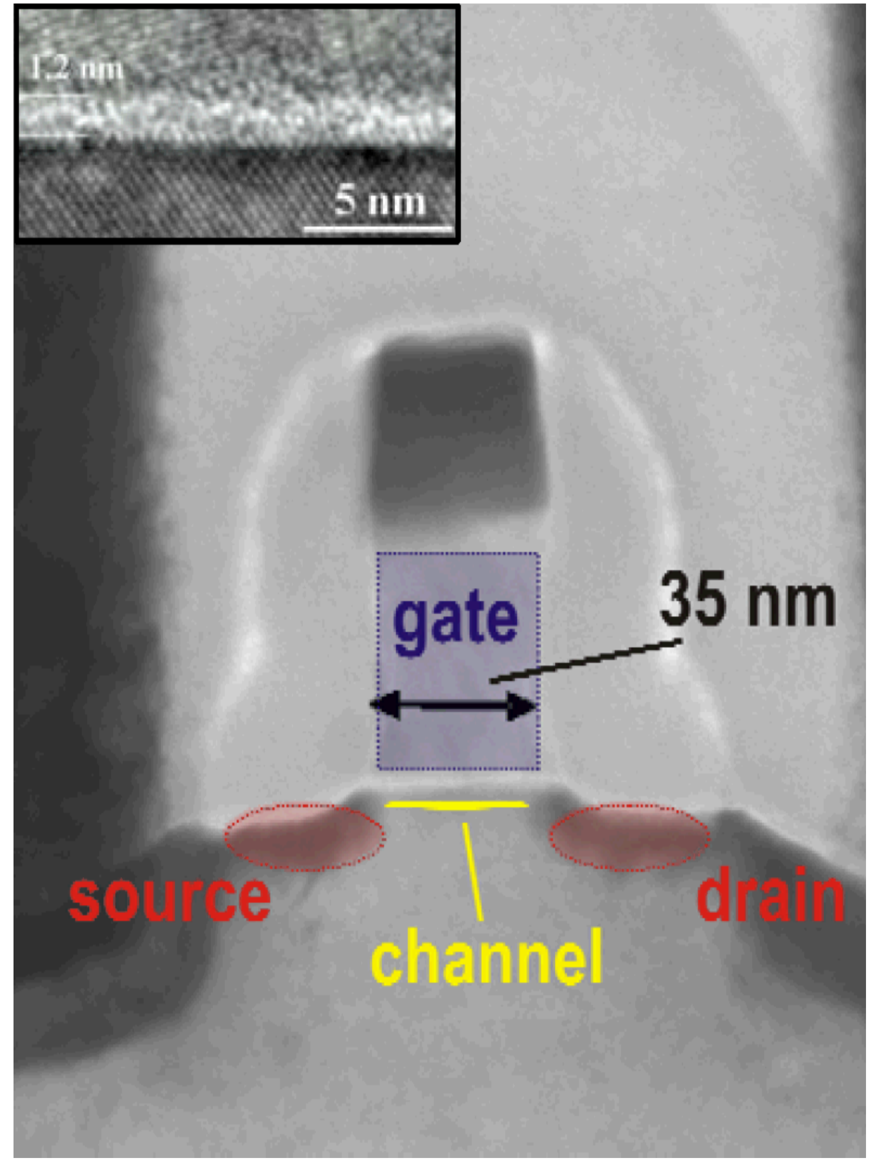
Motivation

- Why silicon QC
- Some general motivati
  - End of Moore's law
  - But can the Si platform be extended with a new function?
  - Why Si QC?



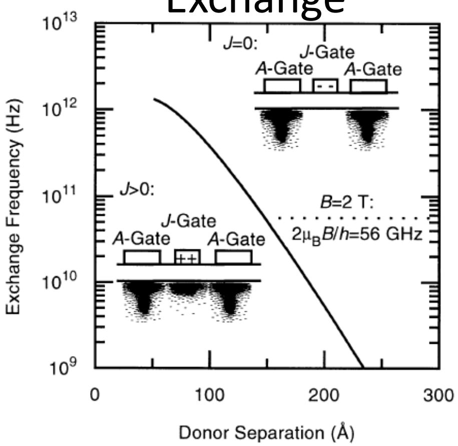






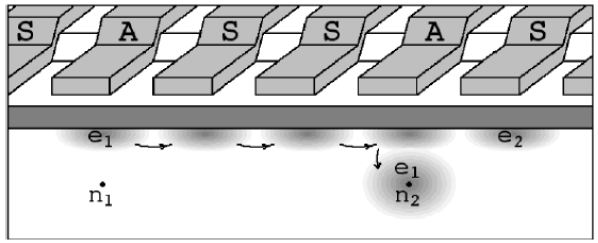
Donor & Donor-QD Architectures

Exchange



Kane (1998)

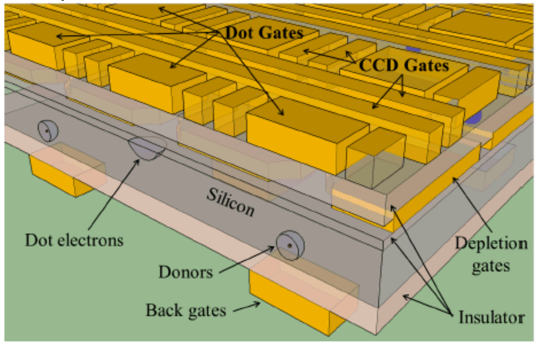
Transport



Skinner & Kane (2003)

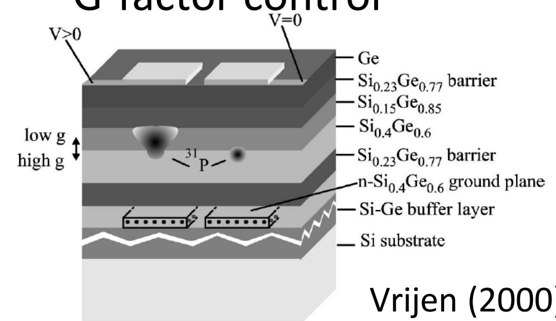
Also transport: Hollenberg (2007), Morton (2009); Witzel (2015)

Quantum Dot Mediated



Lyon (2015)

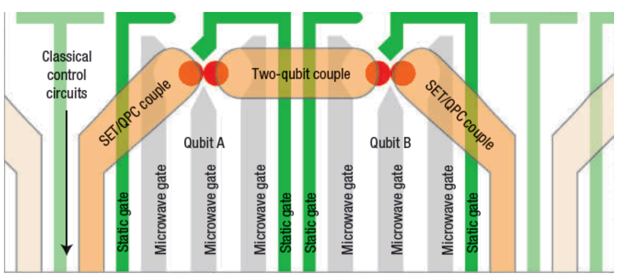
G-factor control



Vrijen (2000)

- Many appeals of donor qubits (e.g., potential for high fidelity, naturally same, compact, nuclear spin, built-in E-field selectivity, …)
- Many different proposals to use them
- Common themes
  - 1-qubit: ESR or NMR (single spin platform & technique)
  - 2-qubit: Exchange or shuttle (double dot platform & technique)
    - Also notable: spin-bus or c-QED coupling
  - Often: quantum dots for assistance
    - If quantum dots, then why donors? D-QD S/T qubit is an example of "if you can, why wouldn't you?"
- SNL effort (generally – advance D and D-QD technology with community):
  - quantum engineering of QD-donor systems (single spin ESR & NMR, D-QD)
  - Advanced fabrication approaches for donors (single ion implant, STM)
  - Device modeling and device modeling tools (e.g., QCAD)
  - Cryogenic electronics (e.g., pre-amplification circuits)

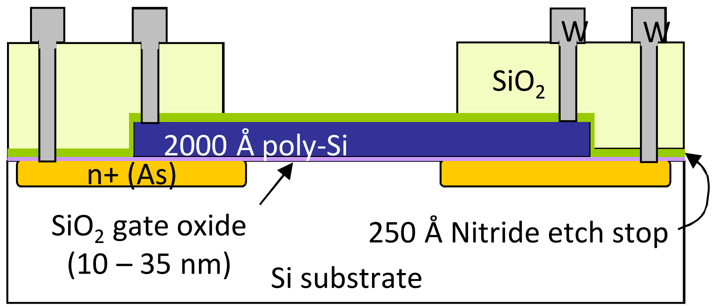
S/T qubit (dB for 2nd-axis)

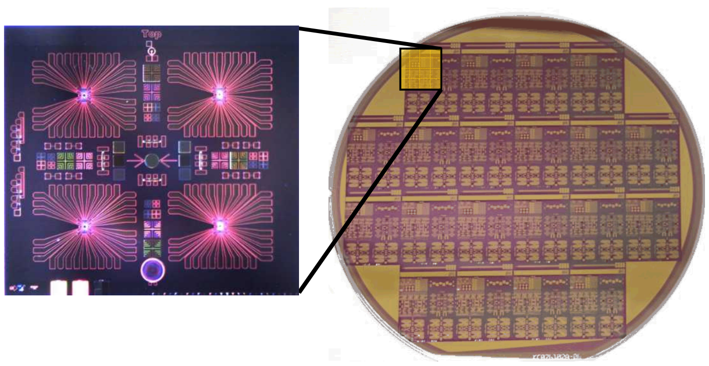


Taylor (2005); Levy (2009); Trifunovic (2013)

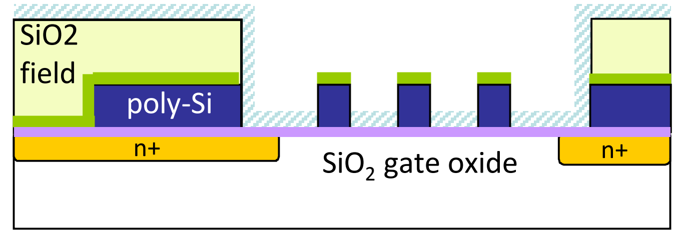
Nanostructure fabrication at Sandia National Labs

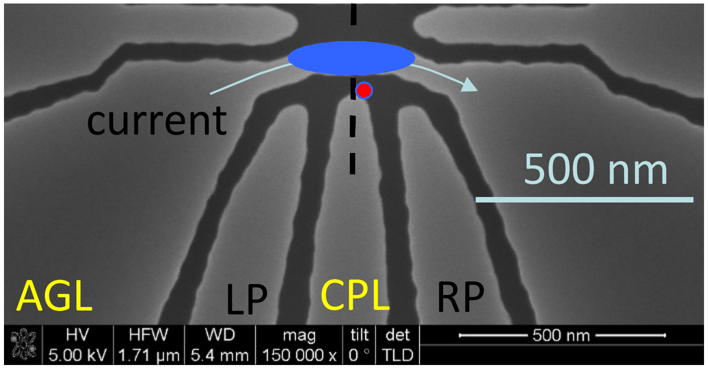
Front-end in silicon fab





Back-end nanolithography



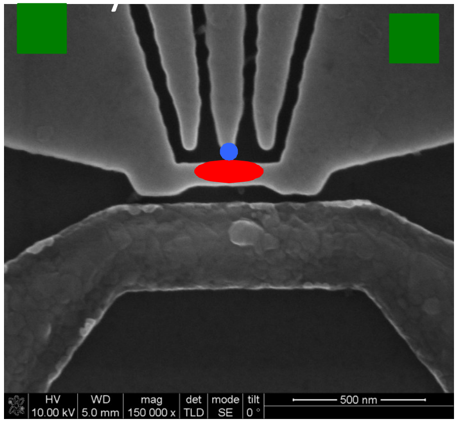


Goal: Use Poly-Si etched structures to produce donor-based qubits

Rationale:

- Self aligned implant
- Foundry like processing
- Potential long term benefits for charge stability

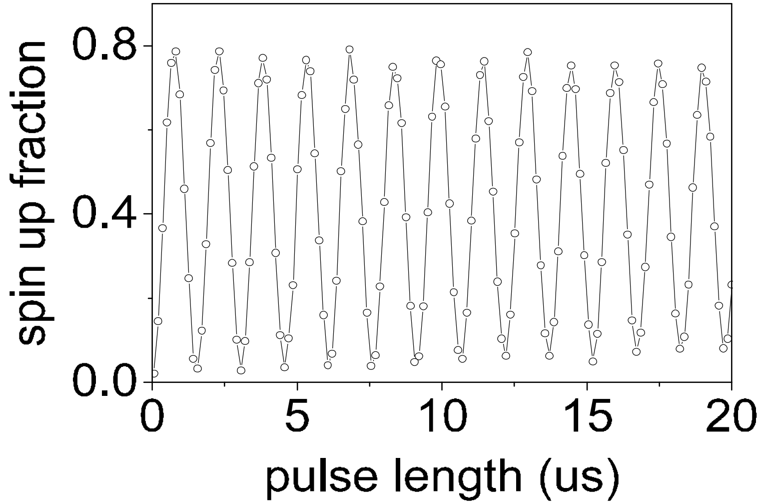
Single donor qubits



Ohmics

Donor

Quantum Dot



^{28}Si epilayer

- 2.5 μm thick
- 500 ppm ^{29}Si (ToF SIMS)

Nominally identical processing

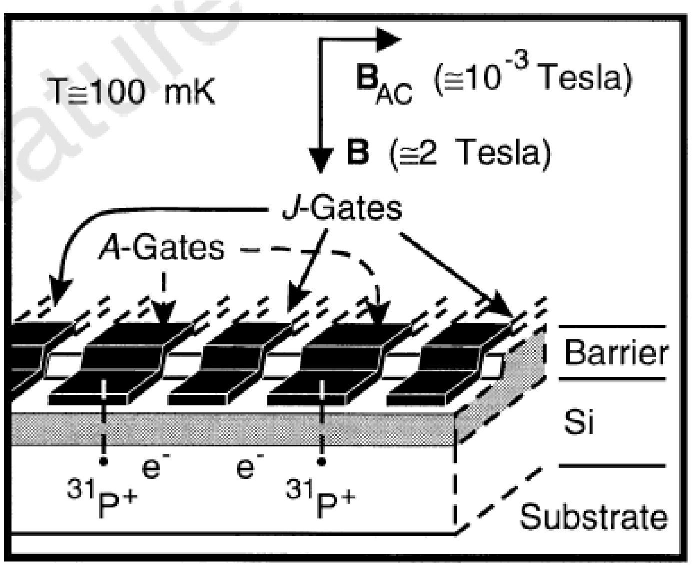
Exception - P Implant:

- 45 keV implant
- Dose: 4e11 cm^{-2}
- This is less than nat. Si case

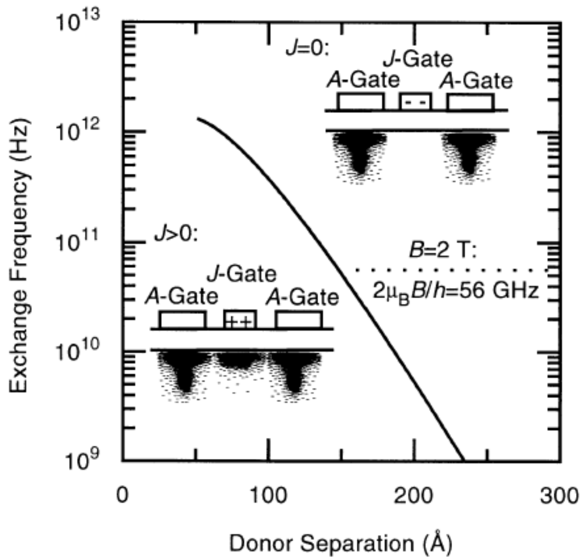
- ESR: T2 = 0.31 ms, T2* = 10-20 us
- For 400 ns gate times and 1.8 us slots
- SPAM error of order 6% & Idle error ~3%
- X/Y rotations are of order 4-5% error.

- NMR of nuclear spin demonstrated at CQC2T
- Very high “control fidelity” NMR rotations (~99.99%)

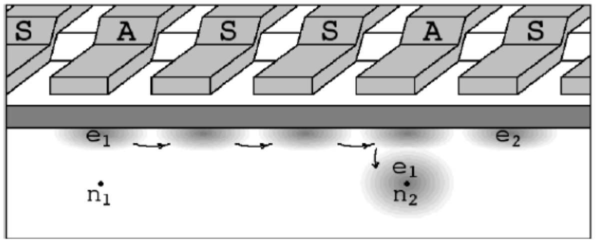
Donor-donor coupling concept



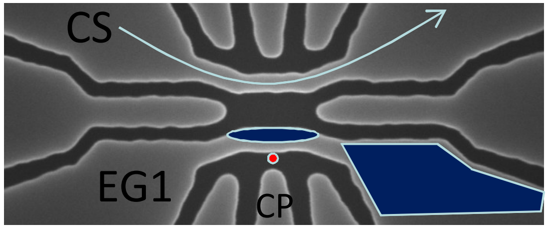
Kane (1998)

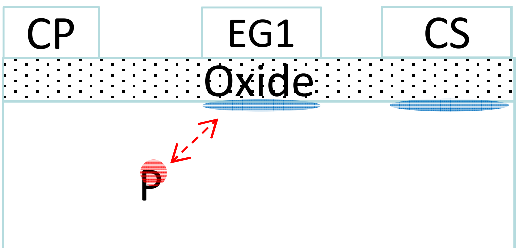


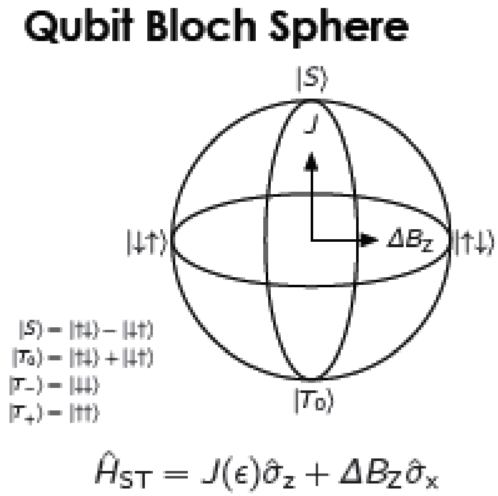
- Donors are a great qubit
- Many architectures consider donor coupling to surface (including QDs)
- Very general question: can a donor practically be coherently-coupled to something at an interface? [Kane-like device architecture]



Approach: Couple a N=1 MOS-QD to a Buried Donor





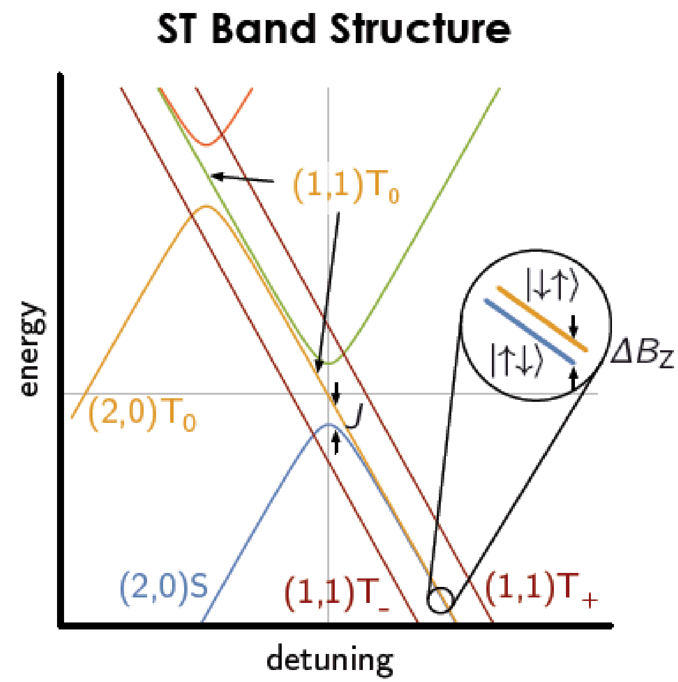


Canonical S/T qubit

$$\hat{H}_{ST} = J(\epsilon)\hat{\sigma}_z + \Delta B_Z(\epsilon)\hat{\sigma}_x$$

