SAND2016-11283C

Comparing SRIM simulations and experimental results for shallow implantation of Sb into Si

Jose L. Pacheco[1], Todd Byers[2,1], [1]Stuart B. Van Deusen, Daniel L. Perry[1], Duncan Weathers[2] and Ed Bielejec[1].

[1]Sandia National Laboratories, Albuquerque NM. 87123

[2]University of North Texas, Denton TX. 76203

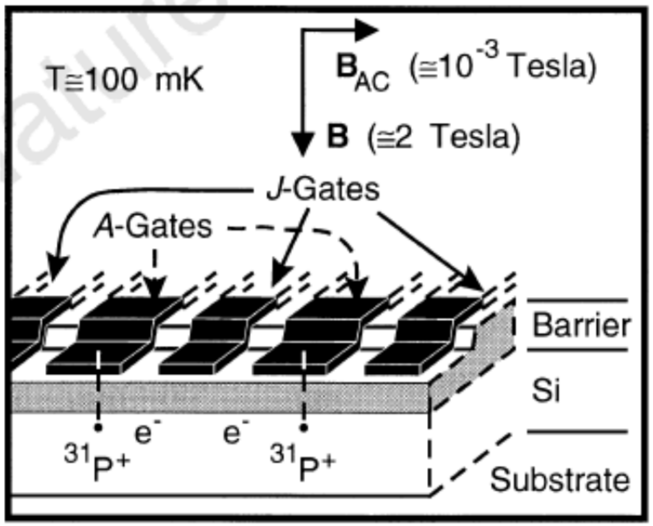
Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Outline

- Single atom positioning with nm-scale resolution
  - Donor based qubits
  - Defect (color) centers in Diamond
- How accurate are SRIM simulations to predict implant range and straggle?
  - Fidelity of SRIM simulations is compromised for low-energy heavy-ion implantation into light targets.
- Experiments to compare SRIM to RBS and SIMS

Single atom positioning with nm resolution: Path to quantum computation

A silicon-based nuclear spin quantum computer

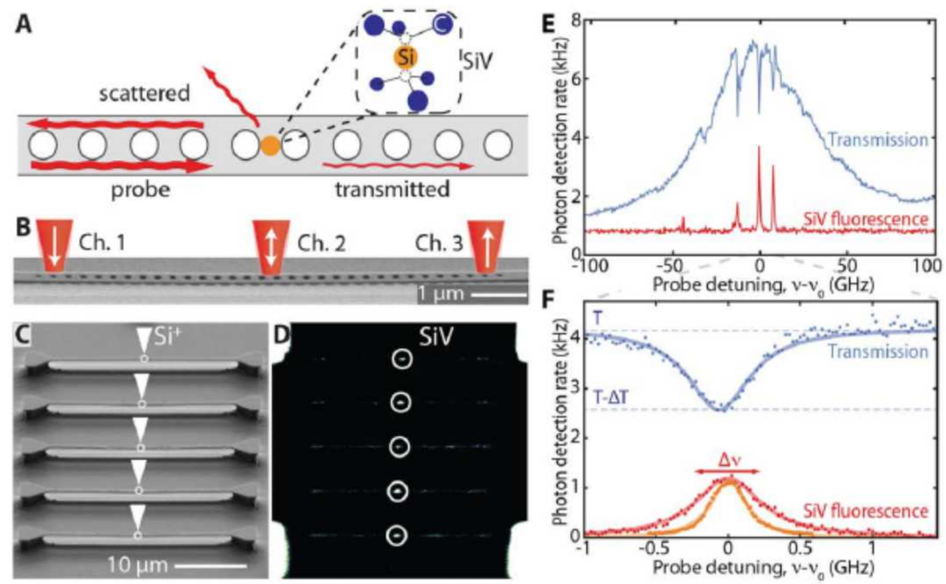


Kane, Bruce E. *nature* 393.6681 (1998)

An integrated diamond nanophotonics platform for quantum optical networks

A. Sipahigil,[1]* R. E. Evans,[1]* D. D. Sukachev,[1,2,3]* M. J. Burek,[4] J. Borregaard,[1] M. K. Bhaskar,[1] C. T. Nguyen,[1] J. L. Pacheco,[5] H. A. Atikian,[4] C. Meuwly,[4] R. M. Camacho,[5] F. Jelezko,[6] E. Bielejec,[5] H. Park,[1,7] M. Lončar,[4] M. D. Lukin[1]†

Science 13 Oct. 2016



Positioning Requirements:

- Donors in Si: 15 nm +/- 5nm from interface** - Defect centers in diamond: < $\lambda/2$ ~ 300 nm

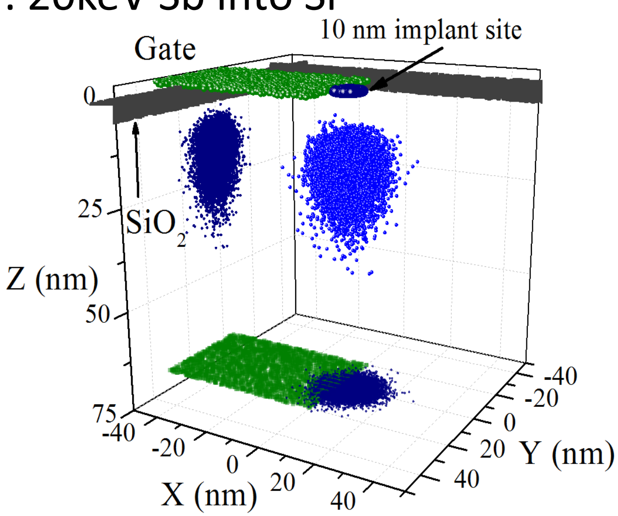
Deterministic, high precision placement of single atoms proposed and demonstrated for quantum computation

Shallow Sb donor implantation: donor based qubits in Si

What is needed:
- Single atom implants
- Range below interface →10 to 20nm
- Minimize straggle

How?
- Implantation of low energy, heavy ions.

