ATOMICALLY PRECISE MANUFACTURING FOR 2D-DESIGNED MATERIALS

DE-EE0008311

Zyvex Labs, NIST, and 3D Epitaxial Technologies

04/01/2018 – 03/31/2021

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U.S. DOE Advanced Manufacturing Office Program Review Meeting
Washington, D.C.
June 11-12, 2019

One of five coordinated 1465 FOA projects in Atomically Precise Manufacturing.

Overview

AMO MYPP Target 5.4.3:

- "Develop a sustained program to design and construct nanosystems for automated, programmable, atomically precise manufacturing using positional assembly".

AMO MYPP Target 16.5:

- "Develop and demonstrate a one square micron (1 μm²) atomically precise circuit."

Project Team and Roles:

- **Zyvex Labs** leads development of automated, atomically-precise lithography. They will create single dopant arrays and increase the yield of dopant incorporation.
- **NIST** leads on whole device fabrication, device modelling. They will develop diborane as a B dopant precursors.
- **3DET** will provide device contacting and measurement for Zyvex devices and develop an alane source as an Al dopant precursor.

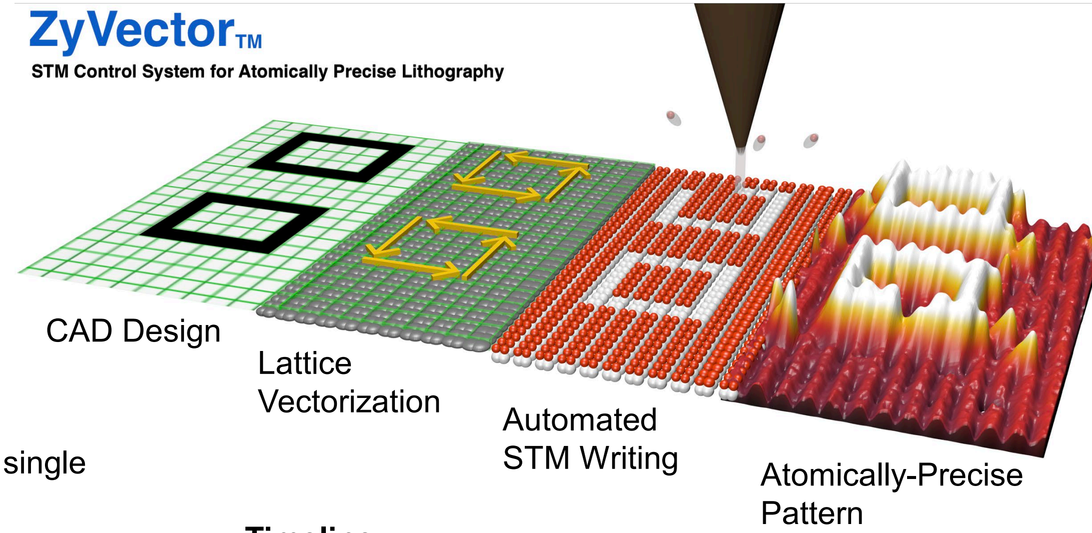
Other related projects

- Working closely with UT Dallas under **DE-EE0008322** and SBIR Phase 2, and ORNL under BES SBIR Phase 1

Barriers and Challenges:

- Atomic-Precision (± 0.4nm) placement of single dopants.
- Avoiding migration of dopants during burial.
- Precursor chemistry for non-P dopants.

Atomically-Precise Manufacturing for 2D-Designed Materials



Timeline:

Project Start Date: 04/01/2018

Project End Date: 03/31/2021

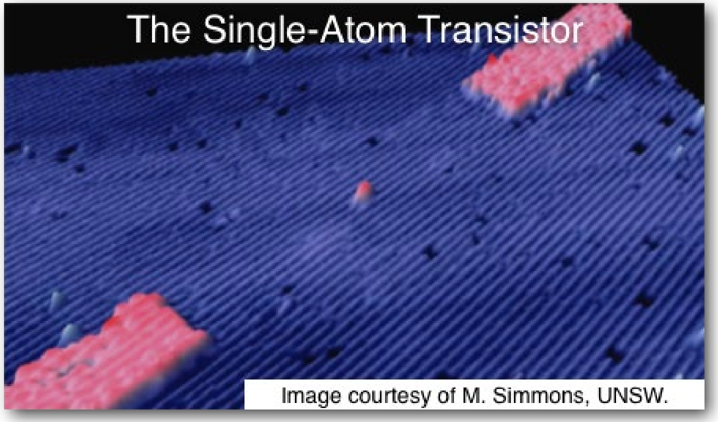
Year 1: Milestones

- All milestones on schedule as per Continuation Report.
- **BP1 Go/NoGo goal: Demonstrated device with sensitivity to single atoms: 100%**

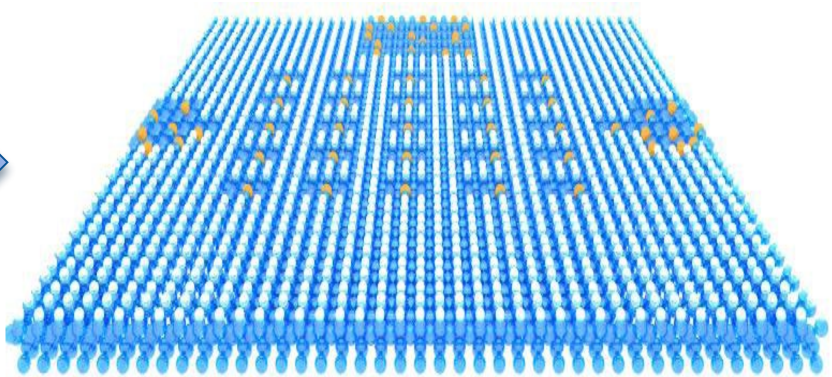
Project Budget and Costs:

Budget	DOE Share	Cost Share	Total	Cost Share %
Overall Budget	$1,521,452	$1,391,951	$2,913,403	47.8%
Approved Budget (BP-1&2)	$1,010,346	$927,255	$1,937,601	47.9%
Costs as of 3/31/19	$491,785	$501,125	$992,910	50.5%

Project Objectives



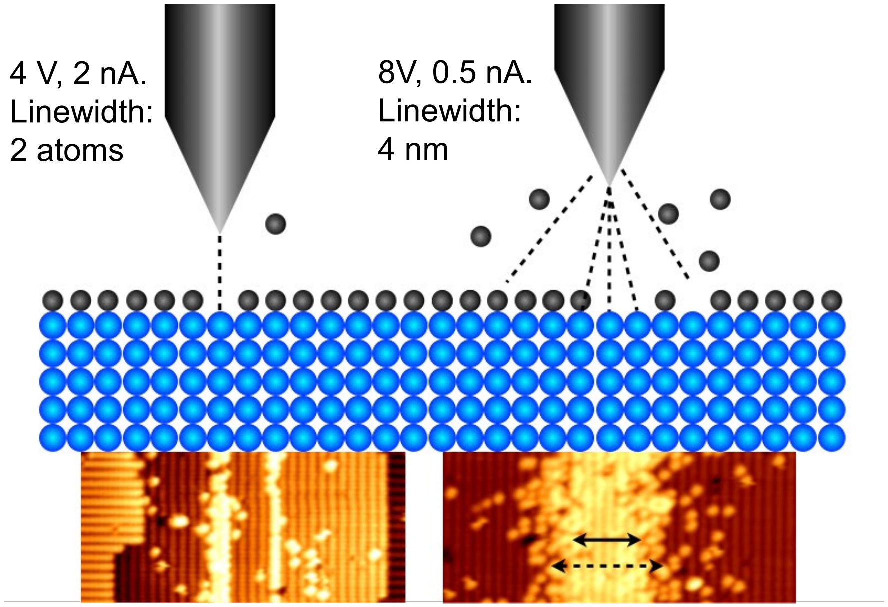
HDL State of the Art – Single Atom Transistor