Donor-QD S/T qubit → $AI \cdot S$

- Encode as singlet-triplet qubit
- Rationale for using this choice as test platform:
  - Platform to examine tuning of the charge & dynamics (e.g., tunnel coupling)
  - Produces an appealing two-axis controlled S/T qubit
  - Rotation frequency is chemically distinct
  - Opens up a potential electrical read-out of nuclear spin
  - Directly probes coherence times of surface-bulk-donor coupling
  - S/T protocols can be used to test adiabatic and diabatic transfer



Carroll

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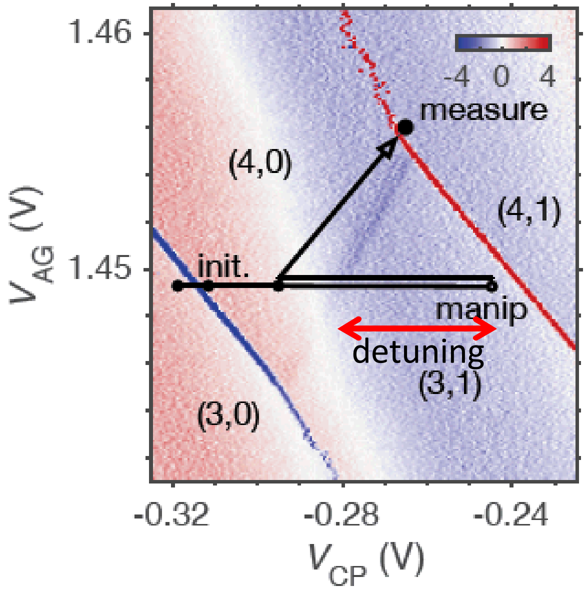
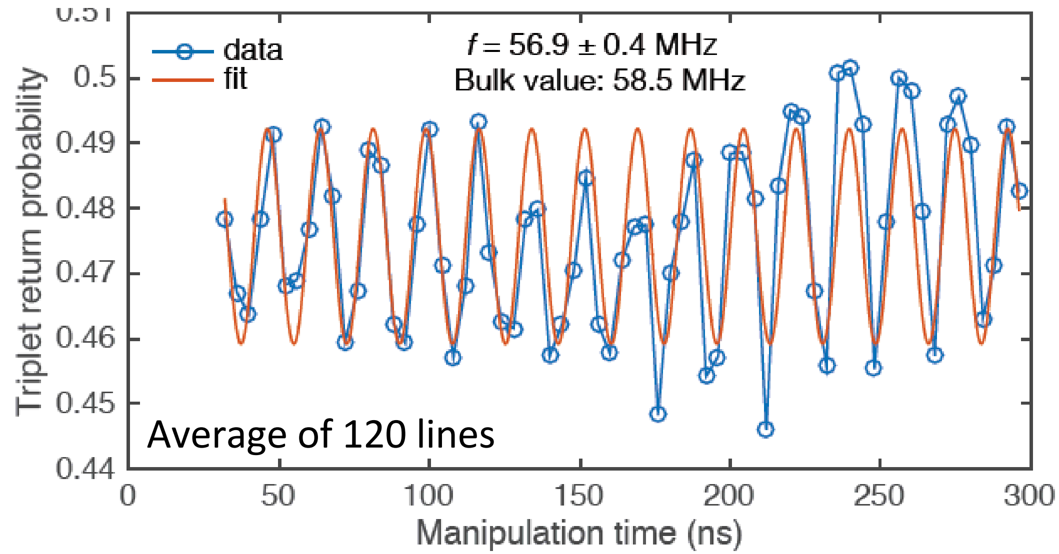
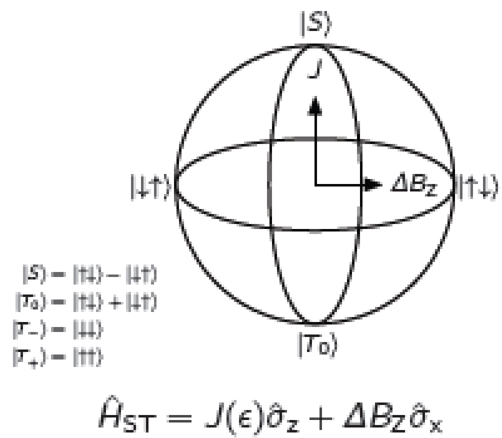
Pulse sequence & singlet-triplet rotations





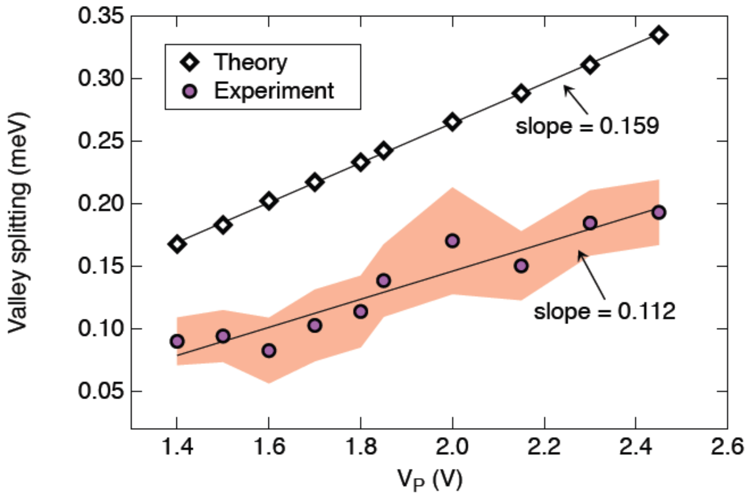
- Coherent oscillations observed for variable time & fixed detuning
  - Note: only the measurement point differs
- Oscillation frequency is close to bulk donor contact hyperfine value of 58.5 MHz
- Frequency is detuning dependent – J changes
- Visibility is ~10%

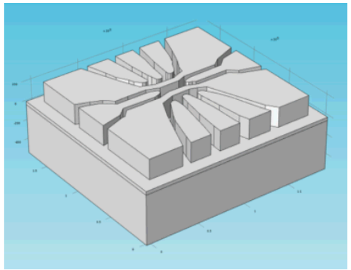
Qubit Bloch Sphere

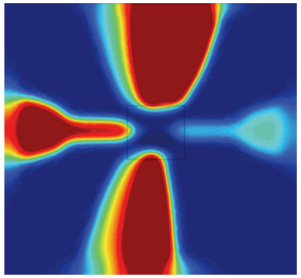


Poster: Harvey-Collard

Valley splitting and pulsed spectroscopy



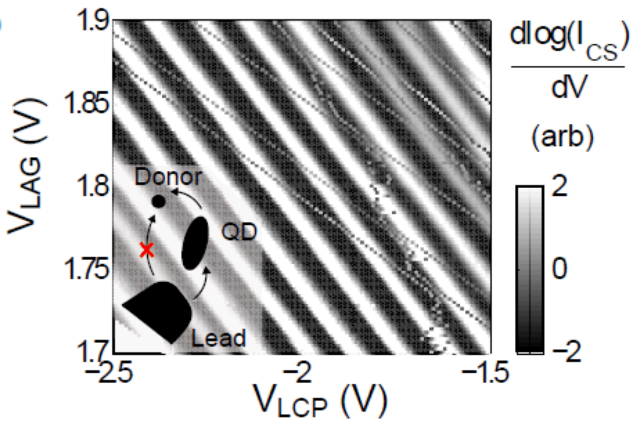


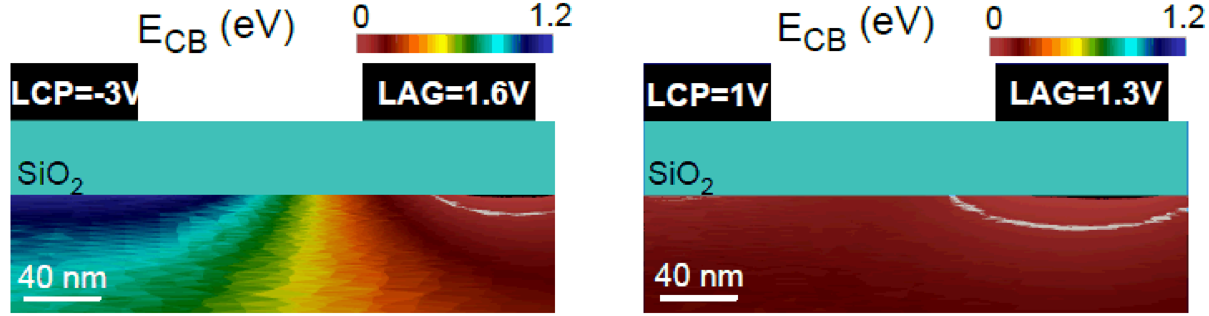


Full 3D calculations to extract vertical field and predicted valley splitting

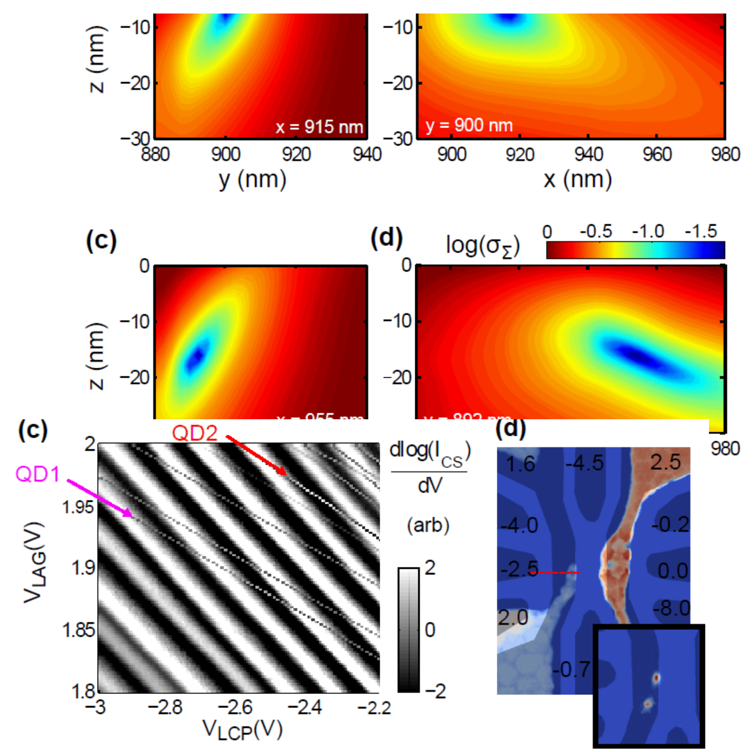
- Reason that N_{eff}=4 was N=2 singlet-triplet spacing too small – valley splitting a concern
- The valley splitting is measured using pulsed spectroscopy
- Valley splitting was measured over large range of voltages (i.e., -8 < CP <0)
- Barrier tuned at each location to enable pulsed spectroscopy
- Disagreement between "ideal" and measured is topic of discussion

Triangulation of donor position





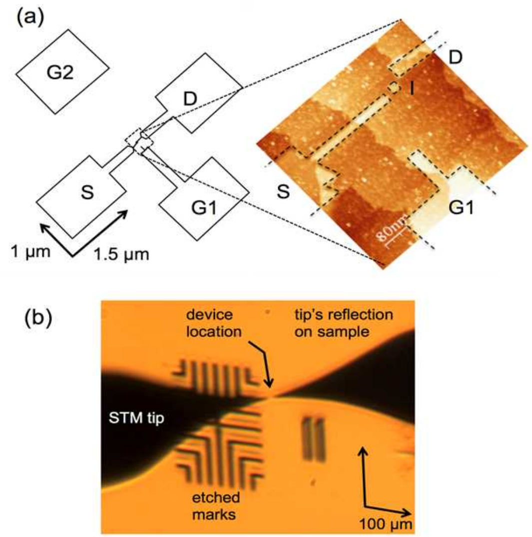
- Modeling of slopes in stability diagrams (against all gates) to help identify position of object
- Capacitances of multi-gate system are sufficient to locate position
- Visible donors are underneath LAG
- Depth of donors:
  $7 < z < 15$ nm
- This observation is also consistent with semi-classical QCAD calculations of 45 meV "ionization contours"



Rudolph, Bureau-Oxton, Singh, Nielsen

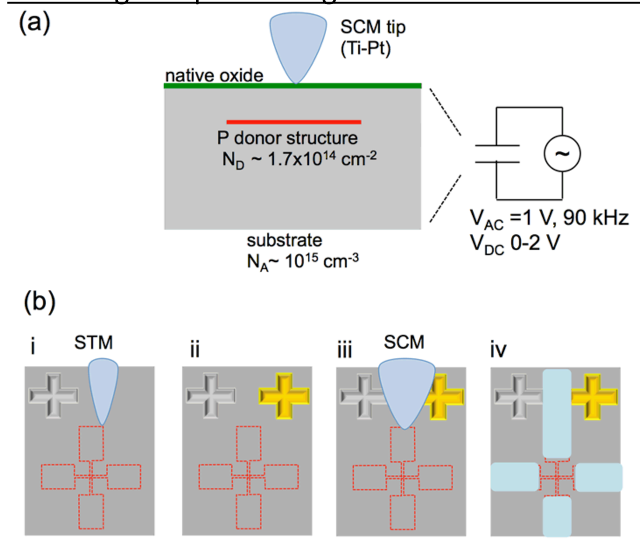
Finding the donors after they are placed

Original recipe: align to trenched Si marks

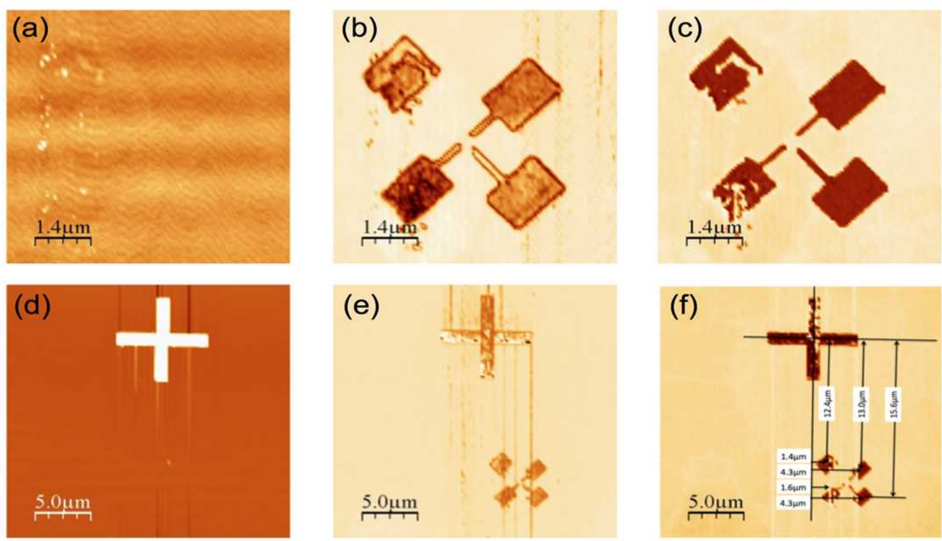


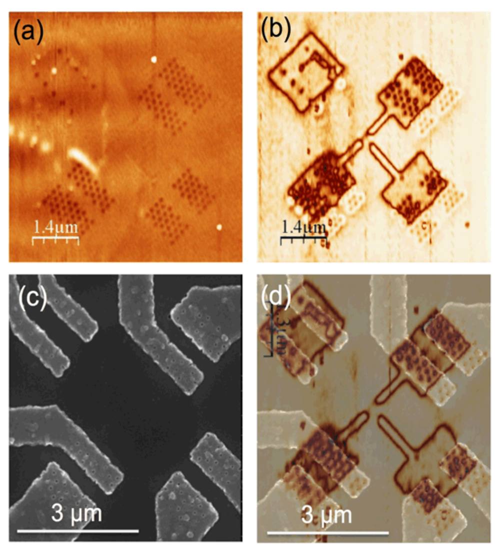
New approach: align to mark after STM fab

Advantage: improved alignment limits & STM fab flexibility



Alignment and post STM fab metrology





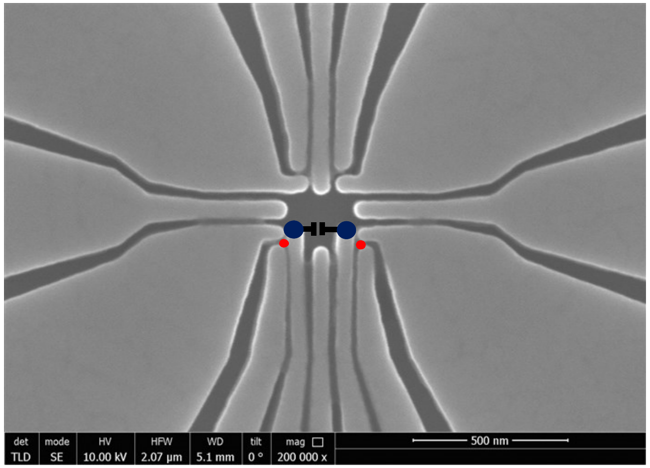
Result:

~300 nm resolution now

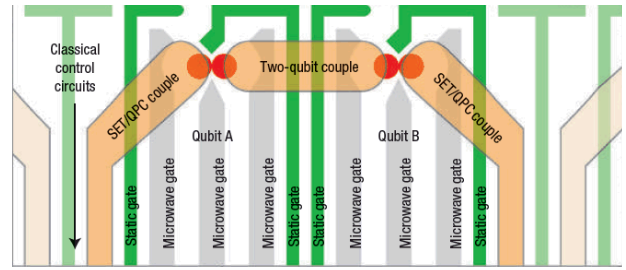
10-20 nm possible at RT

Bussman [Nanotechnology 26 (2015)]

Possible future lay-out for two-qubit coupling

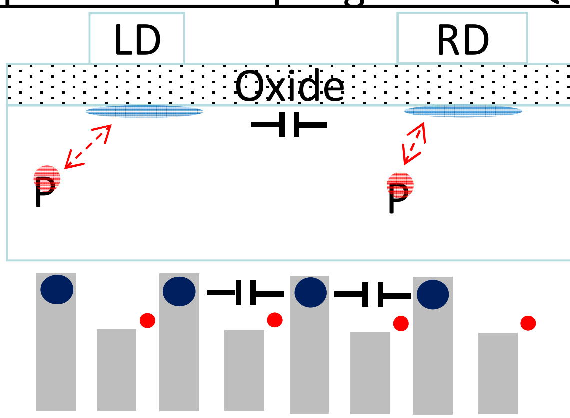


S/T qubit (dB for 2nd-axis)



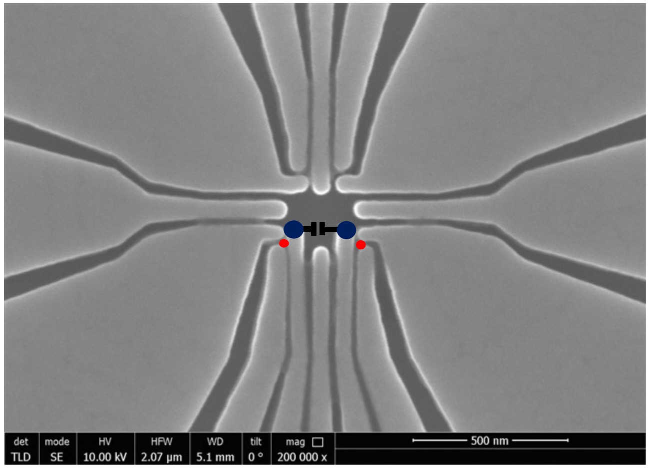
Taylor (2005); Levy (2009); Trifunovic (2013)