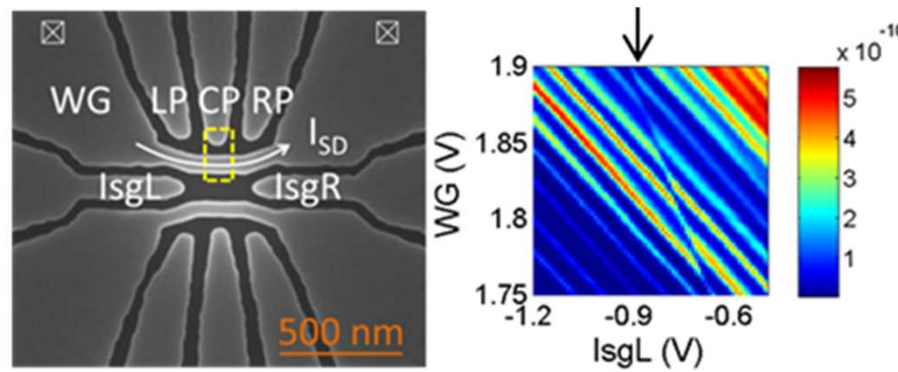
SRIM: 20keV Sb into Si



Electrostatically defined silicon quantum dots with counted antimony donor implants

M. Singh,[1,2,a)] J. L. Pacheco,[1] D. Perry,[1] E. Garratt,[1] G. Ten Eyck,[1] N. C. Bishop,[1]
J. R. Wendt,[1] R. P. Manginell,[1] J. Dominguez,[1] T. Pluym,[1] D. R. Luhman,[1,2] E. Bielejec,[1]
M. P. Lilly,[1,2] and M. S. Carroll[1]
[1]*Sandia National Laboratories, Albuquerque, New Mexico 87185, USA*
[2]*Center for Integrated Nanotechnologies, Sandia National Laboratories, Albuquerque, New Mexico 87175, USA*

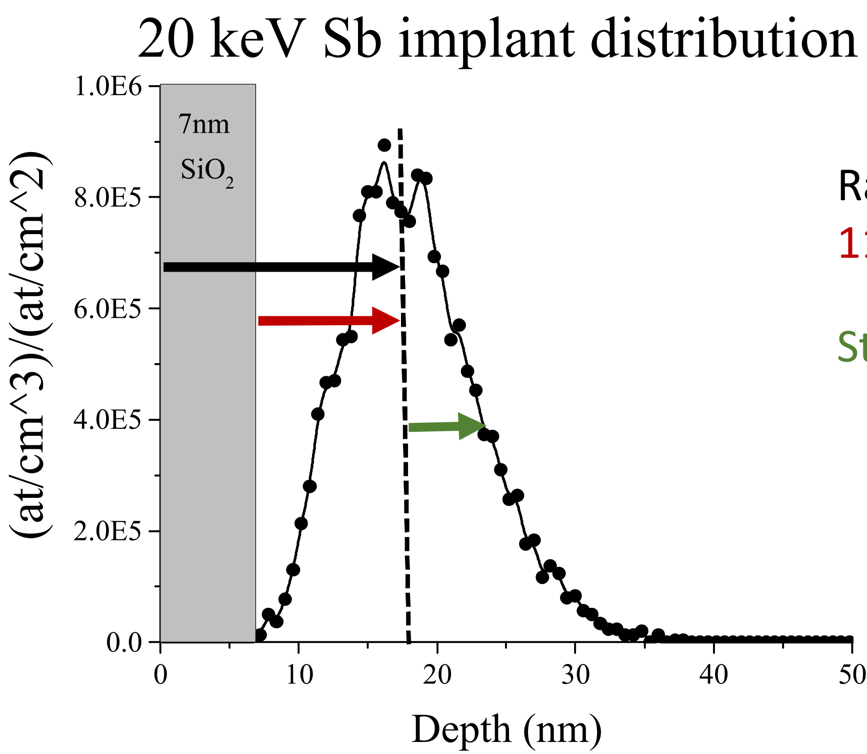
Applied Physics Letters 108.6 (2016)



Electron tunneling events from donor to dot (under gate) cause conductance offsets

Simulation shows a position distribution for high yield fabrication single donor qubits, and it works!!

SRIM simulations are key to determine the final atom position after implantation



Range 18 nm

11 nm from SiO2 interface

Straggle 5 nm

Implant location known to be within a sphere of ~5nm in radius!!

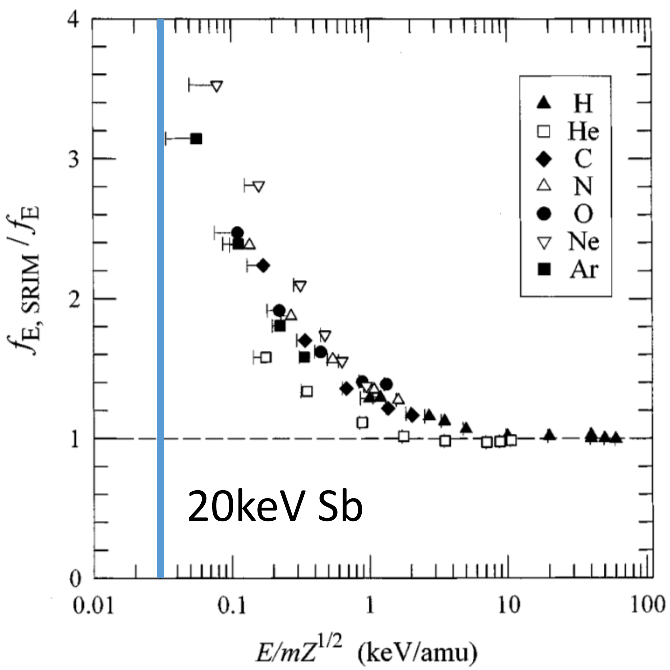
The question is: How accurate are SRIM simulations?