Our Goal –2D Solid State Dopant Devices

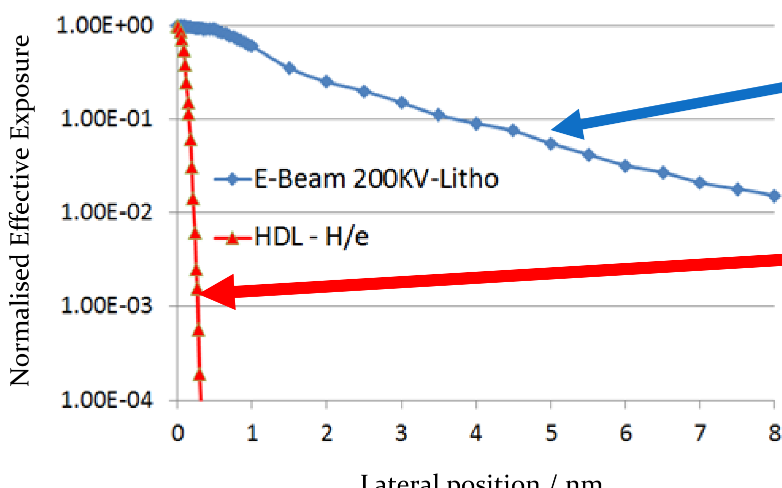
- The challenge of this project is to create uniform arrays of dopants, placed with atomic precision (± 0.4 nm), and to develop devices around these arrays. This project is part of a sustained program to develop patterning and device fabrication technologies for APM using STM-based Hydrogen Depassivation Lithography (HDL). This approach enables rapid commercialization because:
  - It enables automated, programmable tools, and thus satisfy **AMO MYPP targets 5.4 and 16.5**.
  - Early premium R&D markets – Quantum Information Technology accelerated by the National Quantum Initiative Act 2018, other applications including low-noise bipolar analog devices, atomic-scale classical computers, nanoimprint templates, NEMS – will drive costs down.
- Benefits of this technology include:
  - Continuing to scale computing devices down to the atomic scale will continue the Moore's Law trend of reducing energy consumption / computational bit.
  - Radically improved separations technologies such as 100% selective nm-pore-size membranes.
  - Reduction in embodied energy of all fabricated nanoscale devices by using technology such as nanoimprint templates which will aid manufacturing at this scale by increasing throughput.

Technical Innovation - STM Lithography



STM Lithography Modes

- In Hydrogen Depassivation Lithography, an STM tip is used to remove H atoms from a Si(001) surface creating chemical patterns.
- Two modes: Single atoms or wide lines.
- State of the Art in HDL has *atomic resolution* but very *low throughput* or precision.
- State of the Art for e-beam lithography (EBL) has much *higher throughput* but *lower resolution* (6 nm lines).
- With automated, programmable HDL patterning technology, we hope to have *atomic resolution and higher throughput* towards manufacturing scale.



Unprecedented Patterning Resolution

In **e-beam lithography**, the lateral point spread function intensity drops to about 10^{-2} at about 8 nm.

Minimum pattern size ~6 nm.

For **STM lithography**, the tunnel current drops off with lateral distance and the H yield scales by I_t^8, giving the overall depassivation yield $<10^{-8}$ @ 0.5 nm lateral position.

Minimum pattern size: 1 atom (0.4 nm)

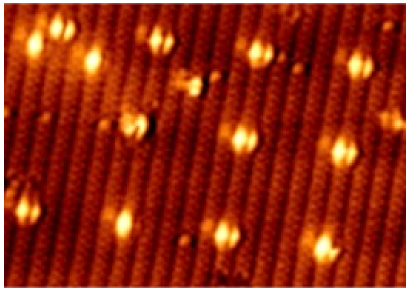
Technical Innovation

Current Practice

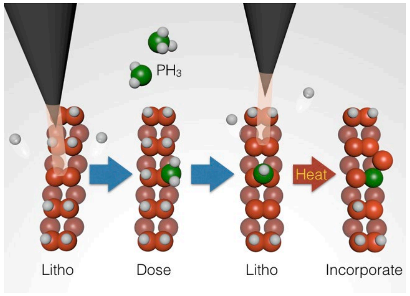
- **STM Lithography:**
  - Manual Positioning by Dead Reckoning
  - Constant dose
  - No detection of H atom removal
- **Dopant Incorporation:**
  - Ion Implantation: large position uncertainty
  - Thermal Incorporation Process: Precise but Yield 70% at most.
- **Sample processing**
  - Device found by indirect reference to optical markers
  - Al spike contact down to a 2D delta layer
- **Si Quantum Computing**
  - Niche market using dopant positioning to create quantum computers