Capacitance coupling of MAJIQ-SWAG



- Capacitance coupling by proximity for two qubit gate
- Approach uses energy selection of one of many donors in an ensemble & poly self-alignment
- Concept might be generalized to more (in a 1D line)

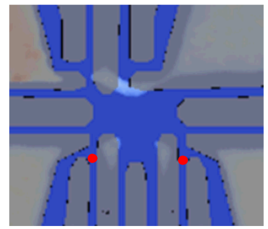
Possible future lay-out for two-qubit coupling



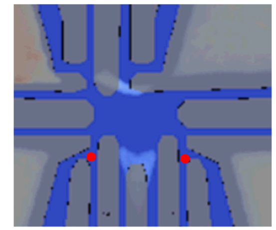
… and other approaches (J or shuttle)

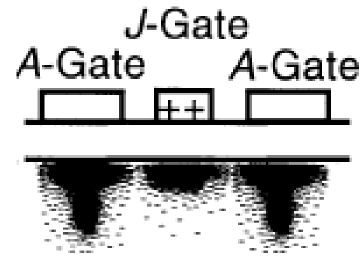
Exchange gate mediated by DQD

Small t

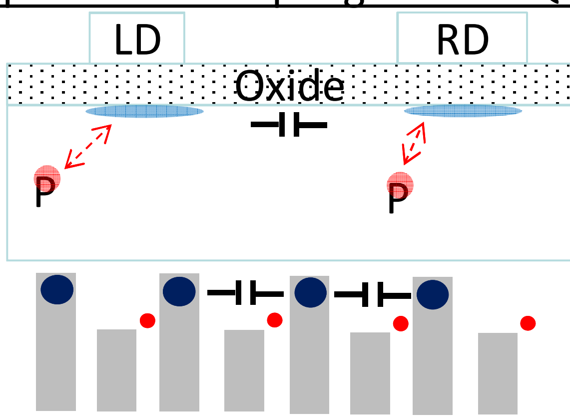


Enormous t

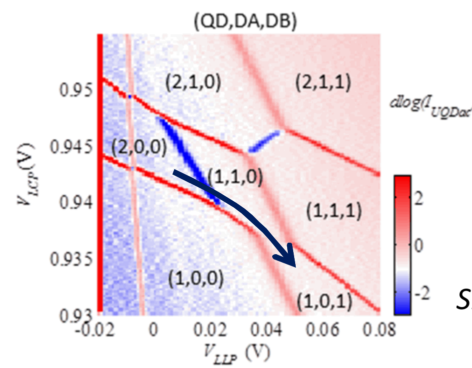


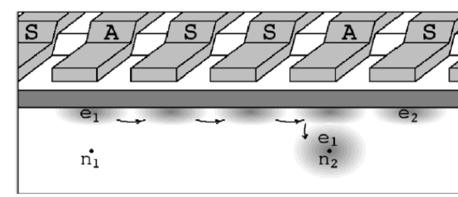


Capacitance coupling of MAJIQ-SWAG



Transport mediated by QDs





Single SWAG case

- Capacitance coupling by proximity for two qubit gate
- Approach uses energy selection of one of many donors in an ensemble & poly self-alignment
- Concept might be generalized to more (in a 1D line)

Outline

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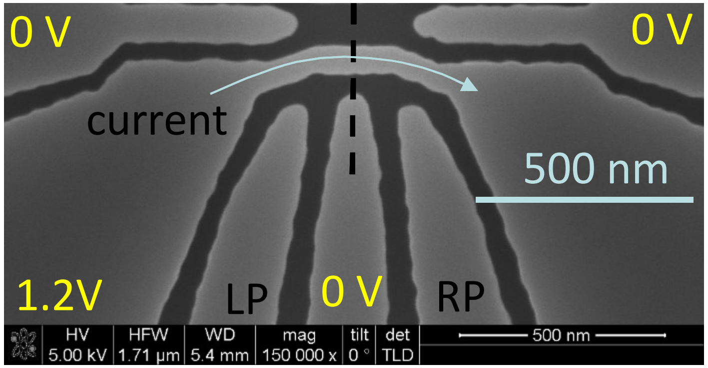
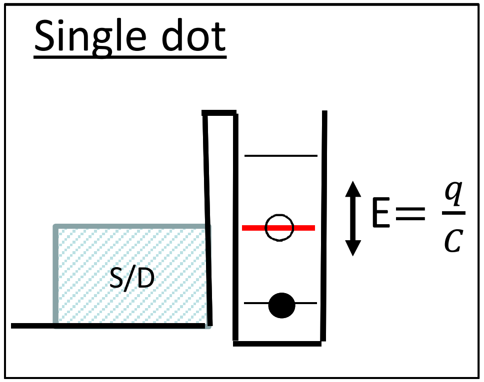
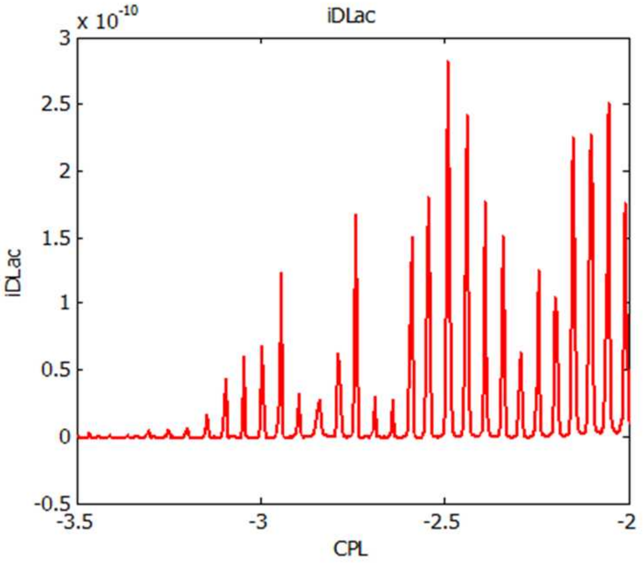
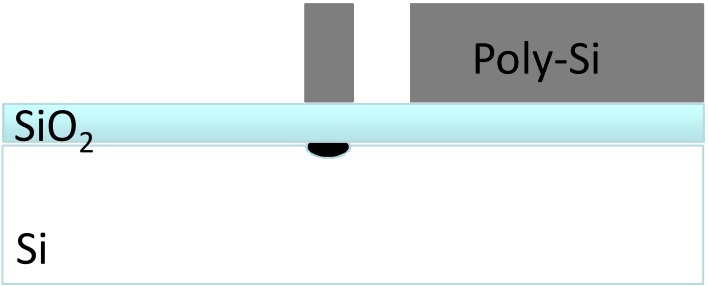
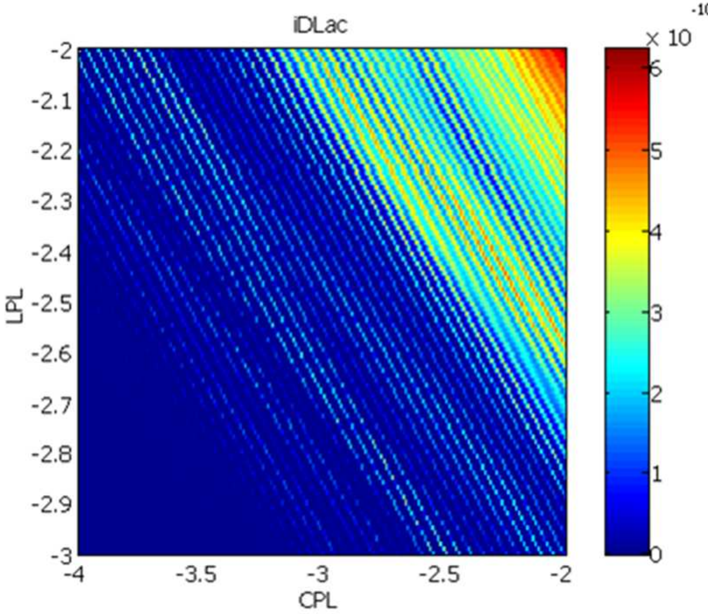
Poly silicon quantum dot







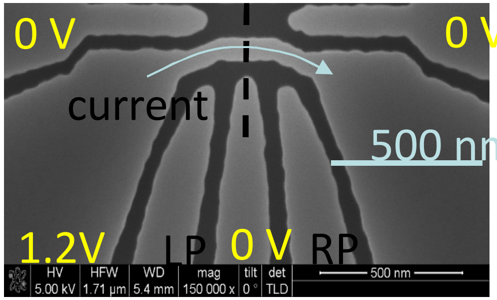


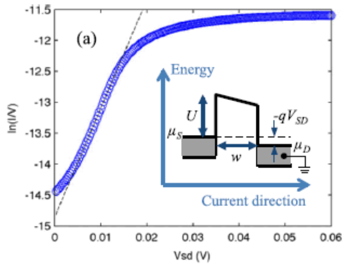


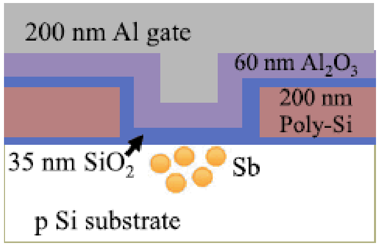
- Relatively regular period Coulomb blockade achieved in poly silicon SET
- Wire width ~50-70 nm with gaps between wire and plunger of ~40-50 nm at tips
- Disorder in potential is still observed in effects on non-linear modulation of tunnel barriers
  - Modulation of conductance not monotonic

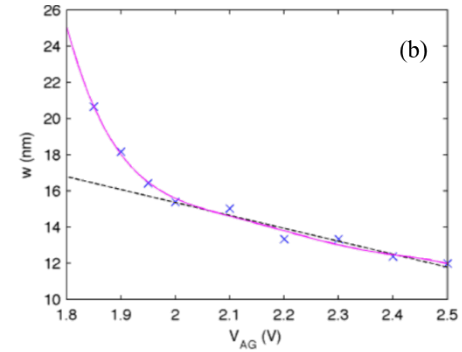
Harvey-Collard

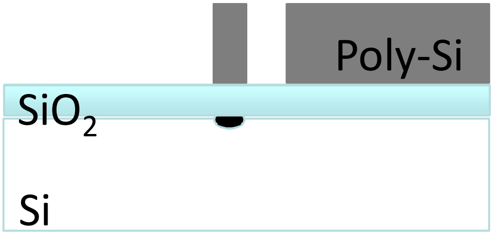
Characterization of tunnel barriers

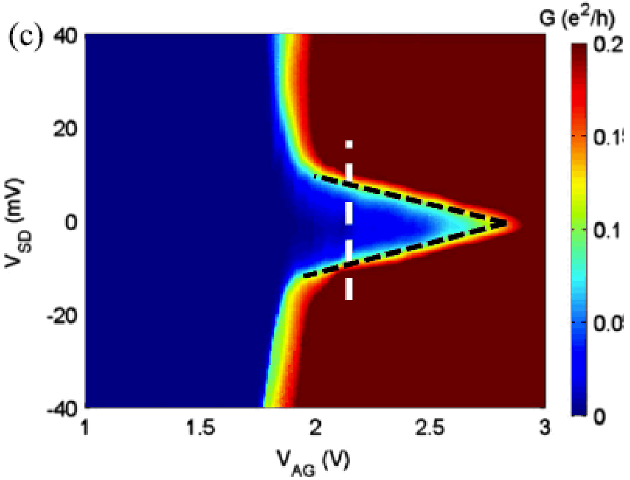


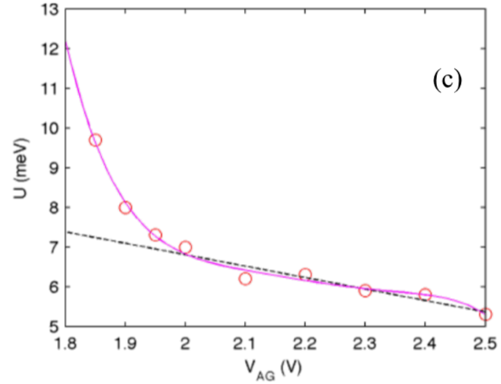


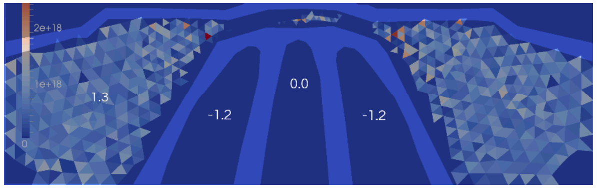






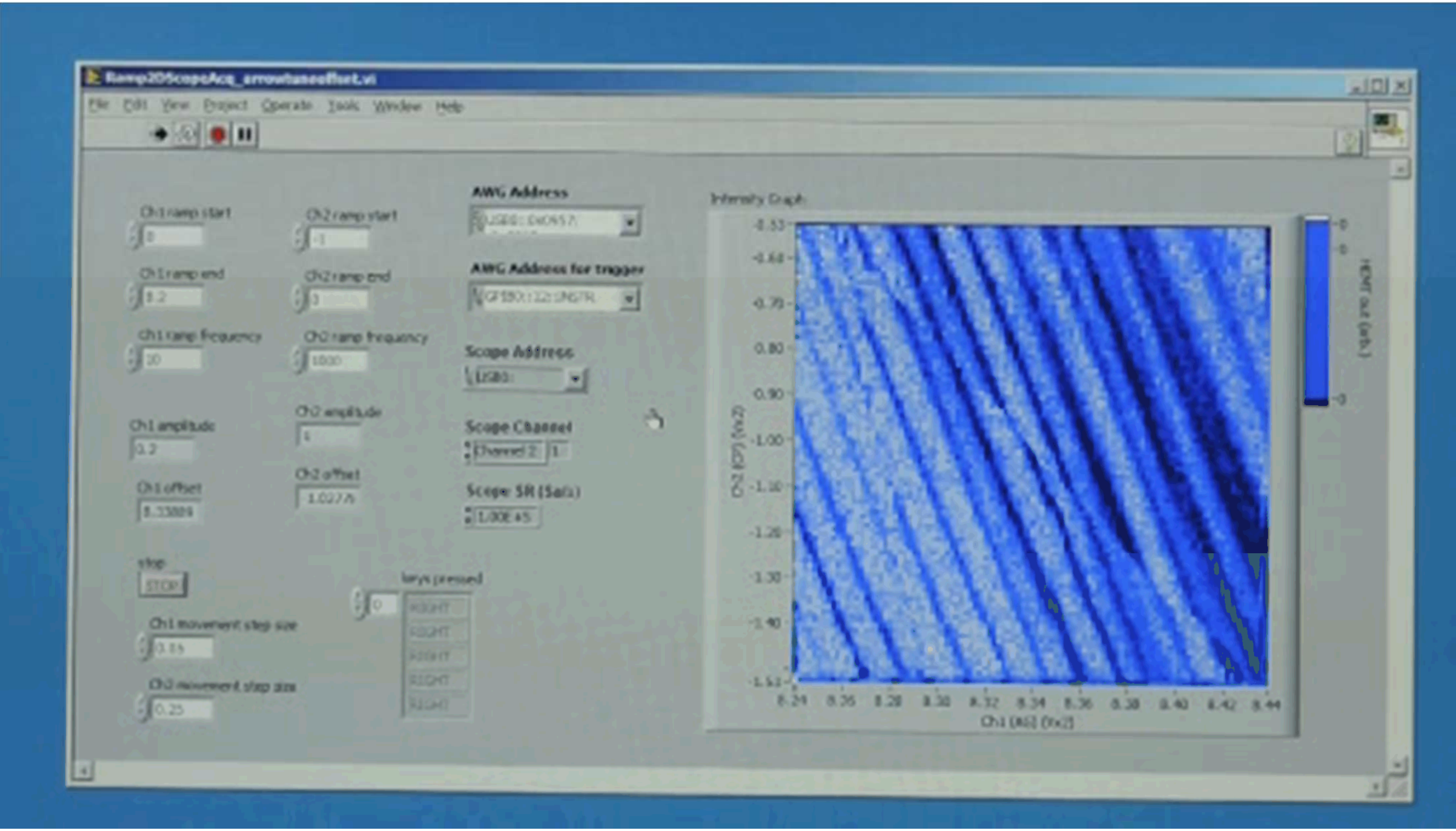






Rapid tunnel barrier characterization is one of the challenges for modeling and fab
Central component of quantum dots – but need a way to rapidly characterize and compare
Challenge: complex dependences on geometry and voltages [Friesen et al., …]
Modeling of tunnel barriers very challenging – difficult to calibrate models to barrier height, width
Approach: use simplified parameteric model that captures barrier height, width, V dependence
Future challenge: understand how to apply to modeling

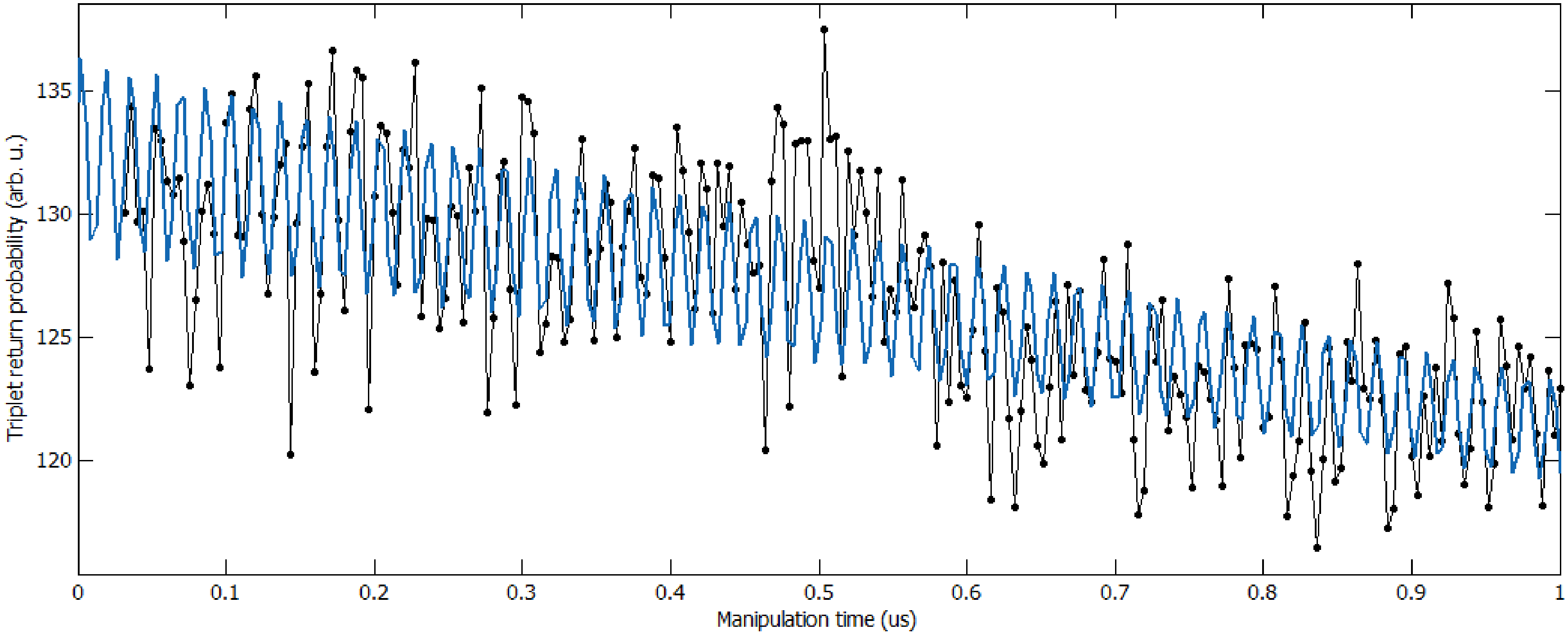
Stability plot movie with "jittery case"



Tracy

Extended time trace & coarse T2* estimate

- Long time trace. Average of 10 lines.
- Decoherence consistent with charge noise – traps?