Low energy electronic stopping and nuclear stopping

SRIM over-estimates electronic stopping

Response of 100% Internal Carrier Collection Efficiency Silicon Photodiodes to Low-Energy Ions

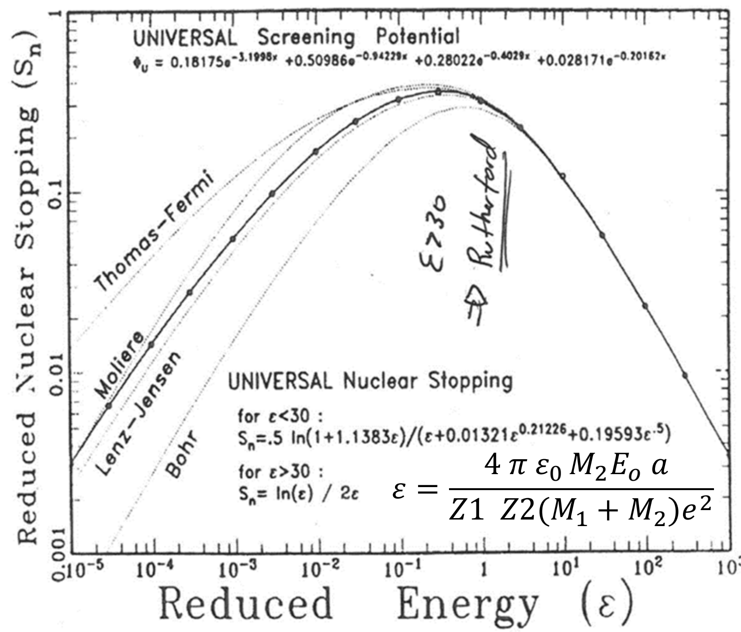
Herbert O. Funsten, *Member, IEEE*, Stephen M. Ritzau, Ronnie W. Harper, and Raj Korde, *Member, IEEE*



IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 48, NO. 6, DECEMBER 2001

Nuclear stopping theories diverge

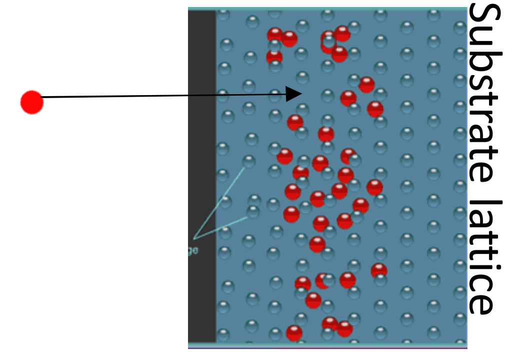
- Universal is a few % accurate over large energy range!!



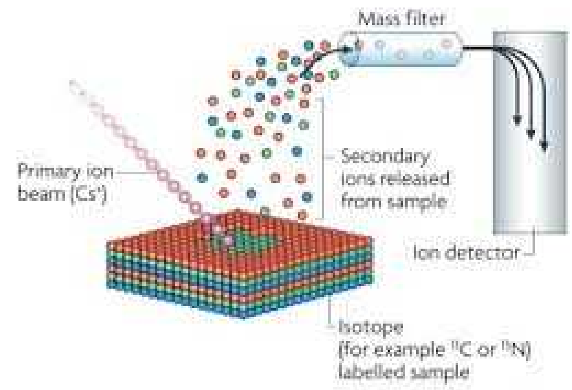
textbook: www.srim.org

Measured vs predicted electronic stopping energy fraction values diverge. Does this affect the range?

Experiments



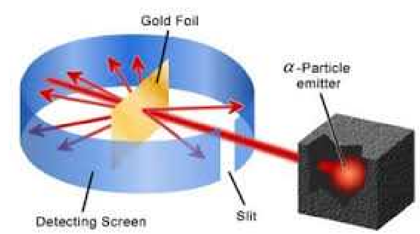
1) Implant Sb into Si
   - Crystalline Si samples with native oxide only
   - Sent to EAG* for implantation of natural Sb (121 and 123)
   - Range of fluences and range of energies
   - Implanted at 7^{o} to substrate normal



Nature Reviews | Microbiology

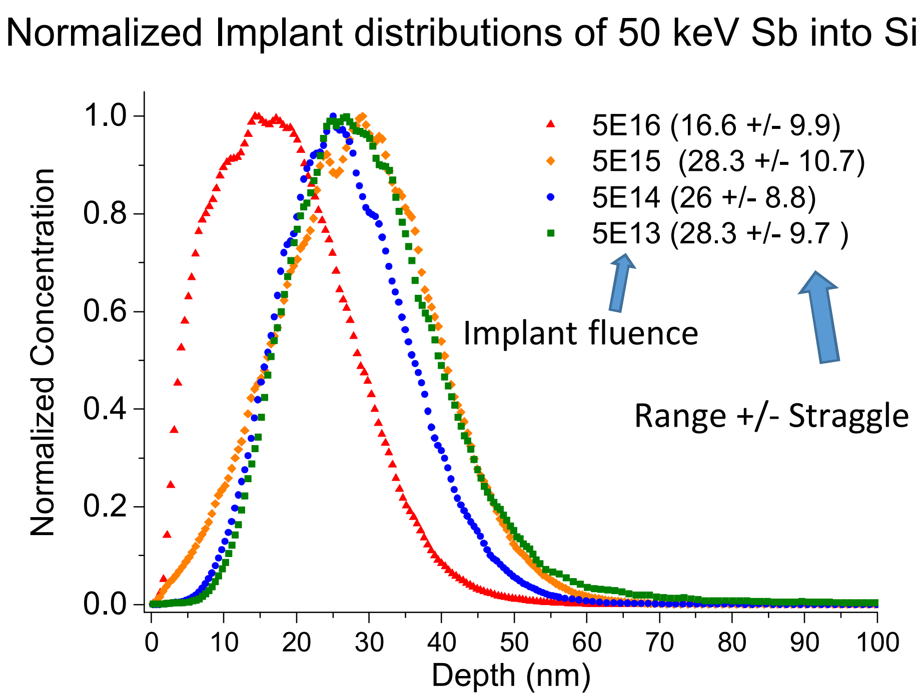
2) Secondary Ion Mass Spectrometry (SIMS)
   - Depth profiling (range and straggle)
   - Determine fluence to implant saturation
   - Incorrect sputtering rate can skew results