What we are developing

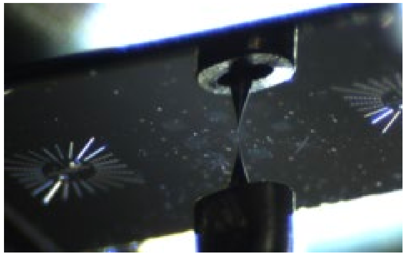
- **Automated STM Lithography**
  - Alignment to atomic lattice grid ✓
  - Creep, hysteresis, drift correction ✓
  - Improved current feedback loop ✓
  - Digital lithography with feedback



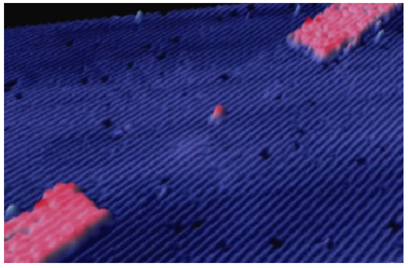
- **Improved incorporation:**
  - Low-Temperature patterning - higher precision ✓
  - Higher-yield incorporation with reduced lateral uncertainty
  - Lower thermal budget –less diffusion



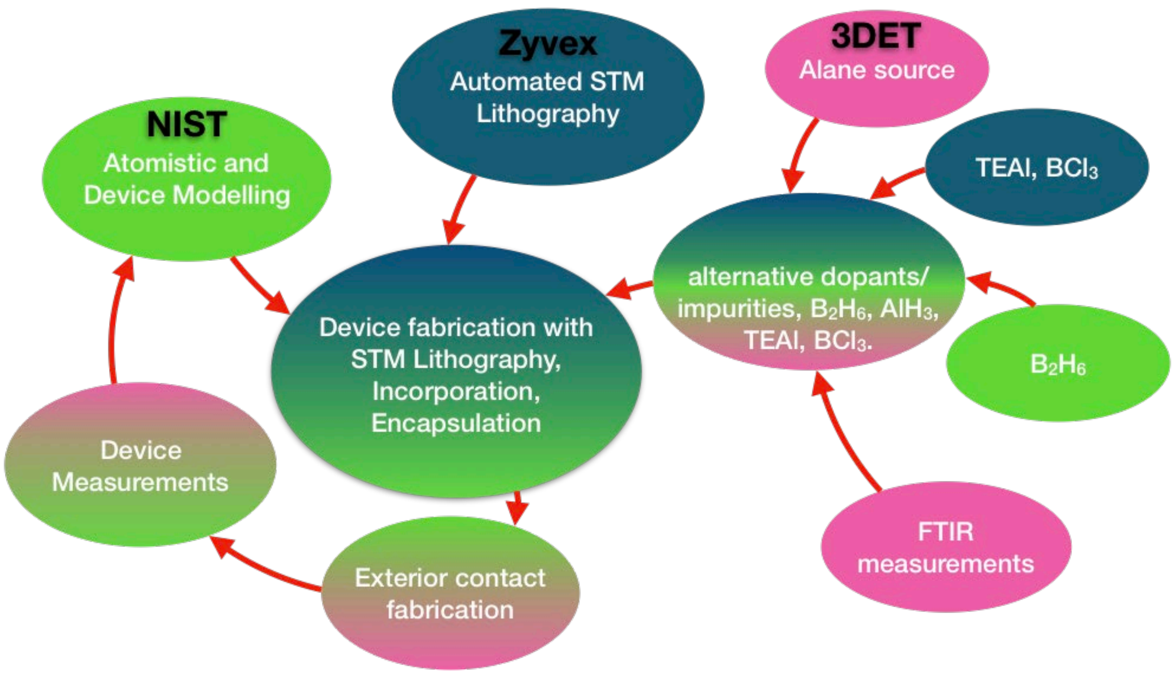
- **Improved sample processing**
  - E-beam defined alignment marks ✓
  - dI/dV STM imaging used to find buried devices directly. ✓
  - 99% yield Silicide contact process ✓