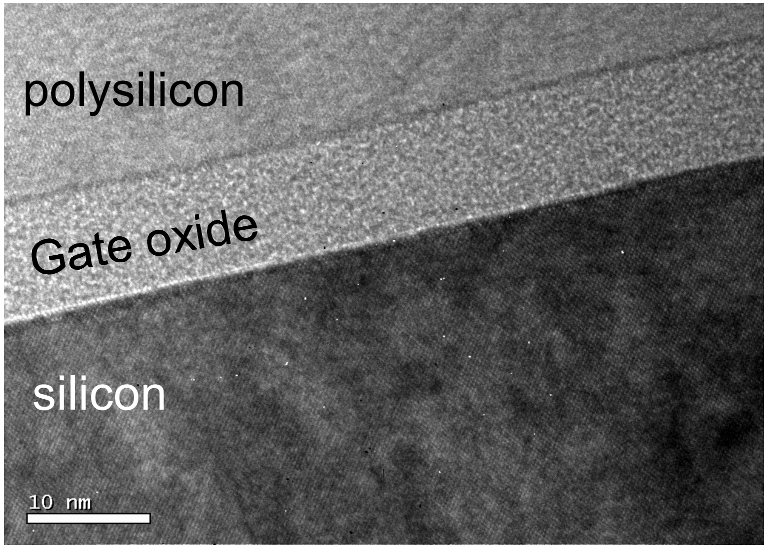


f = 59.5 MHz +- 0.1
T2* = 1.6 +- 0.8 us

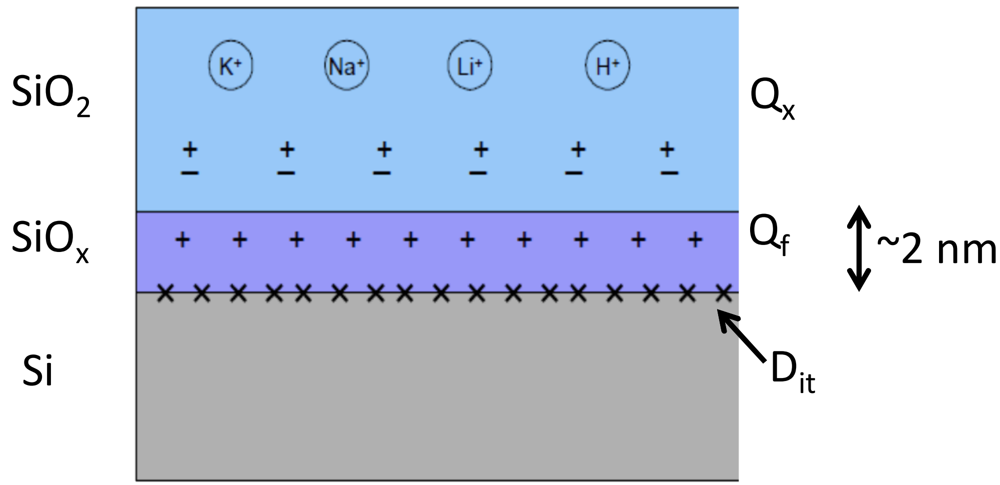
Detuning: 897 μeV

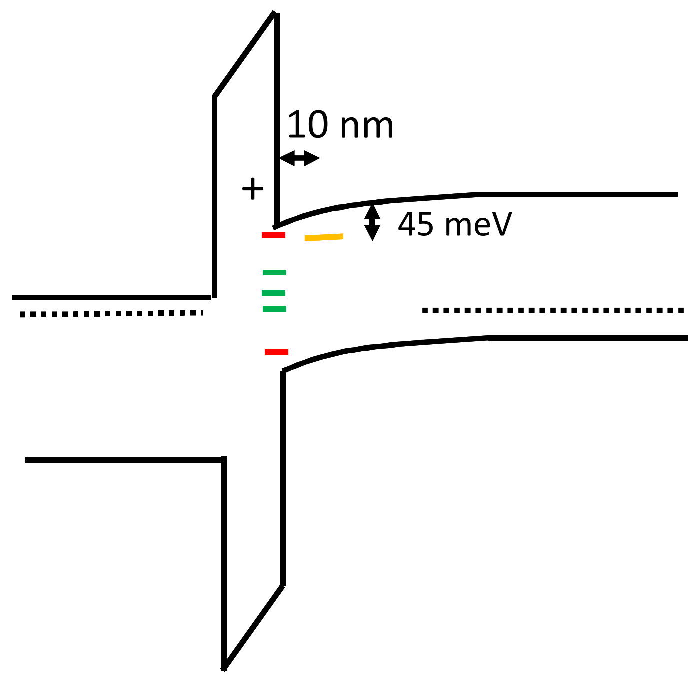
Poster: Harvey-Collard

The MOS interface



Defects





Room temperature picture

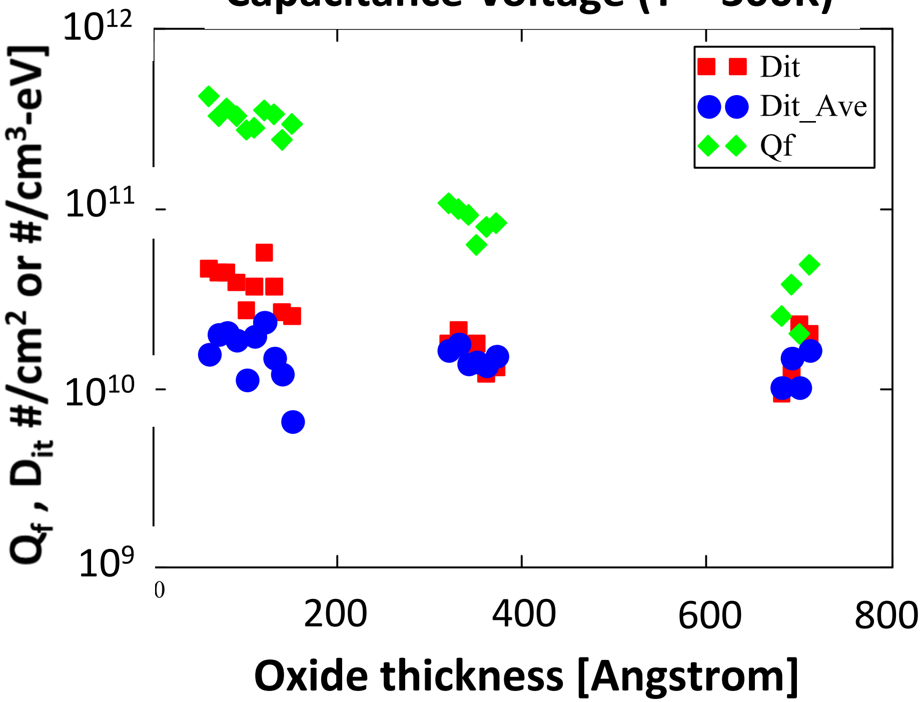
- D_{it} Interface traps and border traps within a "tunneling" distance of interface
- Q_f Fixed charge deeper in oxide

Low temperature picture

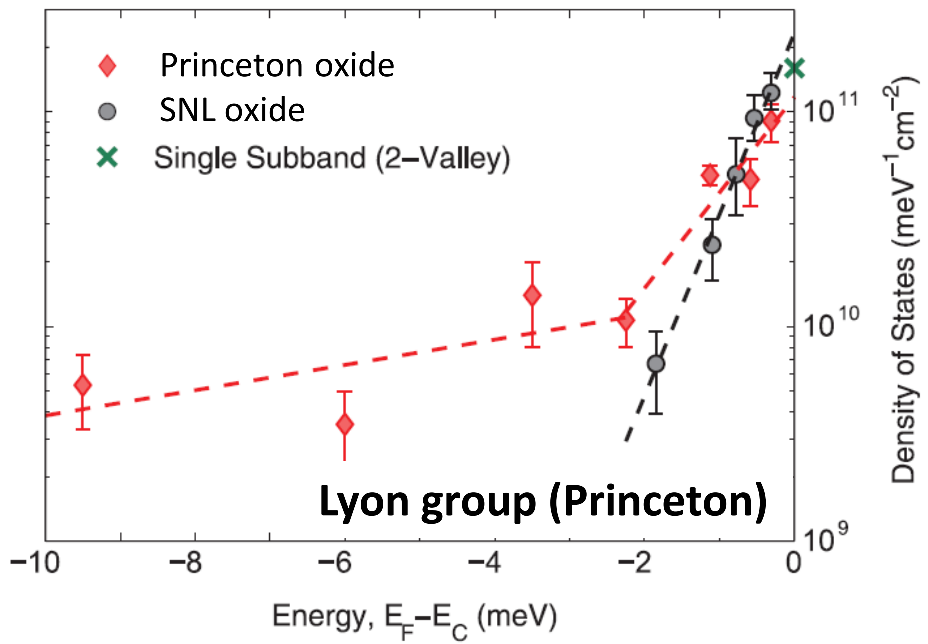
- Shallow traps are most relevant
- Not much known about interface traps close to band edge
- Fixed charge could be producing a dynamic state at the interface

Oxide defect densities

Capacitance-voltage (T ~ 300K)

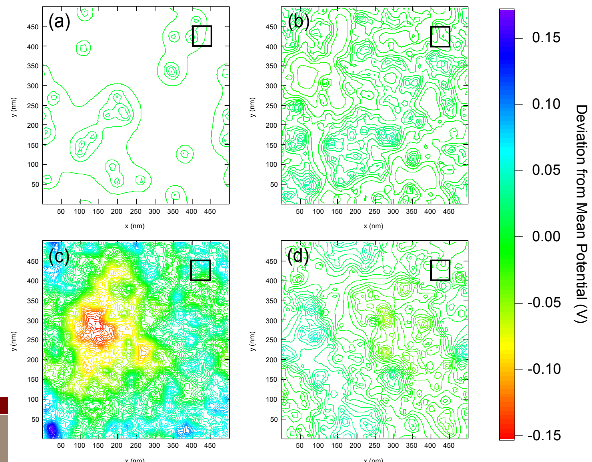


Electron spin resonance (T ~ 4K)

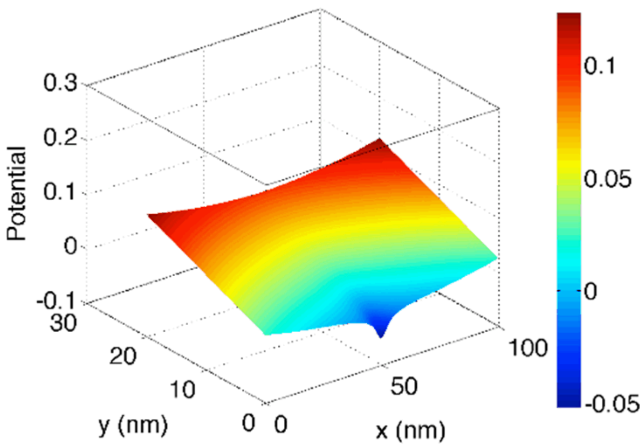


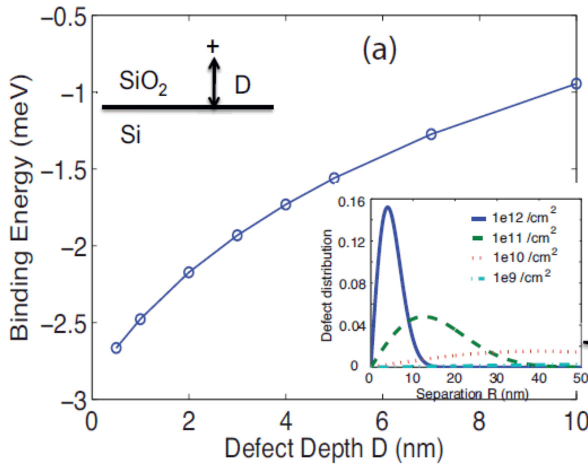
5,000 cm² / V-s < mobility < 15,000 cm² / V-s

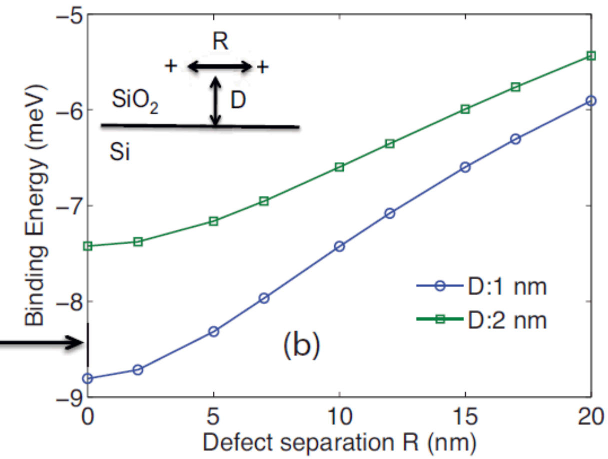
Jock et al., APL 2012



The influence of fixed charge







PHYSICAL REVIEW B **85**, 125423 (2012)

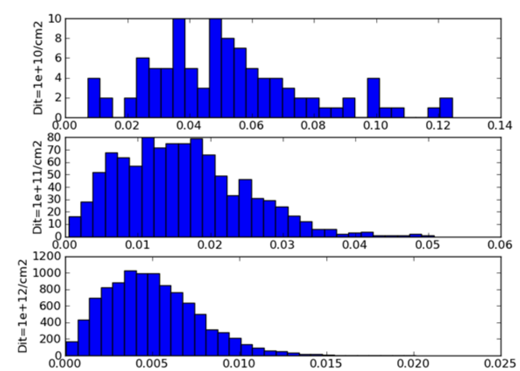
Voltage controlled exchange energies of a two-electron silicon double quantum dot with and without charge defects in the dielectric

Rajib Rahman,* Erik Nielsen, Richard P. Muller, and Malcolm S. Carroll

R (10^{10}) = 40 nm

R (10^{11}) = 13 nm

R (10^{12}) = 4 nm



Sandia National Laboratories

Outline

- Motivations
- MOS qubit fab and overview of performance
- Materials and modeling
- H-litho fabrication
- Summary

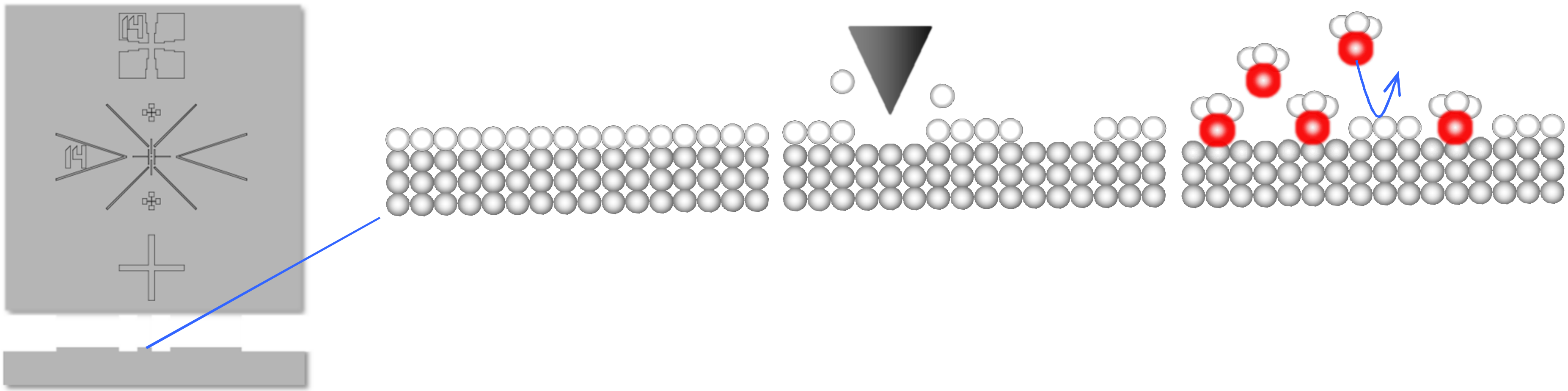
How? Atomic precision fabrication

1. Start w clean Si(001)

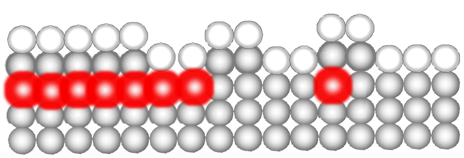
2. Adsorb H resist
Self-limiting 1 monolayer

3. Pattern w STM
Atomic-precision

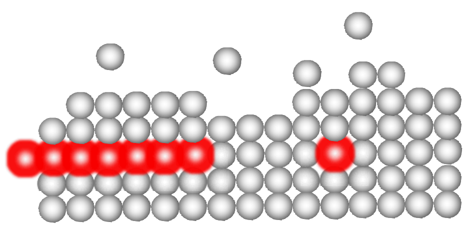
4. Adsorb PH_3



Etched alignment marks

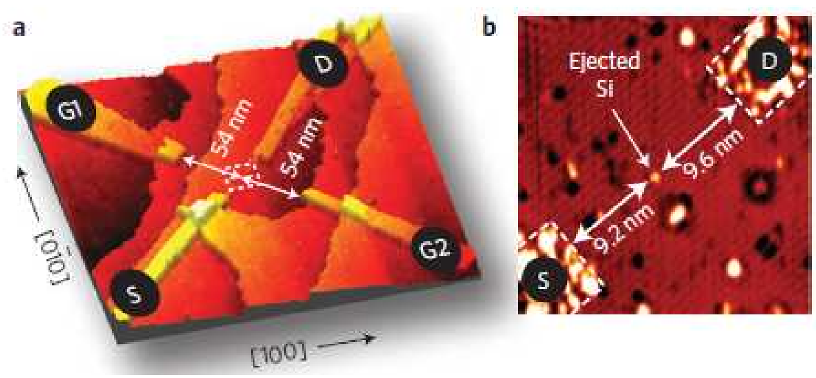


5. Incorporate P
-Anneal➔ Si-P swap
-H resist constrains P

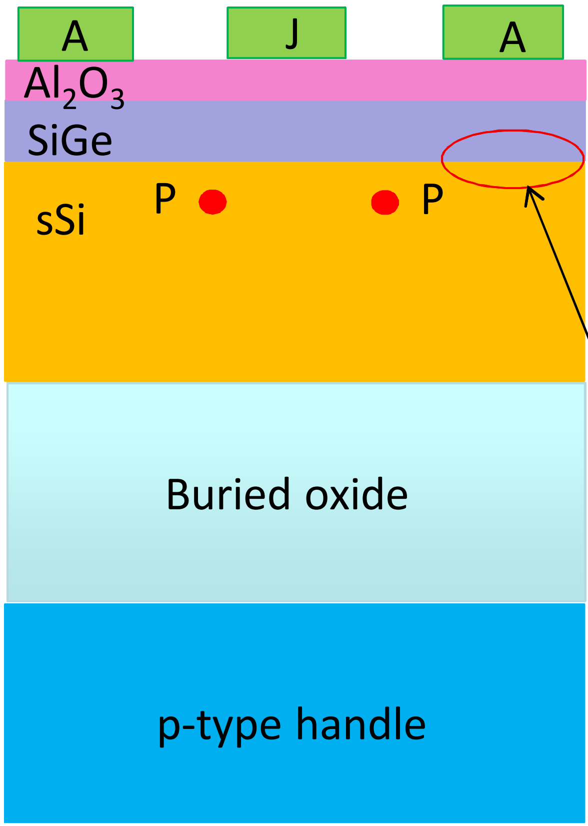


6. Desorb H & bury P in Si

NATURE NANOTECHNOLOGY | VOL 7 | APRIL 2012 |

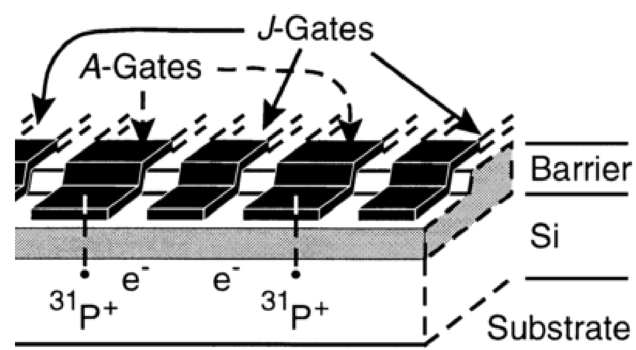


Strained silicon-on-insulator (sSOI)



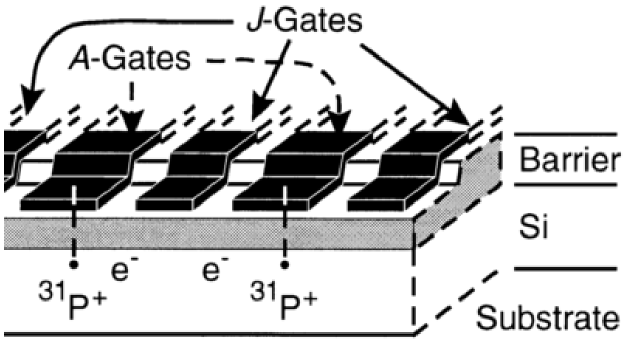
- sSOI to allow for high temperature clean step [Lee et al., Appl. Surf. Sci. 2012]
- We have ~1% tensile strain in films
- Sharpness of interface is important
- Relaxed SiGe can be used as low temperature capping layer instead of a dielectric

Can we make a good interface?