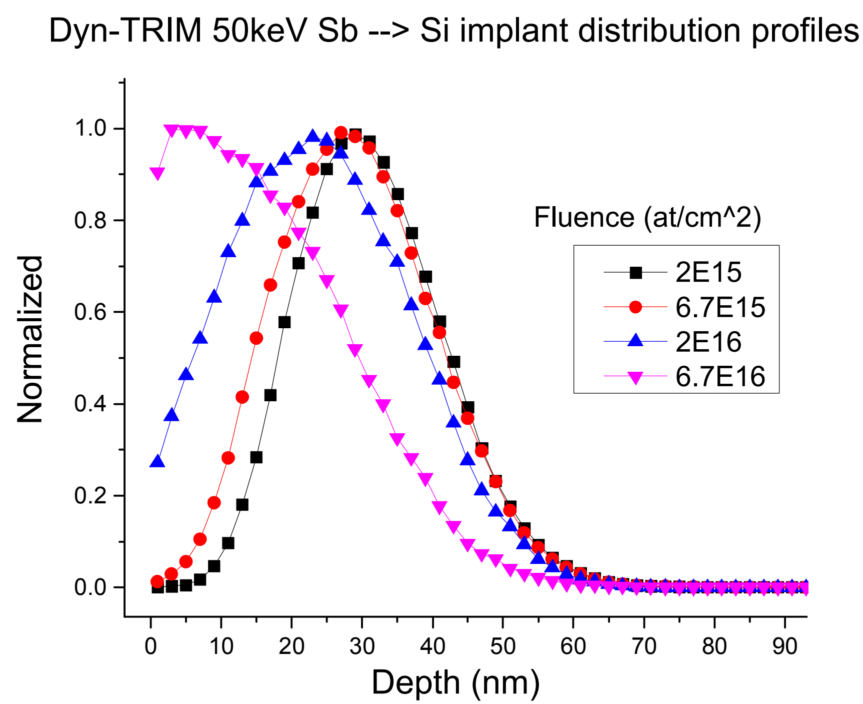
3) Rutherford Backscattering Spectrometry (RBS)
   - Non-destructive
   - Depth profiling (range and straggle)
     - Cross-check SIMS (RBS →SIMS, same sample)
   - Limited depth and mass resolution
   - Large fluence needed for measurable backscattered signal



RBS and SIMS techniques are good complements of each other

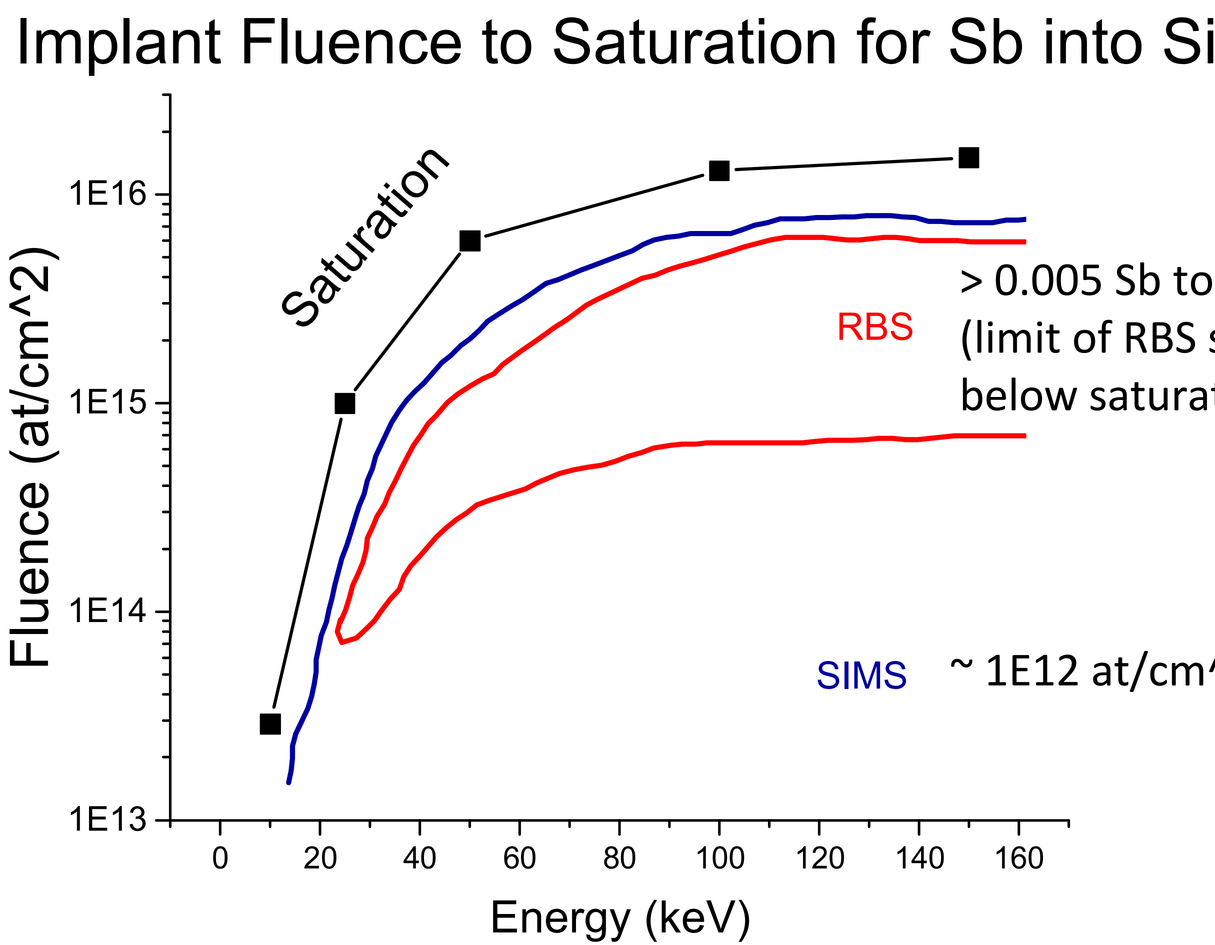
SIMS for implant saturation and Dynamic-TRIM simulation for 50keV Sb into Si