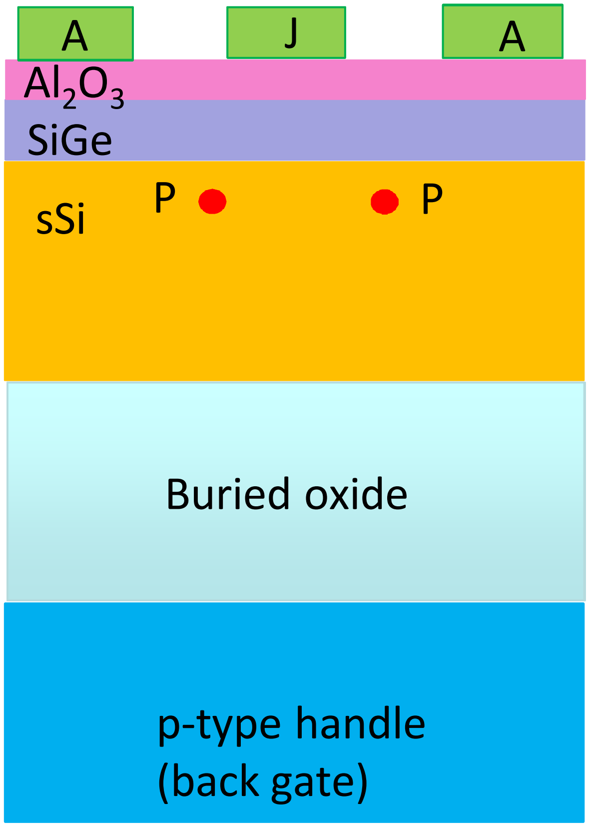


Kane, B., Nature 393, 133 (1998)

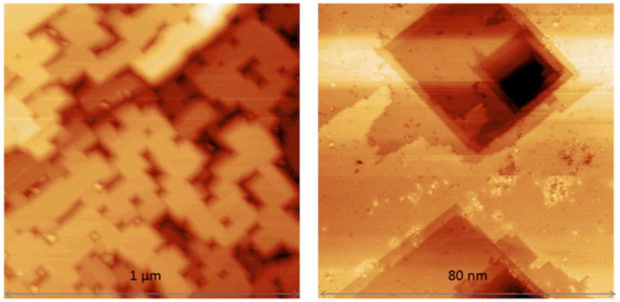
Strained silicon-on-insulator (sSOI)



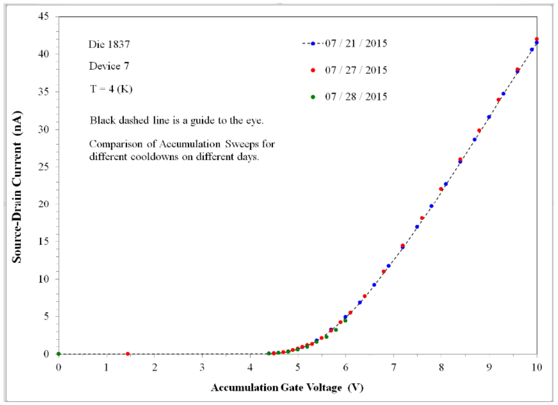
- Approach: Relaxed SiGe can be used as low temperature capping layer and dielectric
- sSOI for thermal budget
- Back-gate for tuning donor tunnel coupling
- This year: SiGe/sSOI Hallbar & H-litho in sSOI



Si buffer layer growth on sSOI to overcome non-idealities. Results: pinning and flats

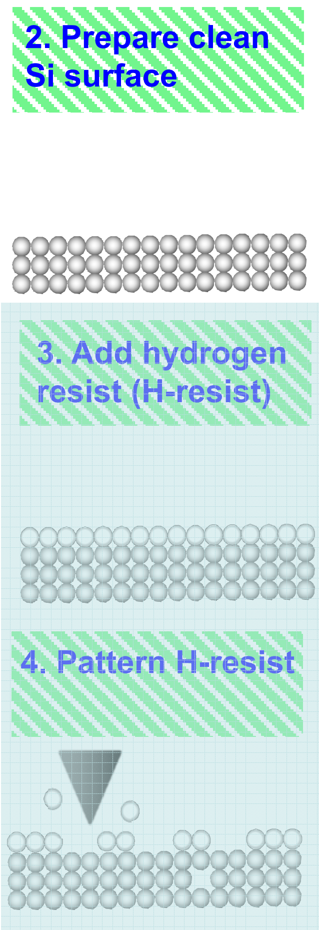


First Hallbar on MBE-STM material demonstrated. ~400 mobility. A good start.



Yitamben, Bussmann, Sharma

Challenges



Low temperature clean & atomically flat surface

No roughness in strained Si

100% incorporation of single donors

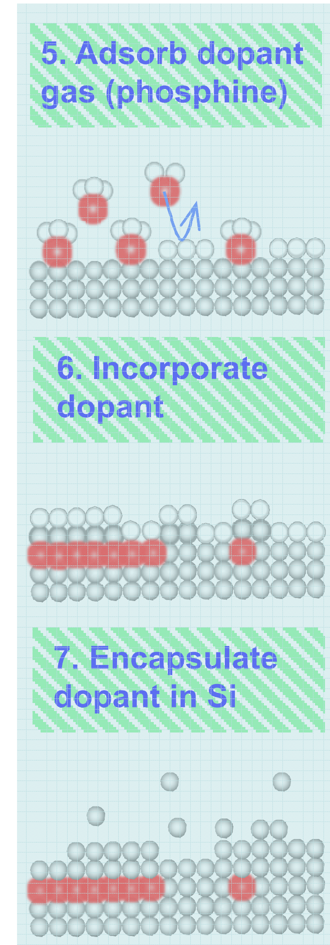
Low defect resist

Atomically accurate pattern (e.g., no H-diffusion)

Low temperature epi, low defect, low segregation

Smoothing epitaxy

Work function of leads – doping concentration



Fab throughput issues in-general

QIST team & external connections

- QIST contributors at SNL

  QD & Timed Implant Qubit Fab: J. Dominguez, R. Manginell, T. Pluym, B. Silva, J. Wendt, S. Wolfley

  Qubit control & measurement: S. Carr, M. Curry, T. England, A. Grine, K. Fortier, R. Lewis, M. Lilly, T.-M. Lu, D. Luhman, J. Rivera, M. Rudolph, P. Sharma, A. Shirkhorshidian, M. Singh, L. Tracy, M. Wanke

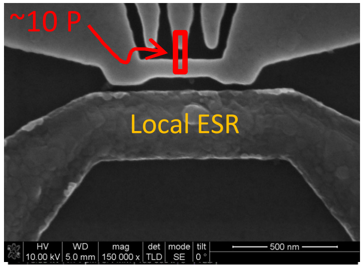
  Advanced fabrication (two qubit): E. Bielejec, E. Bussmann, E. Garratt, J. Koepke, A. MacDonald, E. Langlois, M. Marshal, B. McWatters, S. Miller, S. Misra, D. Perry, S. Samora, D. Scrymgeour, R. Simonson, G. Subramanian, D. Ward, E. Yitamben

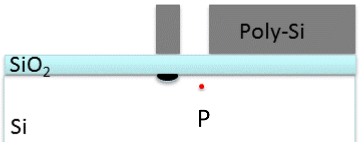
  Device modeling: J. Gamble, S. Gao, M. Grace, T. Jacobson, R. Muller, E. Nielsen, I. Montano, W. Witzel, K. Young

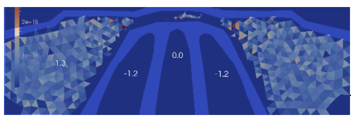
- Joint research efforts with external community:
  - Australian Centre for Quantum Computing and Communication Technology (D. Jamieson, A. Dzurak, A. Morello, M. Simmons, L. Hollenberg)
  - Princeton University (S. Lyon, J. Petta)
  - NIST (N. Zimmerman, M. Stewart)
  - U. Maryland (S. Das Sarma)
  - National Research Council (A. Sachrajda)
  - U. Sherbrooke (M. Pioro-Ladriere, C. Bureau-Oxton, P. Harvey-Collard)
  - Purdue University (G. Klimeck & R. Rahman)
  - U. New Mexico (I. Deutsch, P. Zarkesh-Ha)
  - U. Wisconsin (M. Eriksson, S. Coppersmith, D. Savage)
  - University College London (J. Morton)
  - Zyvex (J. Randall)
  - Chee Wee (U. Taiwan)
  - McGill (W. Coish, D'Anjou)

Summary

28Silicon P donor qubit w/ self-aligned implant

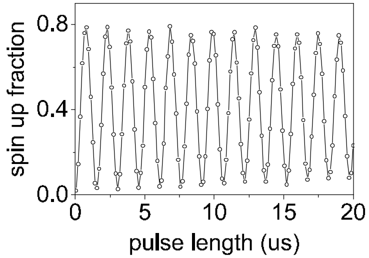




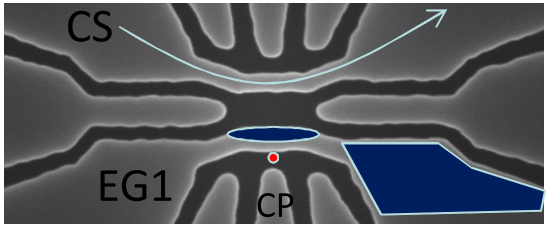


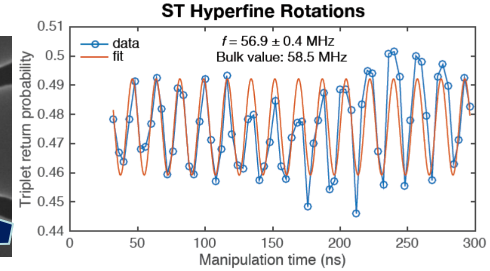
← & Si QD simulation

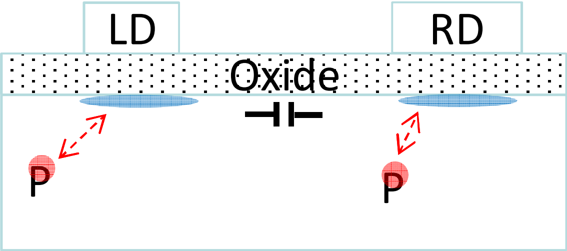
HEMT read-out & Rabi oscillations (28Si)

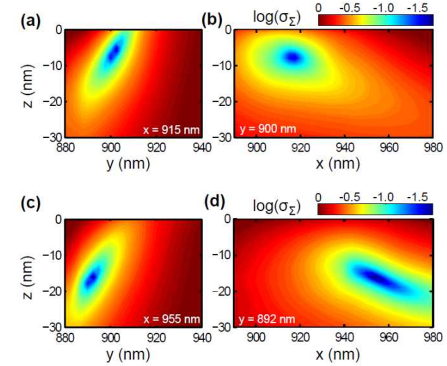


Donor hyperfine driven S/T qubit

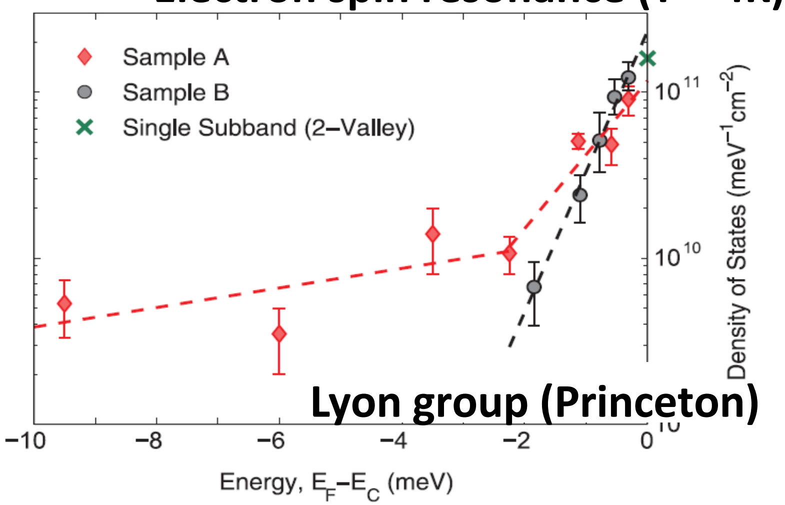




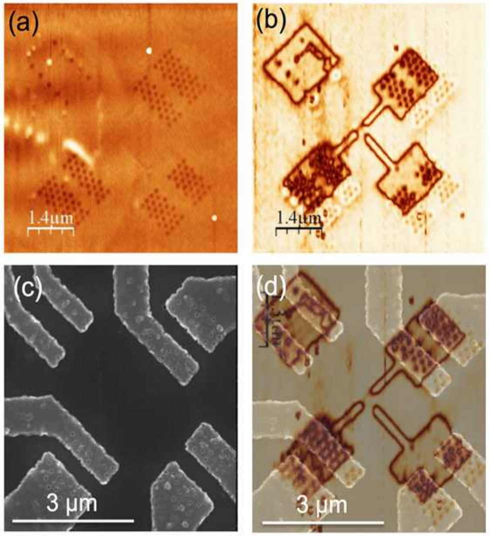




Electron spin resonance (T ~ 4K)

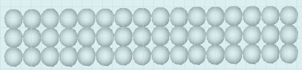


Lyon group (Princeton)

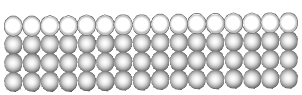


How to do atomically precise fab

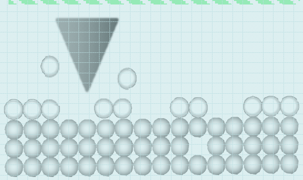
2. Prepare clean Si surface



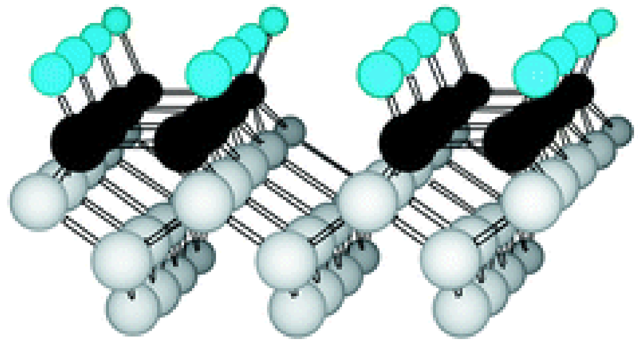
3. Add hydrogen resist (H-resist)

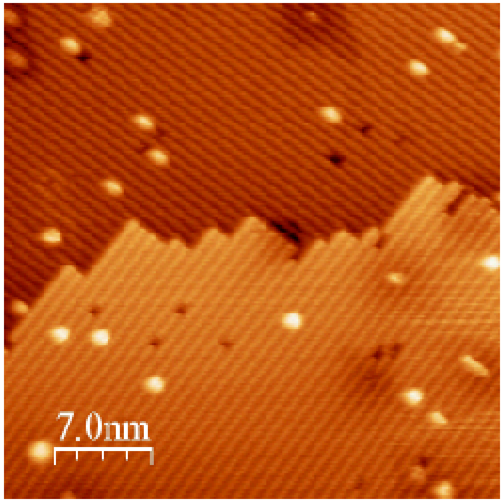


4. Pattern H-resist



H termination

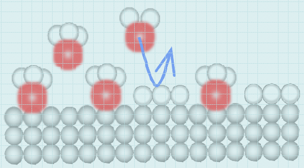




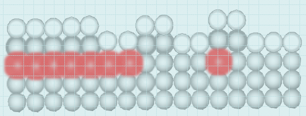
Missing atom defects ("innies")

Single dangling bond ("outies")

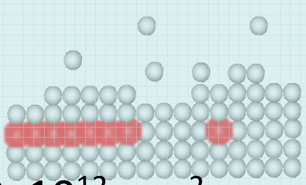
5. Adsorb dopant gas (phosphine)



6. Incorporate dopant



7. Encapsulate dopant in Si



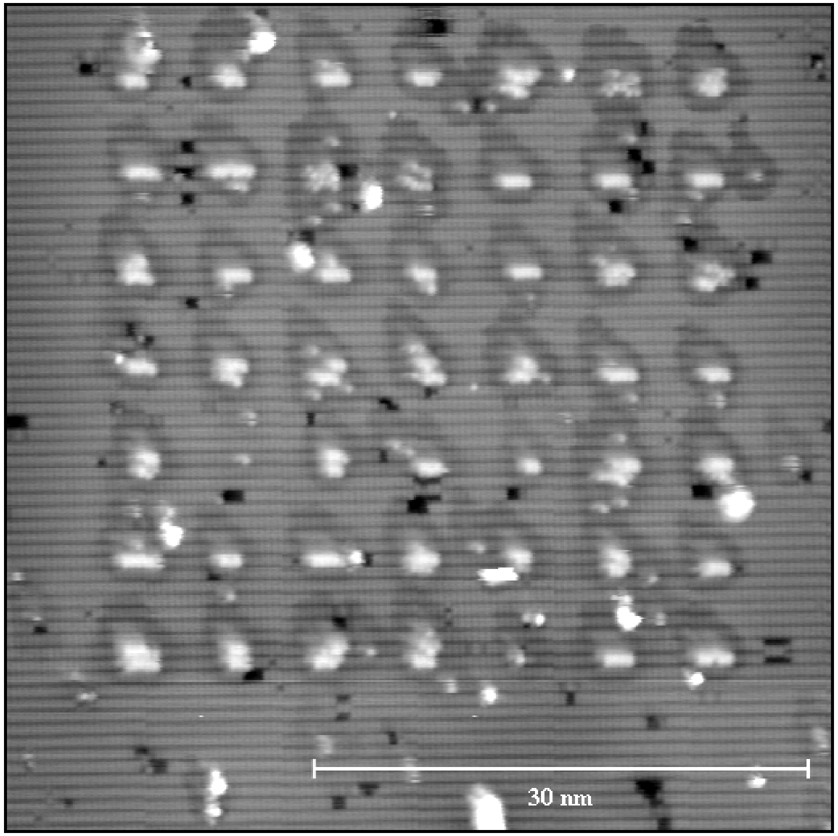
D ~ $3x10^{12}$ cm^{-2}

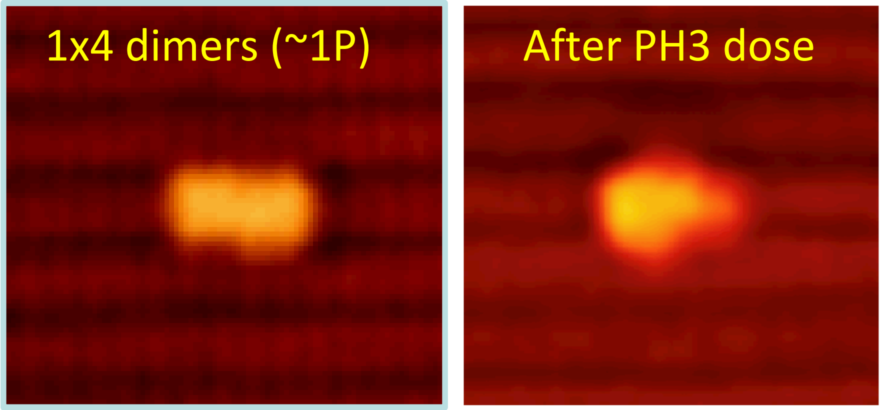
$D_{CMOS-ions/metals}$ ~ $1x10^{10}$ cr

Also better resists?

Single donor placement

H-Si(100) litho array





Precise tip alignment over center of dimer row leads to higher probability of 3-4 dimer openings

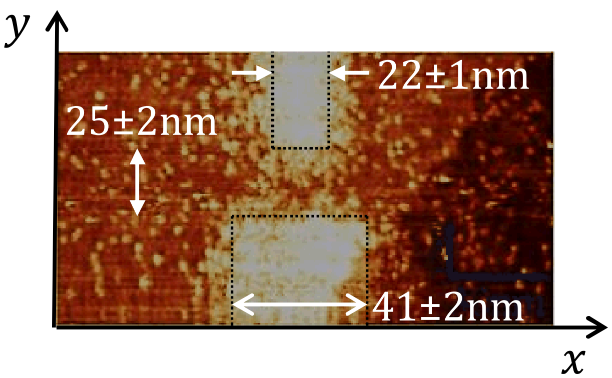
if tip is between dimer rows => poor outcome

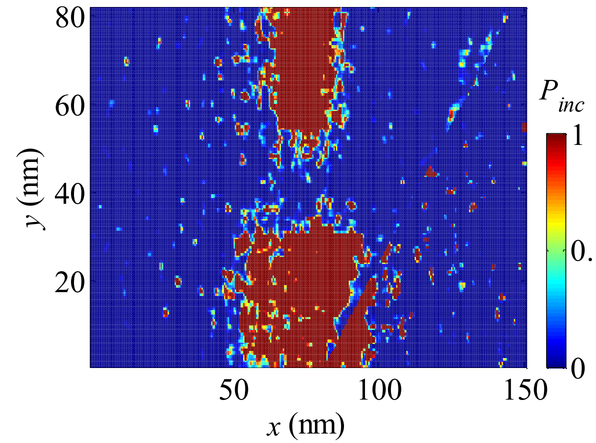
Working with Zyvex on automated control

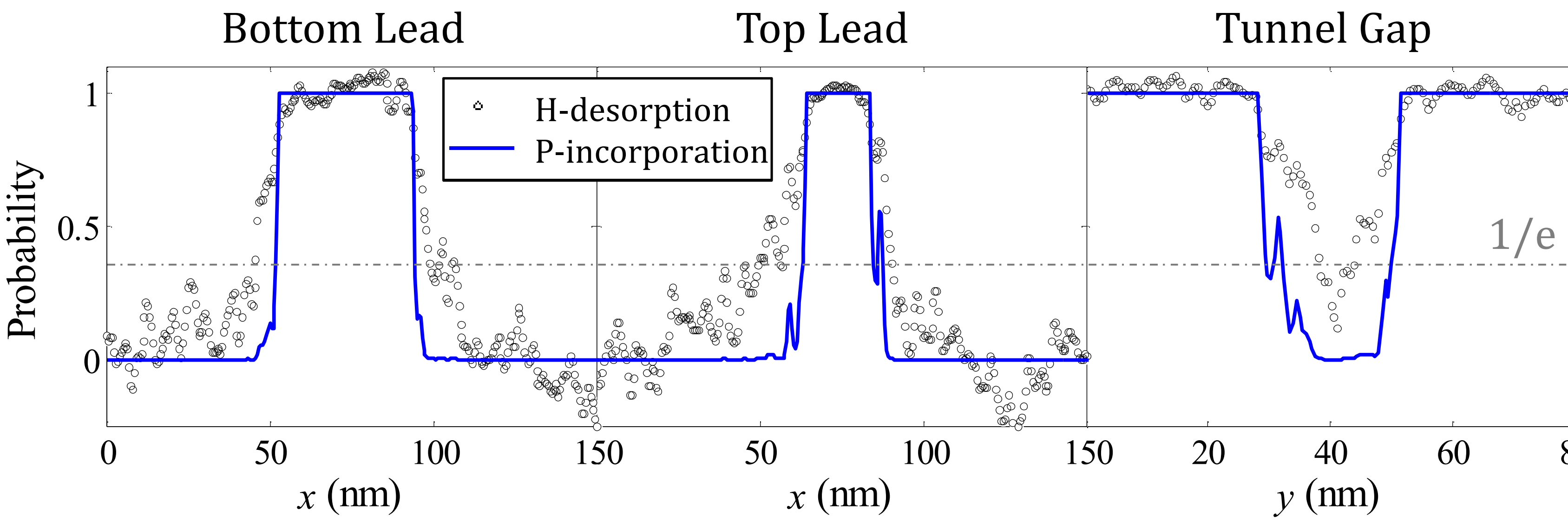
Examined result of PH3 exposure and found evidence of single P species adsorption

How to get 100% incorporation

Tunnel gap device electrical dimensions

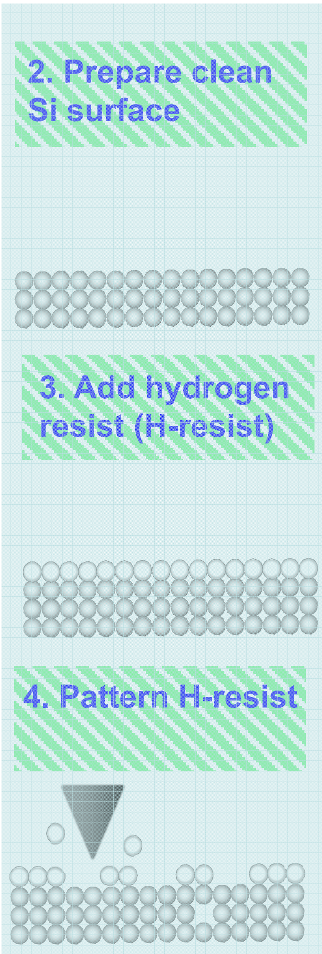


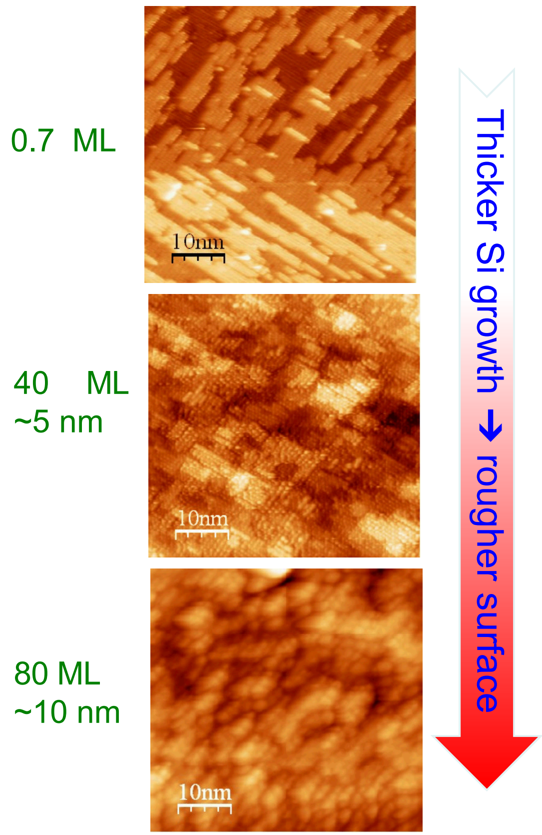


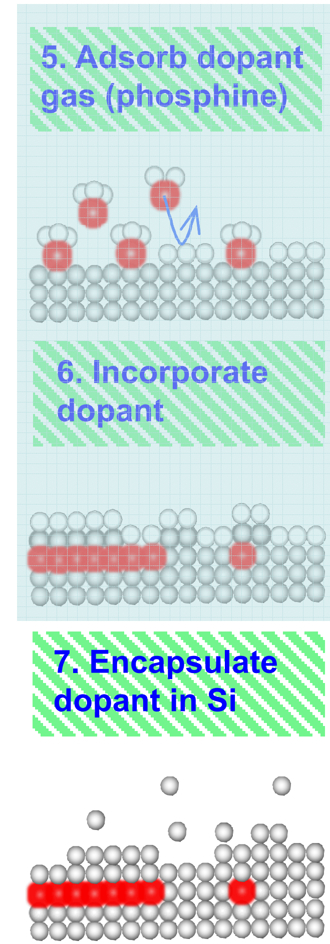


Model of probability of incorporation: Fuechsle (2012)

How to do atomically precise fab

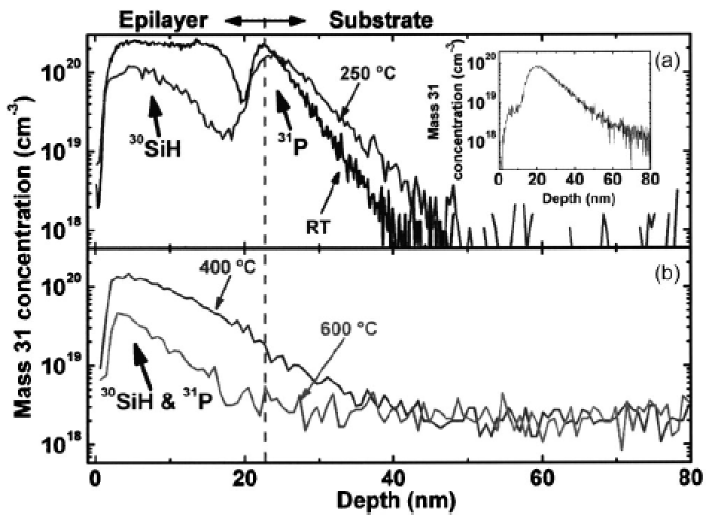




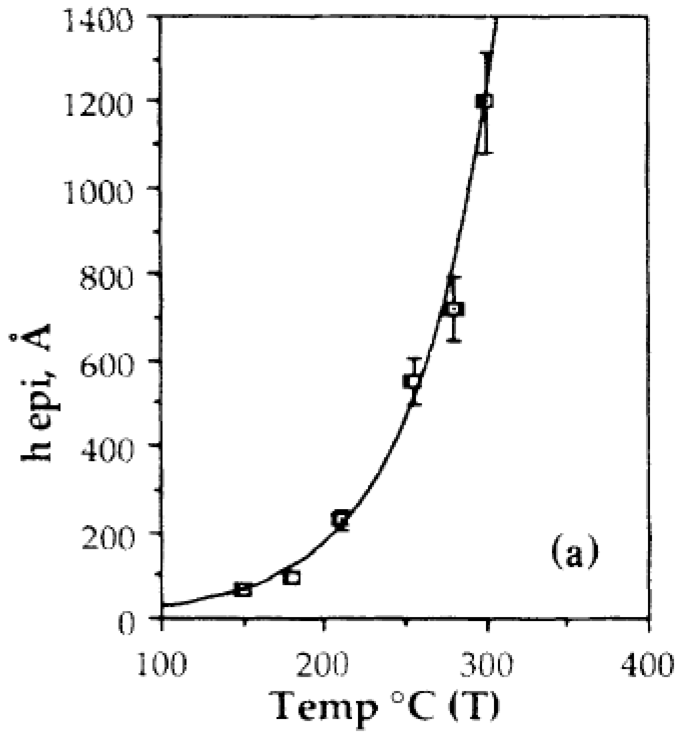


Low temperature/low diffusion Si epi?

T(°C)	RT	250	400	600
ℓ_{seg}(nm)	1.5	2.3	100[a]	1000[a]
n_{31}(10^{14} cm^{-2})	1.3	1.4	1.7[b]	0.4[b]
n_s(10^{14} cm^{-2})	1.67	1.64	0.22	⋯



Goh et al., APL 2004



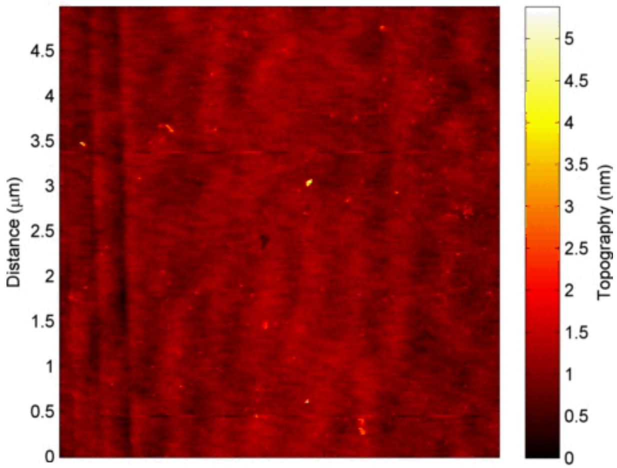
Eaglesham et al., PRL 1990

- Want P to stay in place after incorporation
- Diffusion and segregation work against this goal
- Critical thickness of low T epi also introduces challenges
- Difficult measurement – SIMS is flawed for this characterization
- Better ideas than low T epi + high T epi?

AFM / STM of Strained SOI

AFM

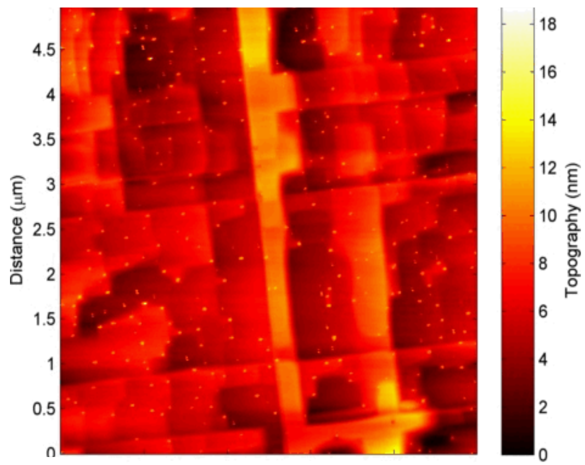
Chemical cleaning +
no Flash



0 Distance [um] 5

RMS roughness = 0.21 nm

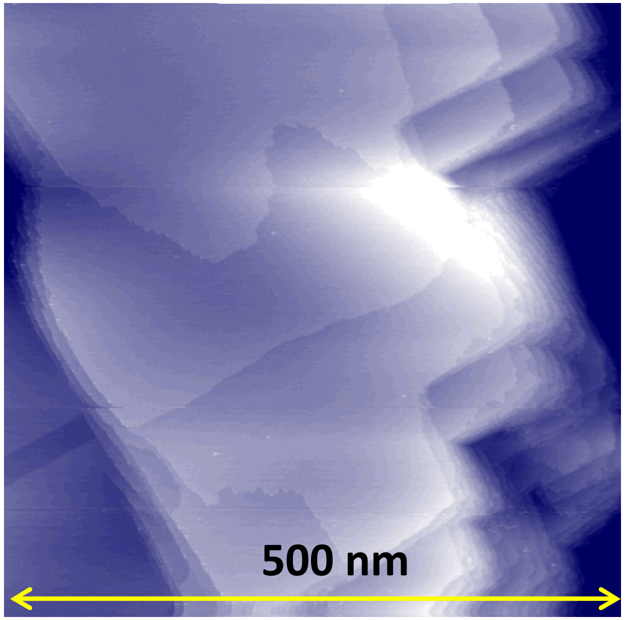
Chemical cleaning + Flash
Anneal at 940°C

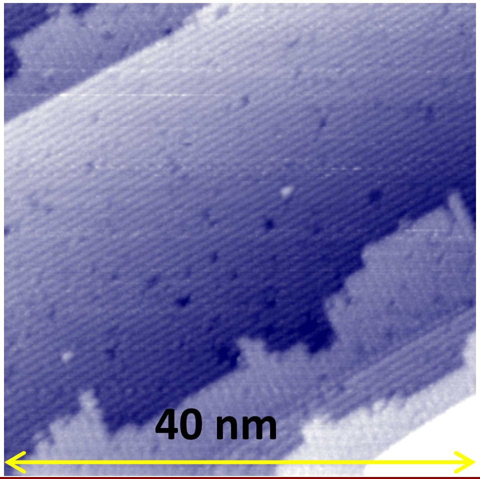


0 Distance [um] 5

RMS roughness = 2.1 nm

STM



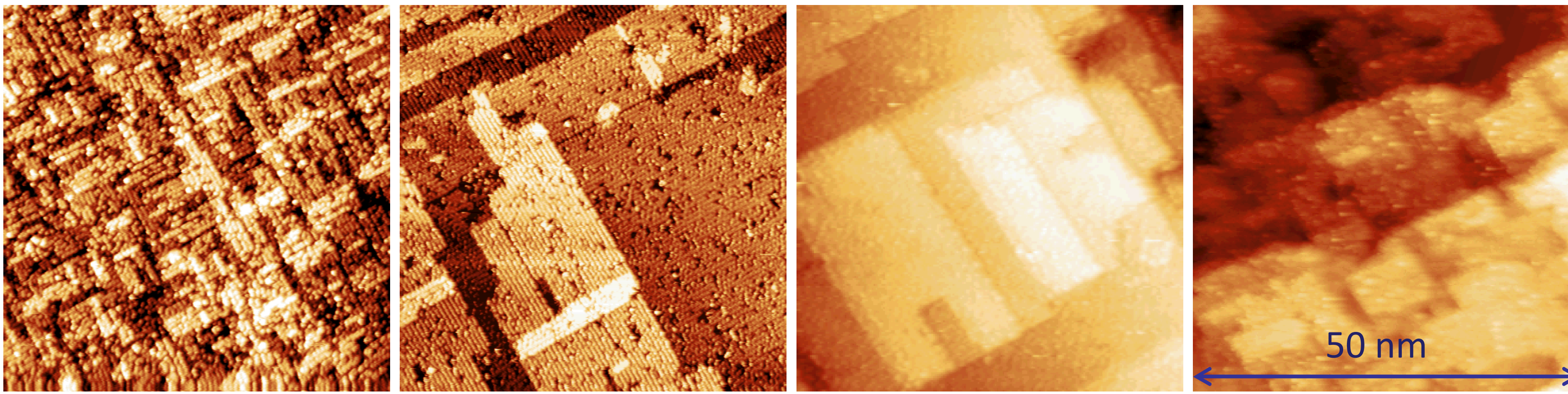


- Surface roughness increases ten-fold once sample is flash-annealed
- Crosshatch patterned island formations, indicating relaxation of strain
- Large terraces form on top of cross-hatch islands a
- Severe step bunching observed on the side of terraces/islands