Dynamic –TRIM predicts the implant profile shift when the local antimony fraction becomes large (10% or greater)

Implant Saturation "turn on"

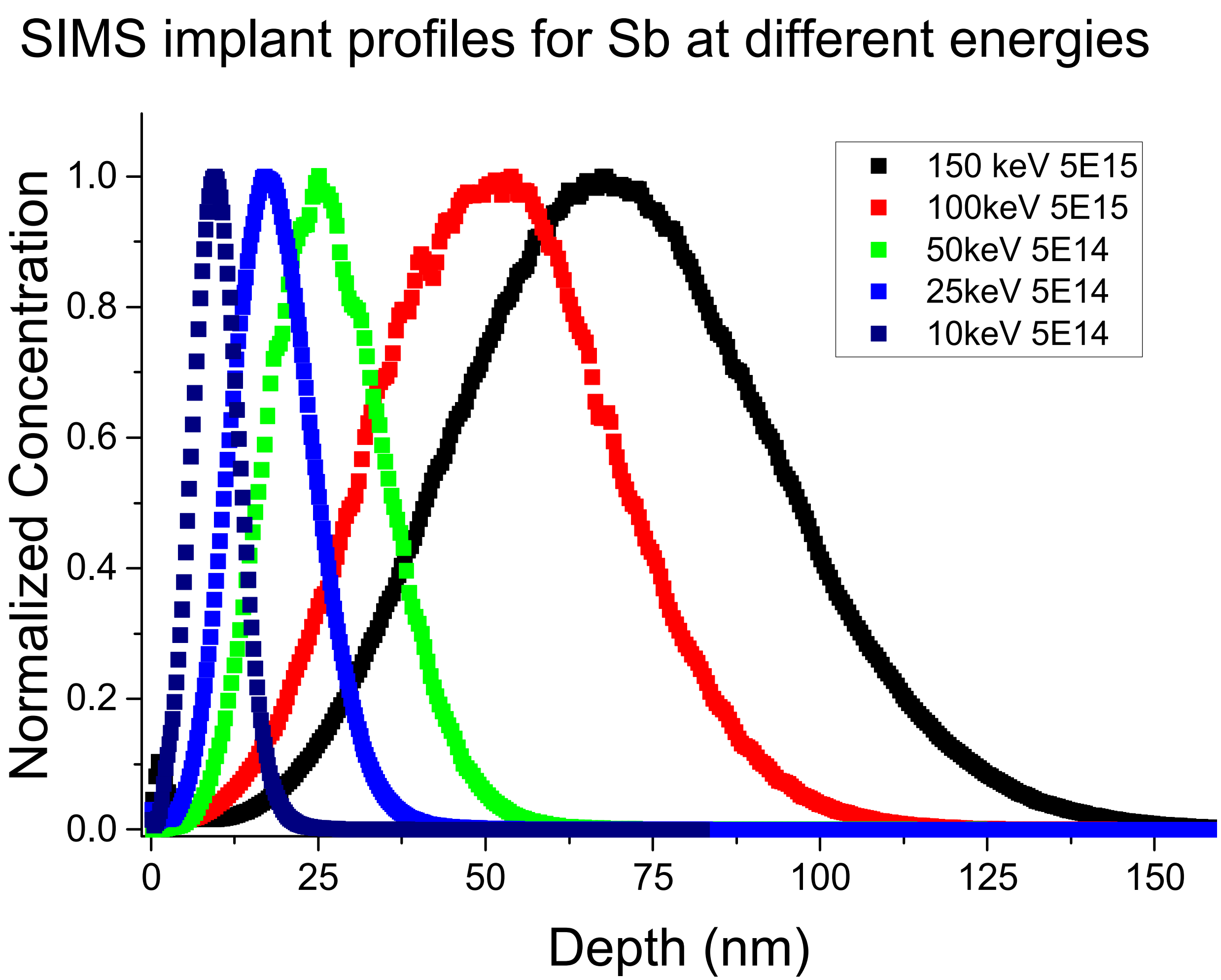


> 0.005 Sb to Si ratio at peak (limit of RBS setup) and below saturation

~ 1E12 at/cm^2 or greater

Cross-check SIMS and RBS measurements: need implant fluence below saturation but high enough to yield an RBS signal

SIMS profiles avoiding implant saturation



Notice all implant profiles tend to zero near surface

Avoiding saturation we can compare measure range to SRIM

RBS: 2MeV α's (SNL Pelletron)

Energy Calibration using Origin
Fitting Algorithms
- Gaussian fits to peaks
- Linear interpolation to edges

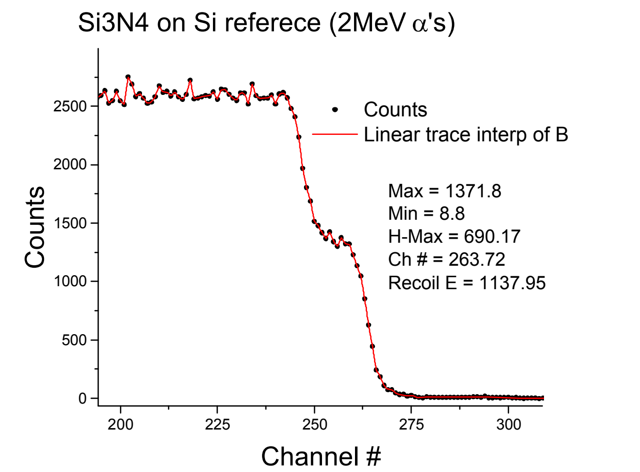
Acquired RBS spectrum for
512 and 1024 channels

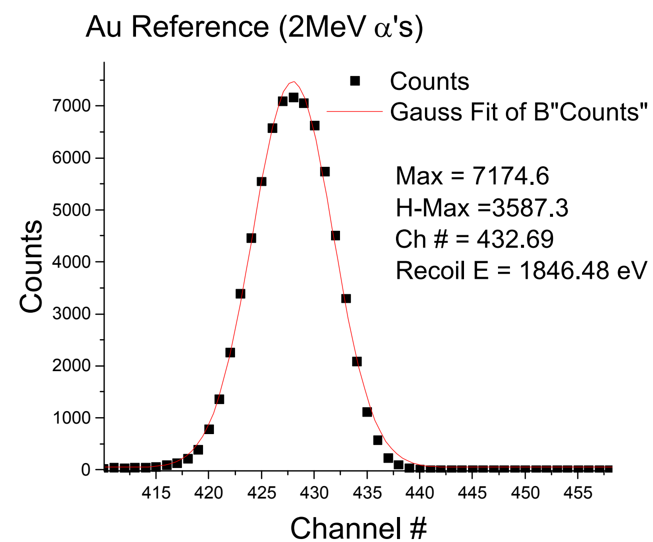
Si target with Sb implant was simulated using
Sim-Target

The best Sim-Target fit to spectrum is then analyzed
to find the range.