Si Growth on sSOI

Increasing thickness

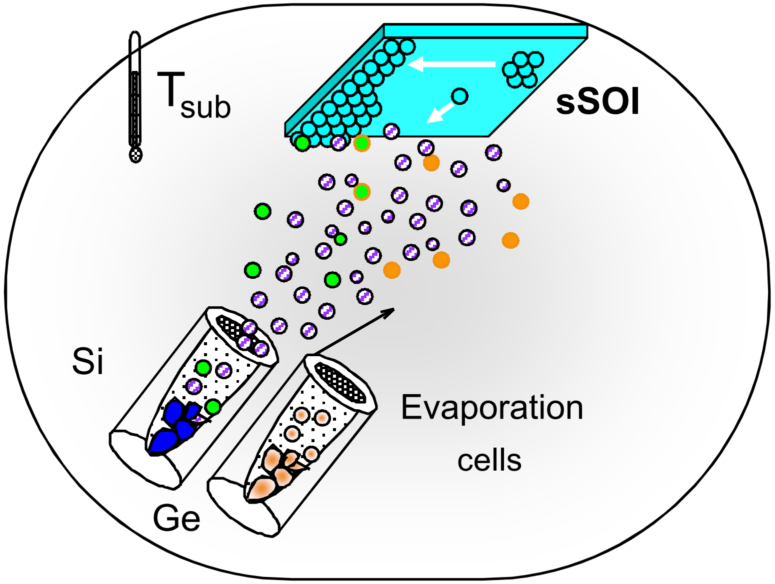
No heat 1.4 ML 3 ML 34 ML



$T_{substrate}$ = ~ 500C

- No heat ➔ the surface is rough ~ 5 Å
- With heat, there is more order on the surface: 2-D islands form
- With increasing thickness, larger islands form, and further, there is an increase in island density

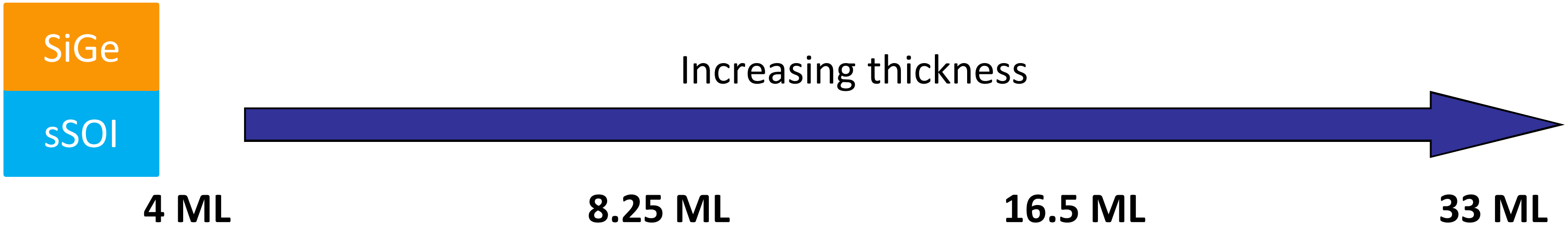
SiGe Growth (~20 % Ge) on sSOI

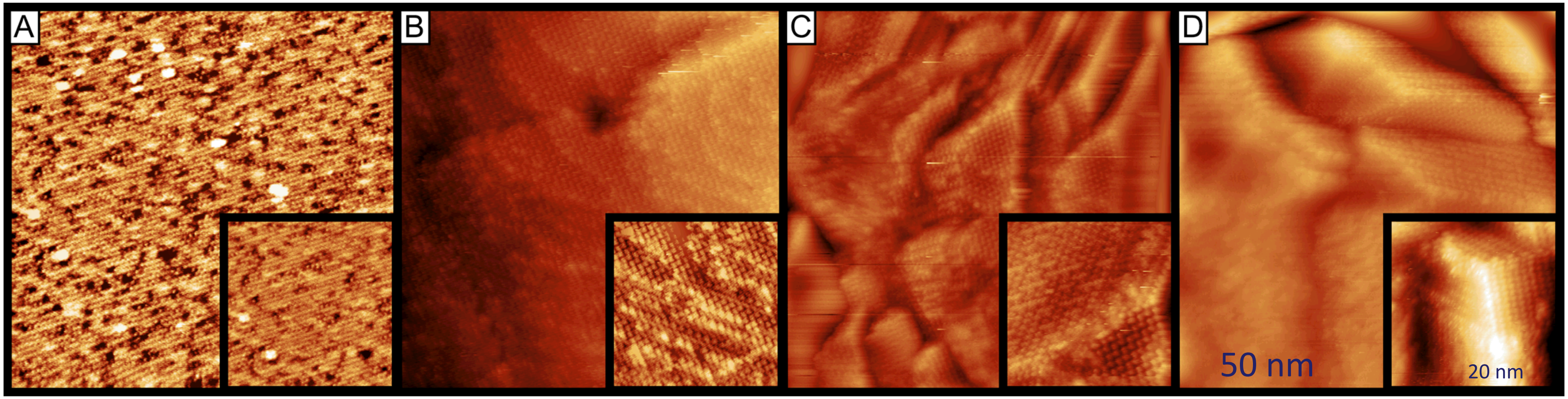


- Sample preparation
  - Evaporation of Si and Ge on Si(001);
  - Si flux is 0.032Å/s and Ge flux is ~ 0.006 Å/s
  - Substrate kept at ~ 500 - 550C during deposition;
- Scanning tunneling microscopy (STM)
  - Sample imaged at room temperature.

20% SiGe is approximately lattice matched with the sSOI

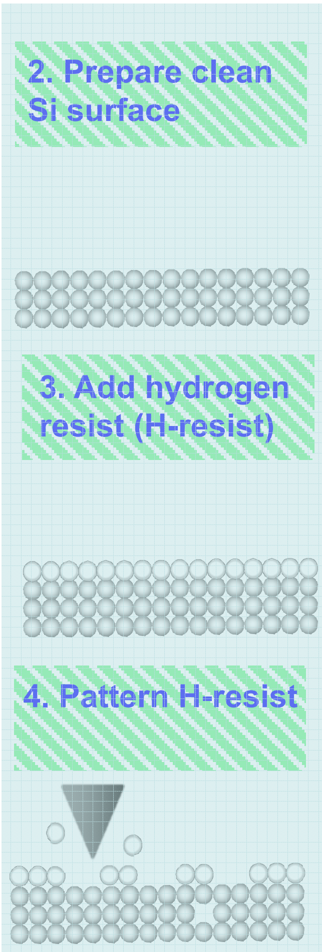
Different Thickness of SiGe (~20 % Ge) on sSOI

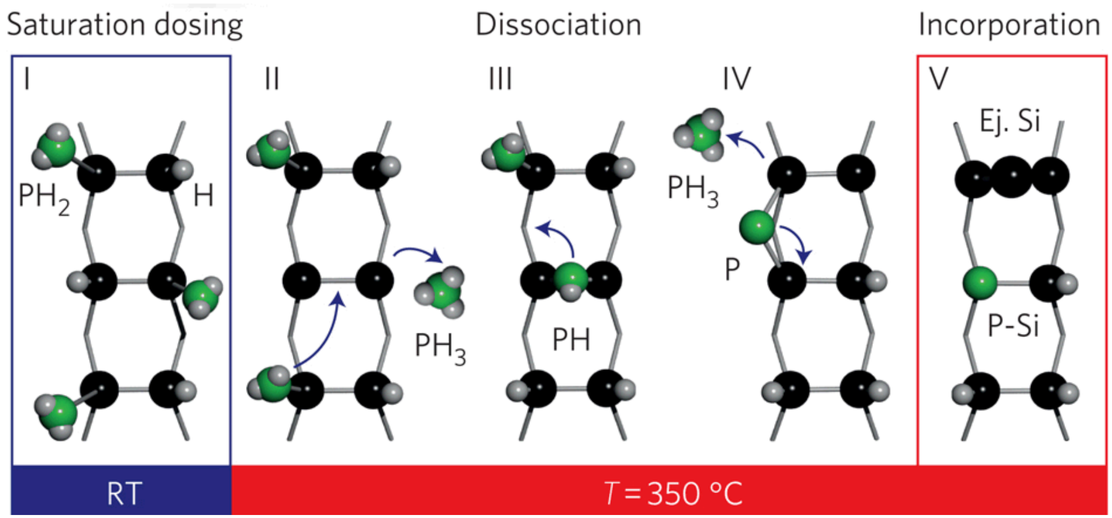


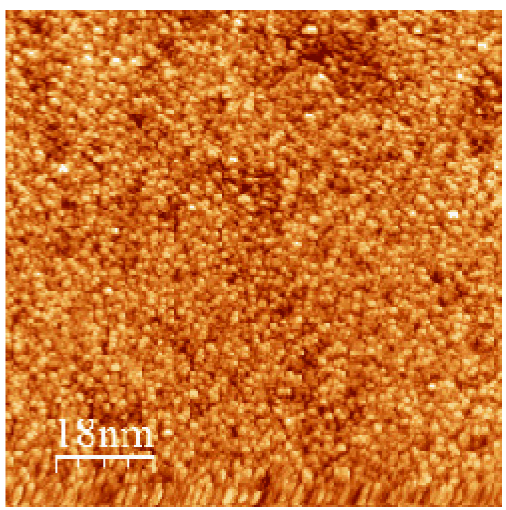


- At low coverage, observation of dimer row reconstruction, although defects in reconstruction is relatively high
- With increasing thickness, shallow 3D islands start to form (~2-3 nm peak to valley)
- MBE of unstrained SiGe on Si reported flat for these conditions [Bean et al., JVST A 2(1986)]
- TEM shows defect free interface
- Next: make devices and work on smoother growth conditions

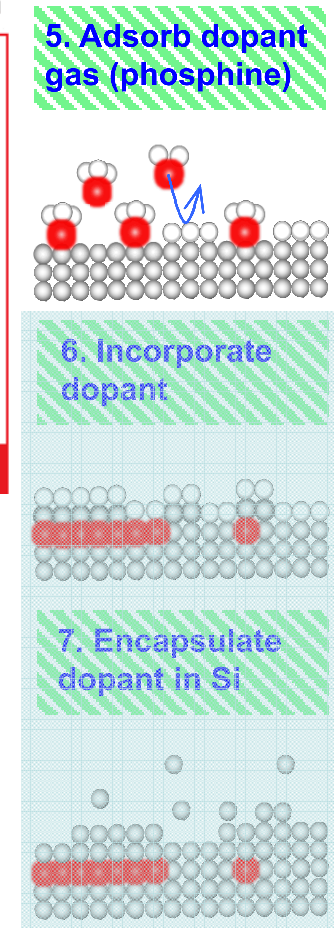
How to do atomically precise fab



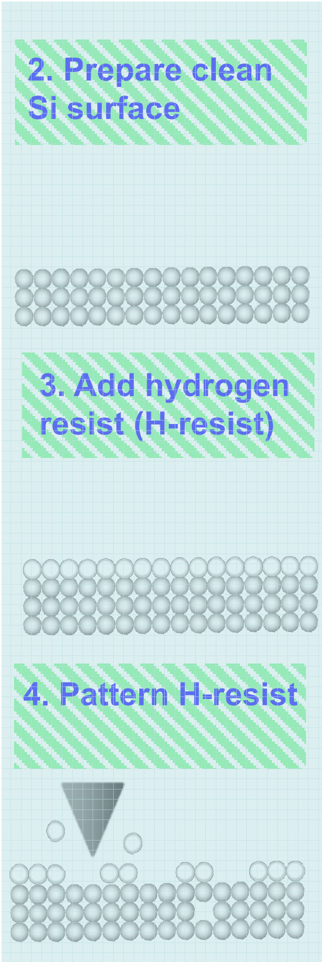


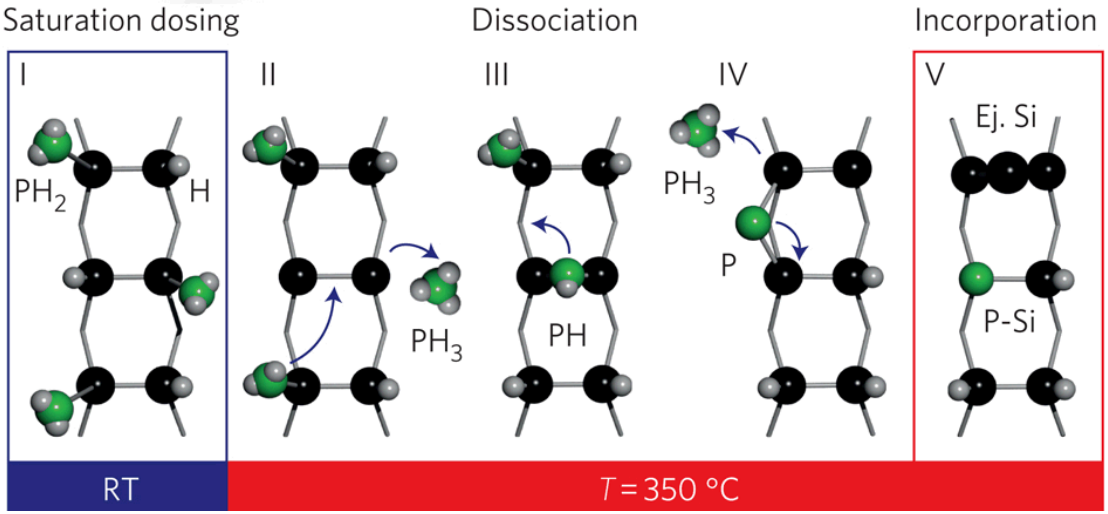


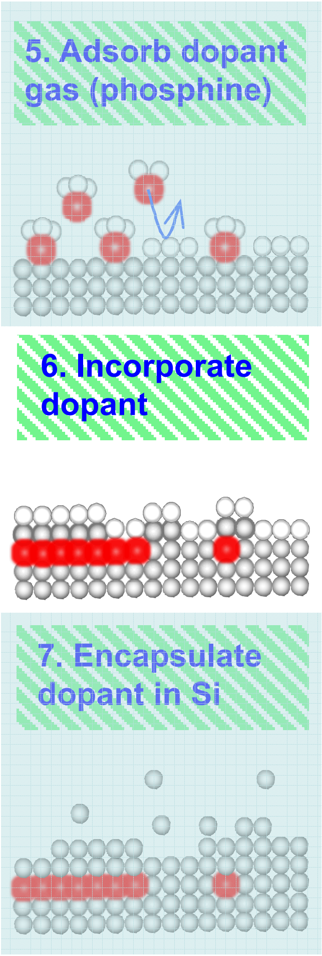
H/ PH_x looks disordered

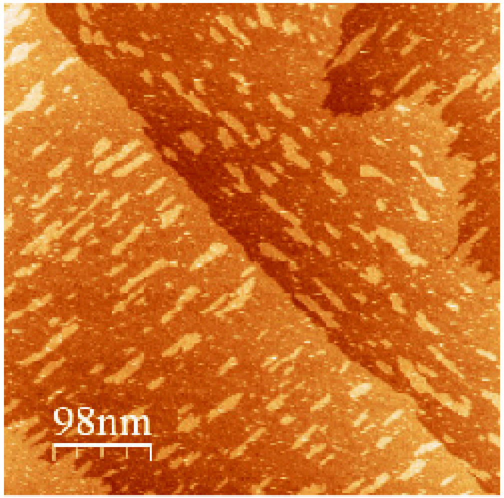


How to do atomically precise fab

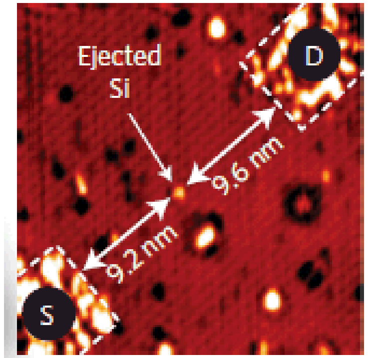








See ejected Si



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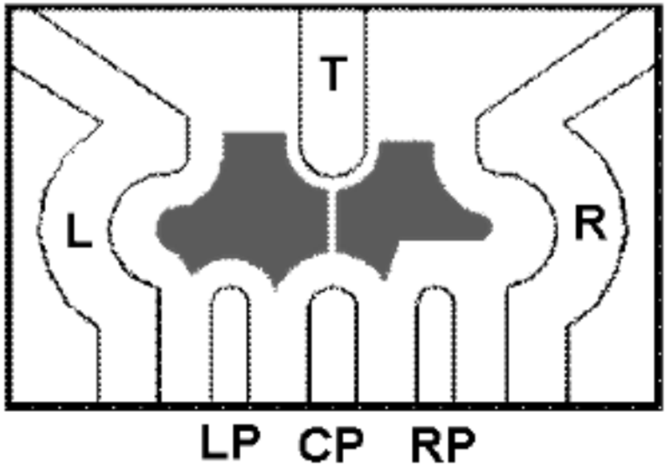
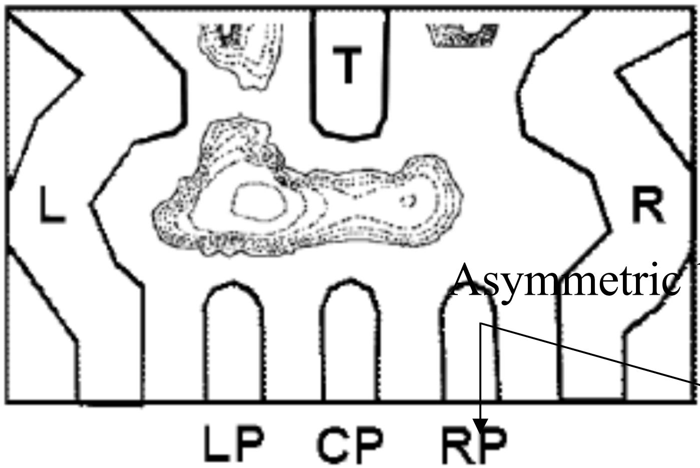
High accuracy single donor writing?