The RBS range shown (next slide) is for implant
fluences below saturation

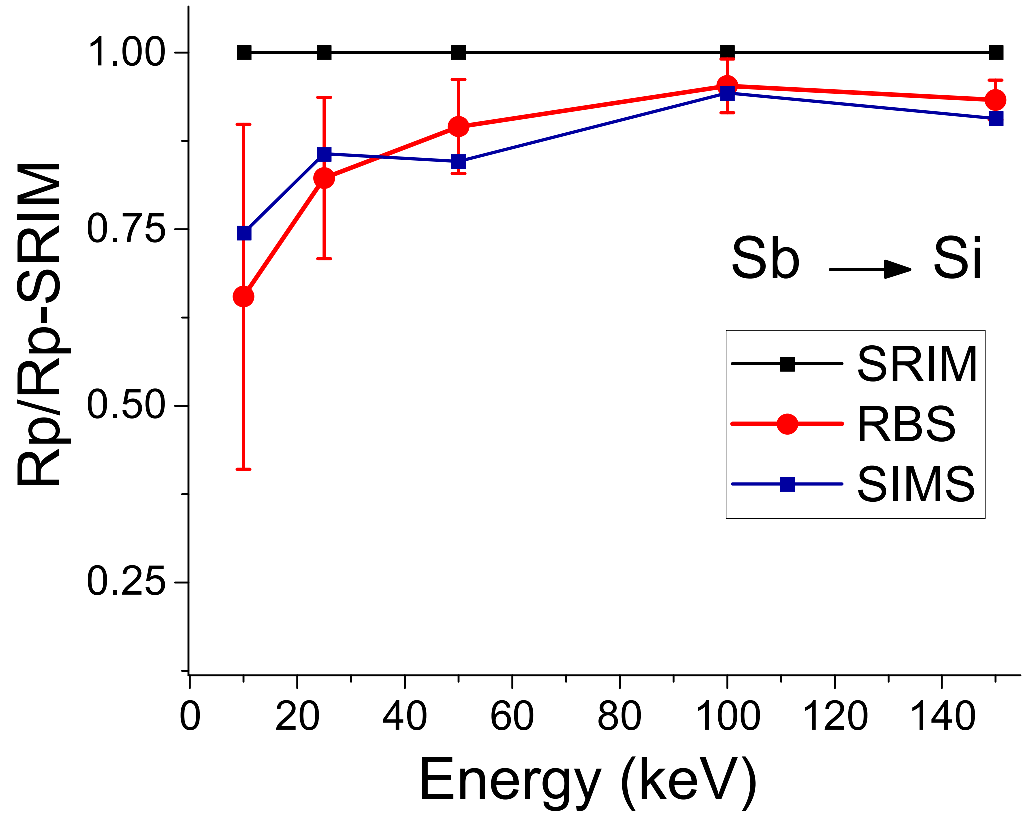
Energy Calibration





- Fitting error for Gauss fits is < 0.1 typically

Apples to apples comparison:
Avoid channeling and implant saturation



"good" agreement is found between SRIM predictions and experientially measured range values using SIMS and RBS

In conclusion

- SRIM does gives accurate predictions for the projected range of Sb implantation into Si if:
  - Channeling is avoided
  - Implant dose is lower than implant saturation "turn on"

- SRIM simulations show a general trend where the predicted range is larger what we measured
  - the experimental error has a magnitude similar to the difference observed.

- Other studies suggest SRIM range predictions should be shallower than the actual ion range.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Extra slides

Outline

Slide 1 – Title and author list
Slide 2 – Outline
- Single Atom positioning with nm resolution
- Is SRIM a good predictor of the range +/- straggle
- Experimental results comparing SRIM/RBS/SIMS
- Conclusions

Slide 3 – Single Atom Devices (EIPBN intro)
- Si qubits (Kane)
- Diamond nanophotonics (reference Alp Science 2016)

Slide 4 - Shallow Sb donors in Si
- Pathway to donor-donor coupling
- Defines what energies and depth we are interested in (reference Singh APL 2016)

Slide 5 - Graphical picture of Range +/- Straggle
- Two issues
    - Nuclear stopping – figure from slide 8
    - Electronic stopping – figure from slide 7
- Take-home → How good is SRIM

Slide 6 – Design of experiments (outline of the rest of the talk)
- Predict range with SRIM
- Implant Sb
- Measure with
    - RBS
    - SIMS

Slide 7 – Range with SRIM
- 50 keV Sb into Si, what is the issue → implant saturation
- Compare Dyn-TRIM to datasets – range vs. implant fluence and compare

Slide 8 – Implant with Sb
- Balance saturation turn on with high enough fluence to measure
- Saturation curve