- The challenges:
  - Keep tip resolution over entire writing time
  - Accuracy/precision opening of 3 dimers (writing parameters, drift, …)
  - No H re-passivation
  - 100% incorporation into 3 dimer region (get the right temperature)
  - Encapsulation without motion/segregation (next slide)

- Best results communicated
  - ~80% yield
  - Painful verification process

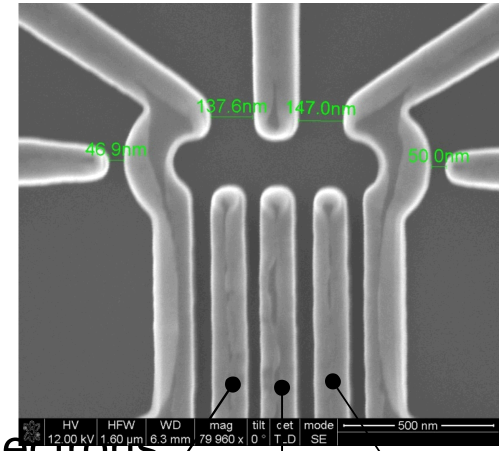
Overcoming Non-uniformity through Tuning in Open Lateral Geometry





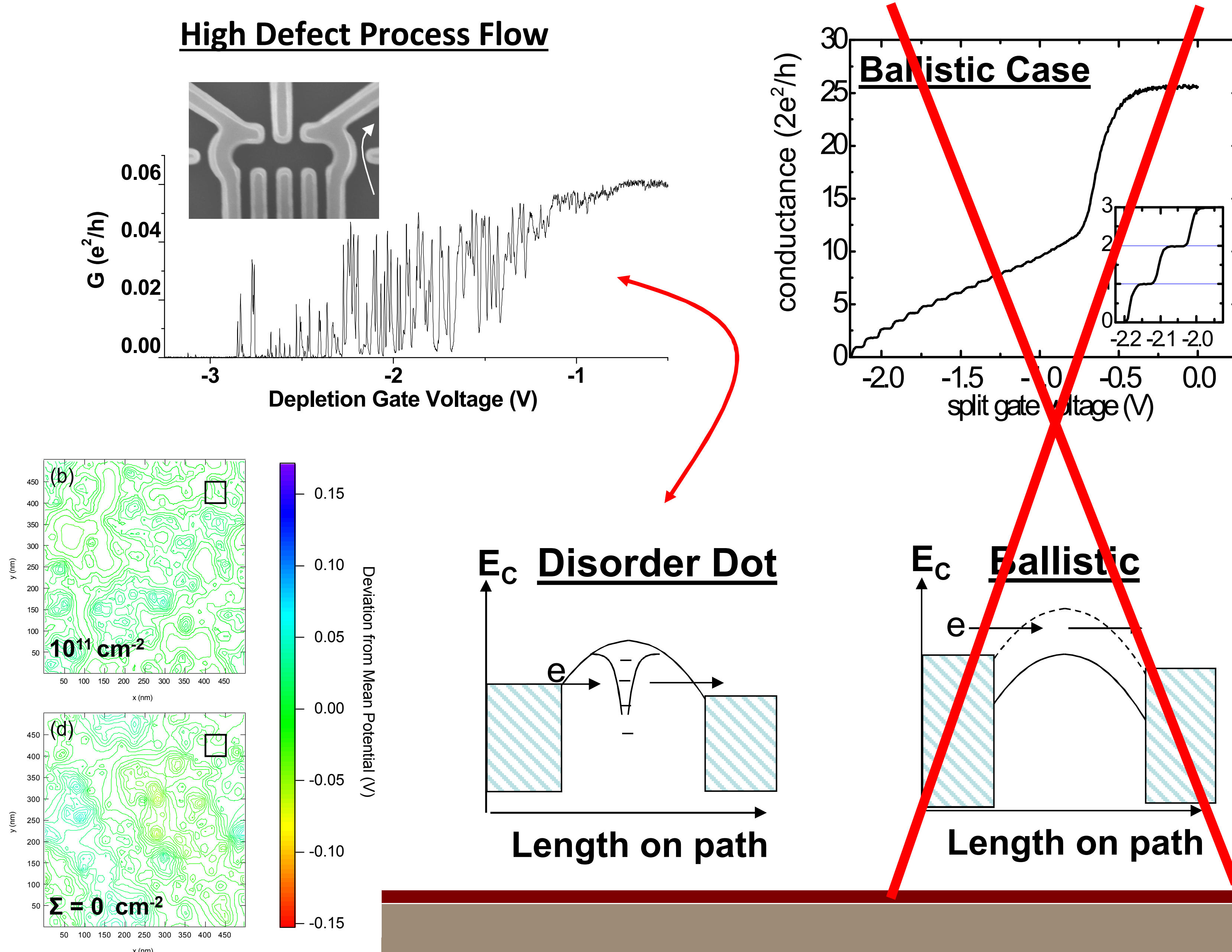
gate – dot	C_{MEAS} (aF)	$C_{Sentaurus}$ (aF)	$C_{CFD-ACE}$ (aF)
RP - RD	5.3 ± 0.1	3.3	5.5
RP - LD	1.8 ± 0.1	1.6	1.6
LP - LD	8.1 ± 0.1	9.4	8.0
LP - RD	1.6 ± 0.1	0.7	1.2
R - RD	11.6 ± 0.1	4.6	11.2
L - LD	17.3 ± 0.1	34.4	17.2
T – RD	7 ± 1*	8.8*	7.0
T – LD	8 ± 1*	9.2*	8.0
CP – RD	5 ± 2*	[illegible]	[illegible]
CP – LD	6 ± 1*	[illegible]	[illegible]
TG – RD	21 ± 5*	[illegible]	[illegible]
TG – LD	23 ± 2*	[illegible]	[illegible]

L. Tracy, et al.
(APL in progress)

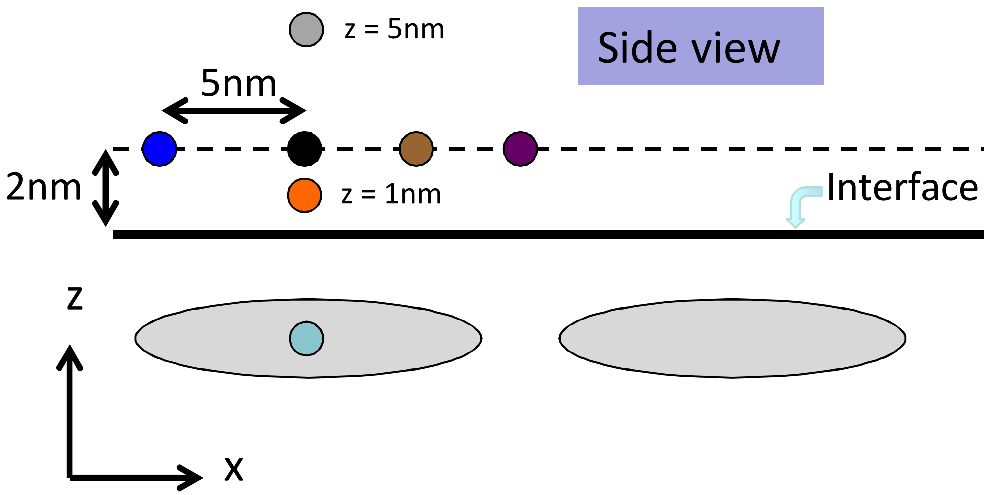


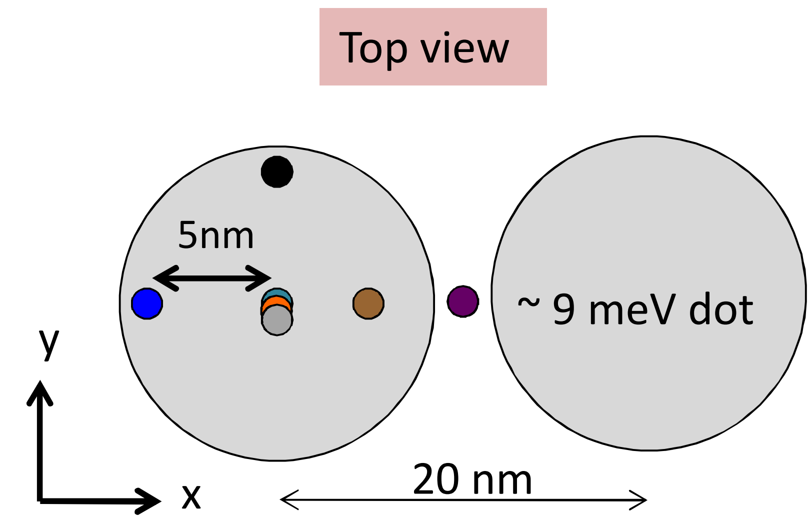
Left dot: 238 electrons
Right dot: 63 electrons

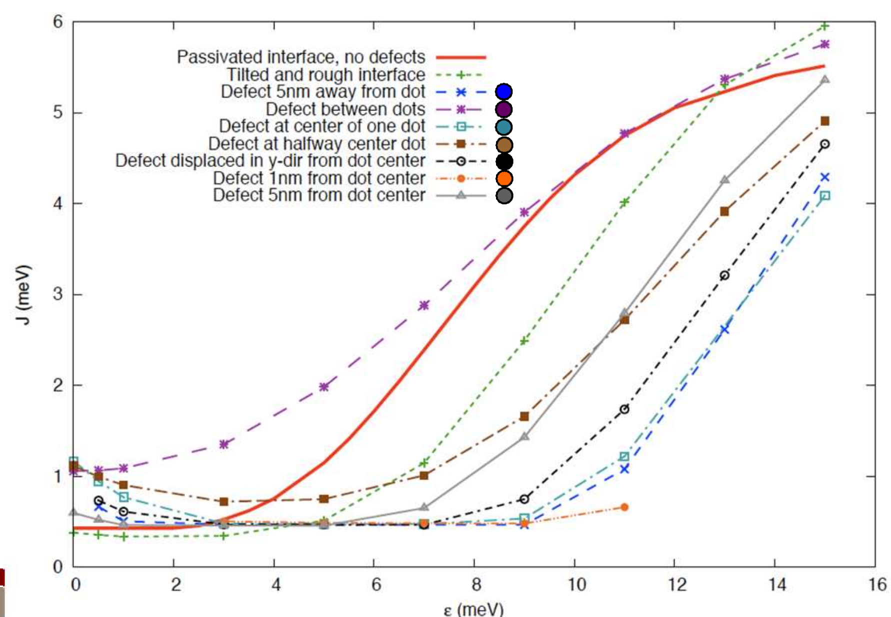
Disorder Potential Produced Quantum Dots



Implications for J curve (NEMO3D & CI calculations)







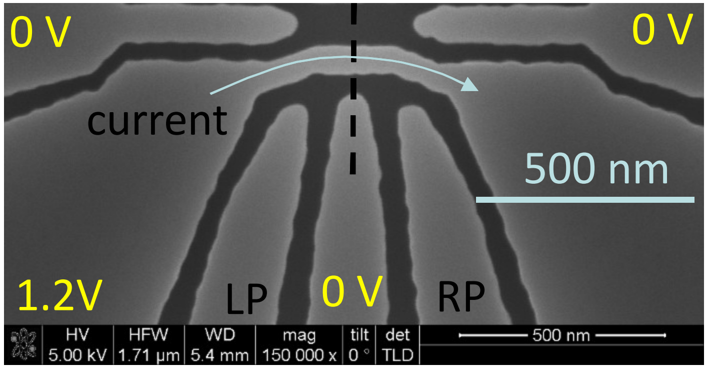
Conclusions:

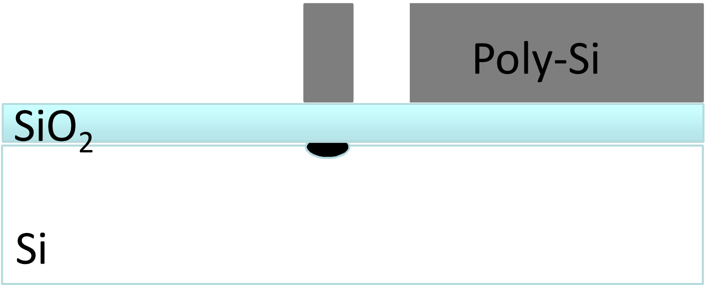
1. Defect produces offset in detuning
2. Tunnel coupling (slope of curve) can be perturbed
3. Result is statistical variation that will require tuning.
4. Possible challenges to control of dJ/dV

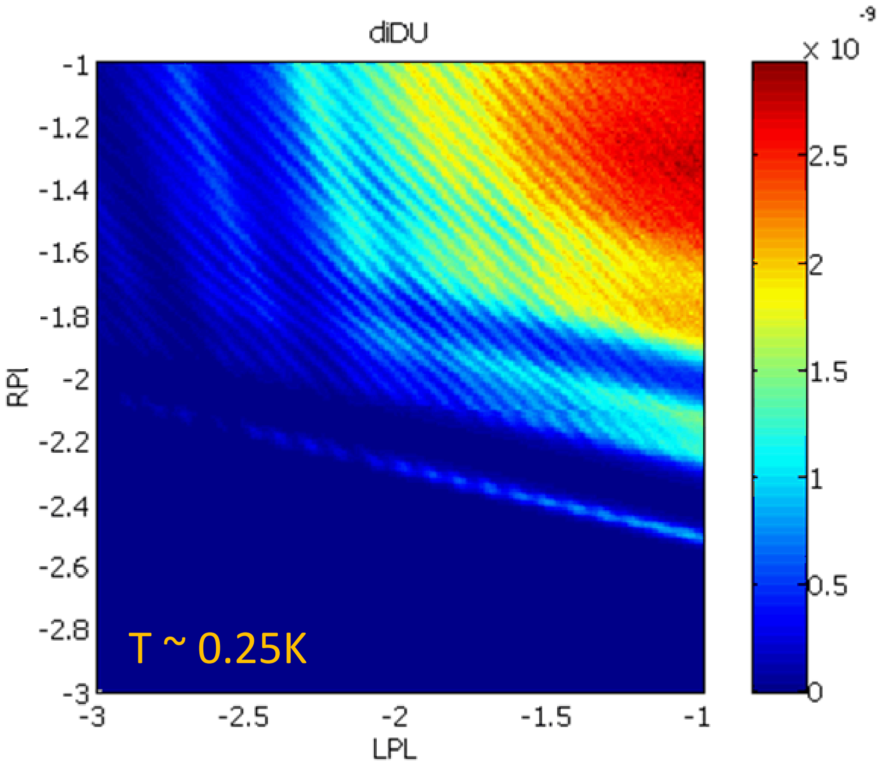
Calculations done using NEMO3D single wave functions & CI code

Rahman, Nielsen

Poly silicon quantum dot





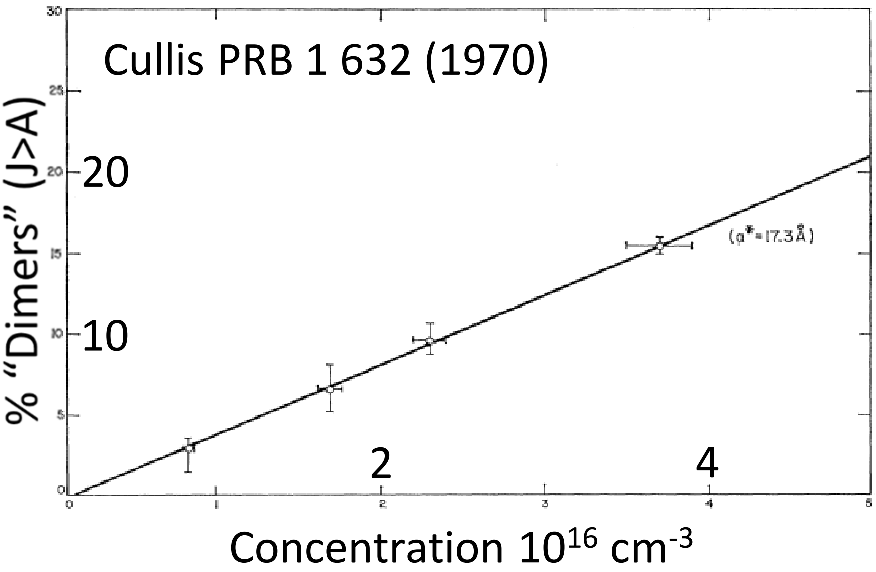


- Simplify SET for donor read-out
  - Implant is still self-aligned
- Relatively regular period Coulomb blockade achieved in poly silicon SET
- Wire width ~50-60 nm with gaps between wire and plunger of ~40-50 nm
- This structure can regularly be used for read-out

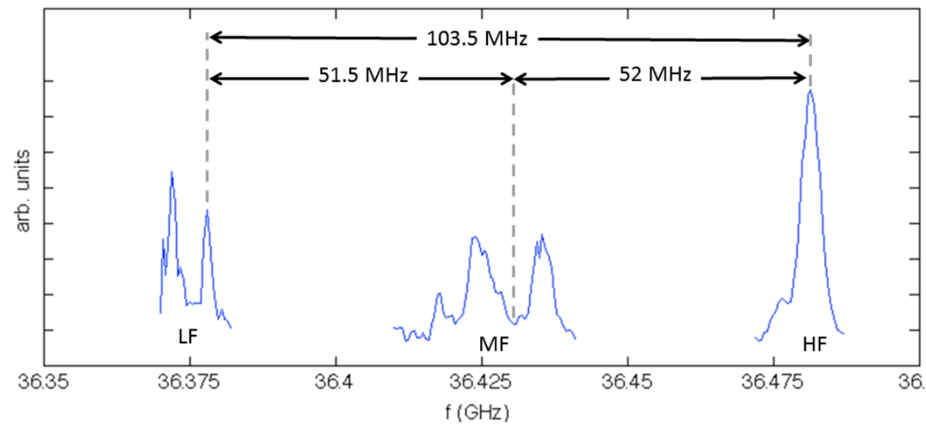
Harvey-Collard

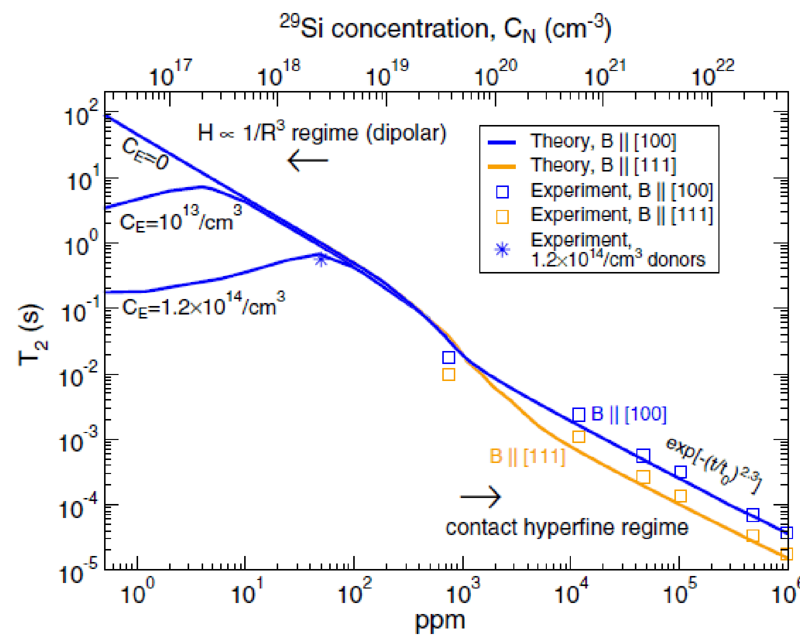
Sandia National Laboratories

Motivation for Single Donor Placement



Complex ESR spectrum from dimerization?





- Often assumed that single donor placement necessary for reasonable two qubit path
- Timed implant combined with tunable D-QD coupling would relax this strict requirement
- Down side of timed implant – the others can still introduce undesired effects
- Precision placement of single donors still the way to go
- Higher yield and performance path (long term view)
  - Place one and know you have one in zone
  - Better QD lateral shift or D vertical gate

Materials science wish list

- Metrology of single atom location
- Low temperature surface cleans and fabrication
  - 111
  - CVD techniques
  - Surface behavior after anneals
- Segregation suppression
- Interface characterization with respect to valley splitting
- Tunnel barrier characterization?
- Defects/traps and dynamics of defects traps
- Modeling
- Work function of donor leads