Slide 9 – RBS
- Intro RBS and show what we can get from it
- RBS limitations

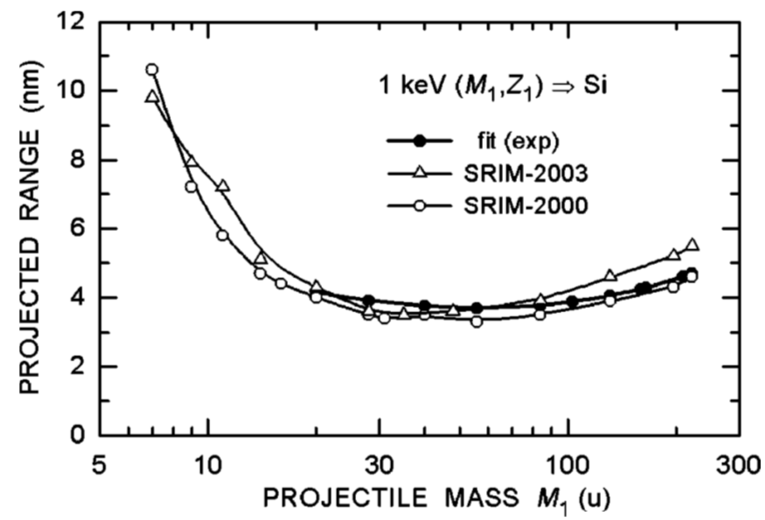
Slide 10 – SIMS
- Intro SIMS and show what we can get from it
- SIMS limitations

Slide 11 – Results
- Range measured over Range predicted vs. energy for Sb implantation
- Correct the figure – use the below saturation datasets

Slide 12 - Conclusions

The problem: incorrect range predictions for low energy of implantation

- Low-energy electronic stopping powers of SRIM-2003 were found to be much too low.
- Differences between detailed and quick calculation modes identified.
- Problems by nonrandom target-atom spacing
- For energies below 5keV, the projected ranges of heavy ions in light element targets increase with increasing projectile mass

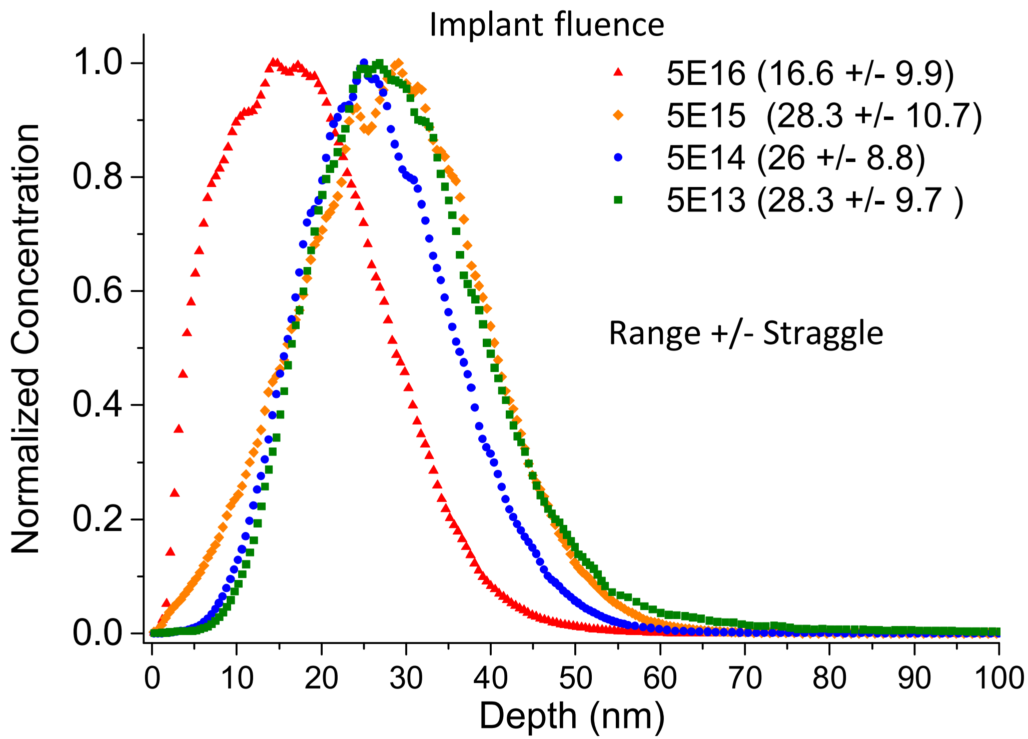


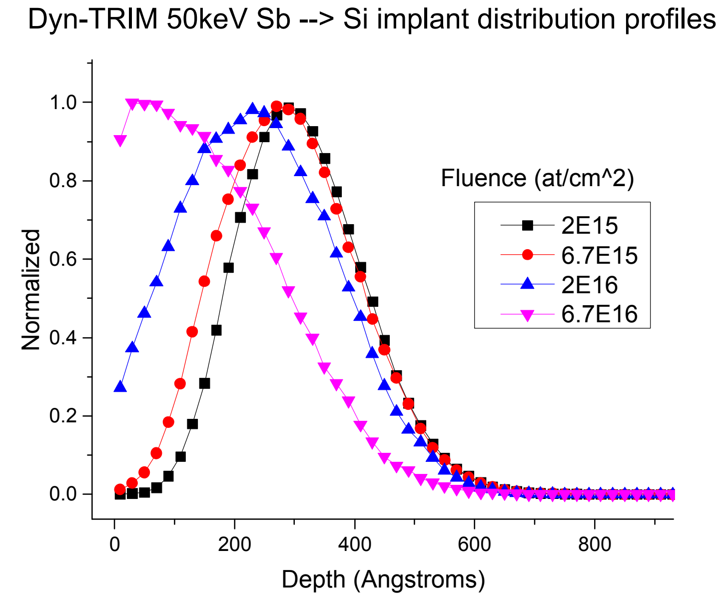
Wittmaack, Klaus. "Reliability of a popular simulation code for predicting sputtering yields of solids and ranges of low-energy ions." *Journal of applied physics* 96.5 (2004): 2632-2637.

Predicted range incorrect for low energies

SIMS* for 50keV Sb into Si: Multiple Fluences

Normalized Implant distributions of 50 keV Sb into Si



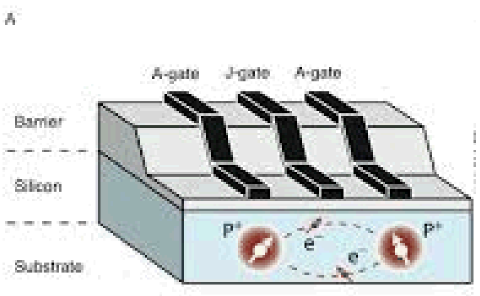


- SRIM predicts a fixed range and straggle vs energy.
- Observed a dependence on implant fluence.
- Agreement found for low implant fluences

*Secondary Ion Mass Spectrometry

The real challenge: donor-donor coupling

Surface gates mediate interaction between two donors near surface

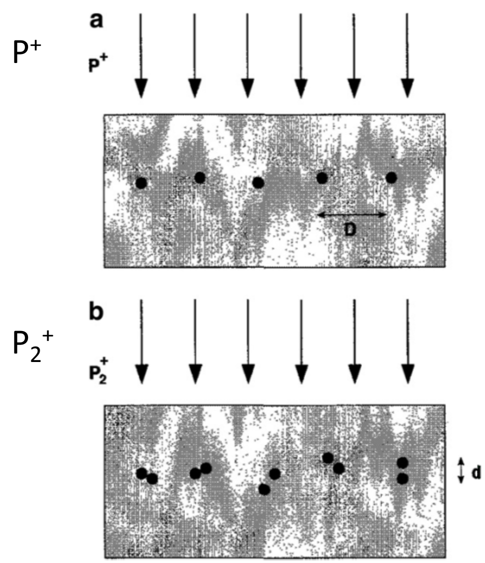


www.cqc2t.org/silicon_qubit_environ

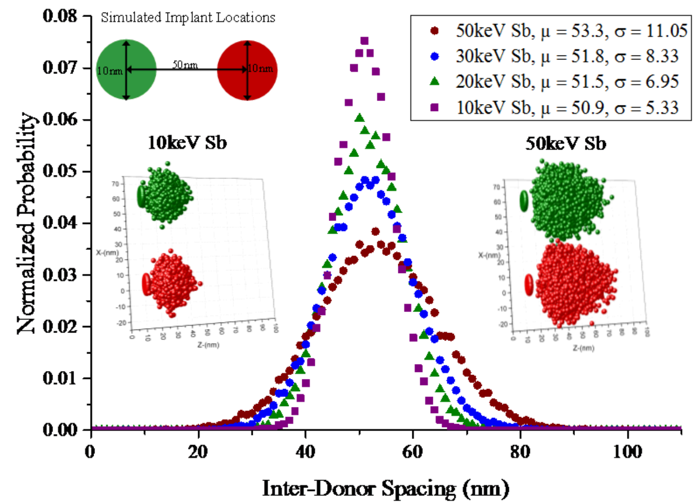
Theory: need <10nm for observable spectral splitting

Ion implantation approaches:

Phosphorus dimer implant



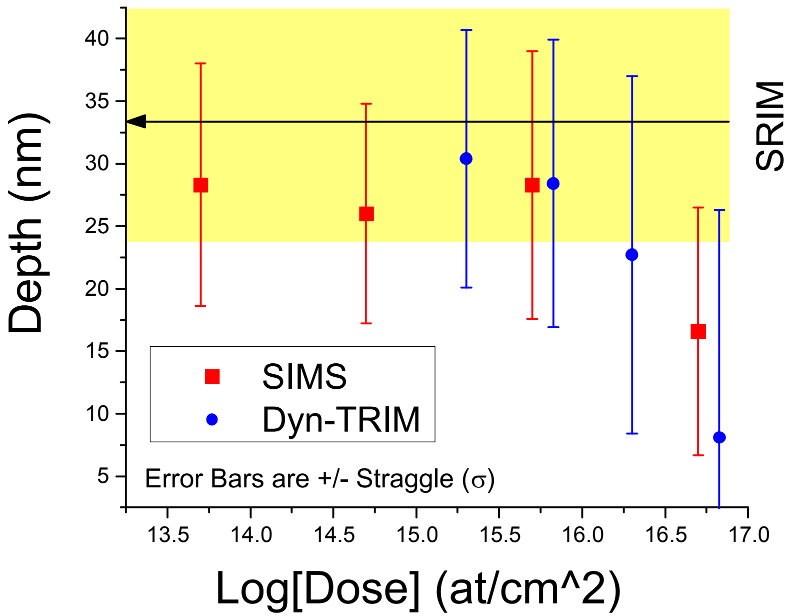
Single atom implant in adjacent sites



Low-energy heavy-ion high precision implantation may offer a road to two-qubit prototypes

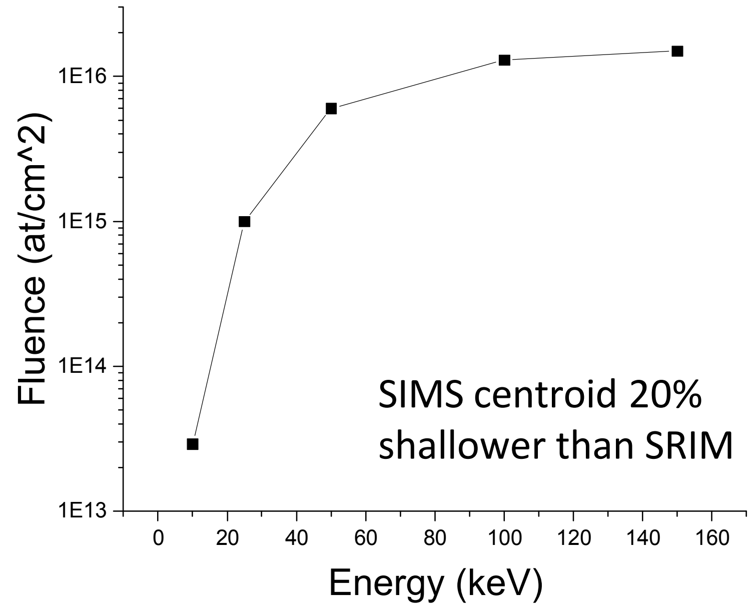
Implant Saturation turn on

Compare: SRIM, Dyn-TRIM, SIMS for 50keV Sb into Si



50keV Sb

Implant Fluence to Saturation for Sb into Si



All energies

- Dyn-TRIM tends to SRIM predictions as the fluence is lowered
- For comparison, stay below implant saturation