- **APM R&D markets**
  - Bipolar analog devices
  - Quantum Simulators
  - Nanoimprint templates
  - NEMS



Technical Approach



- Zyvex Labs:
  - Automated STM lithography.
  - New dopant incorporation processes.
- NIST "single atom devices" program:
  - Making quantum devices
  - Making external contacts
  - Measuring quantum devices.
  - developing models of the planned devices.
- NIST has low temp measurement systems for quantum transport in high mag fields including 3K system, 300 mK 10 T system, and 20 mK dilution fridge.
- 3D Epitaxial Technologies:
  - in-situ Al precursor dosing system
  - Making external contacts.
  - Measuring devices

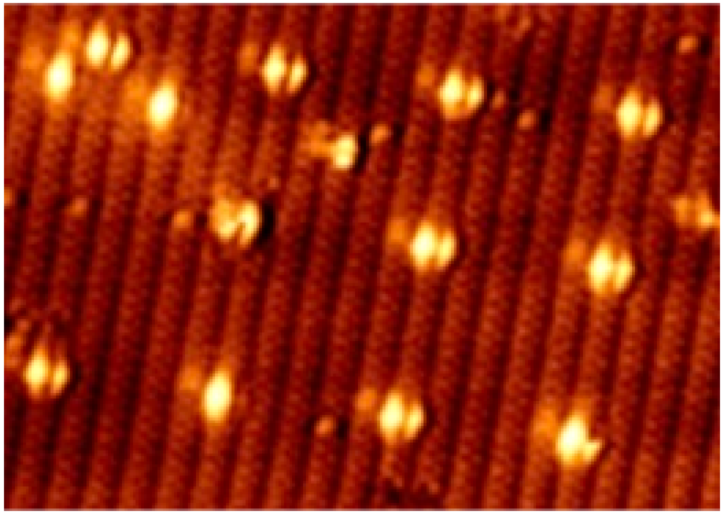
Project Risks

- **Atomic-Precision placement of single dopants continues to be challenging. ZyVector improvements are focussed on position precision at this scale.**
- Similar designer quantum materials can be made using larger patches, each containing several dopants.
- **Precursor chemistry for non-P dopants still to be developed.**
- Multiple candidates for acceptor dopants are being tested; the most promising will go forward to device fabrication in the third year.

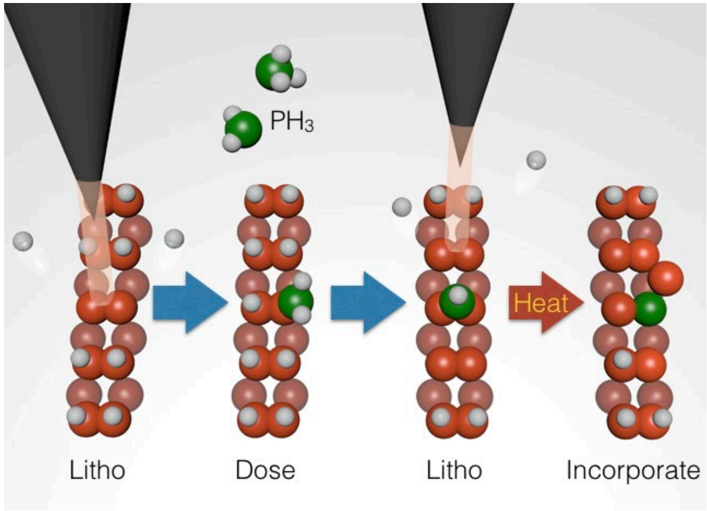
Technical Approach

Challenges for single-dopant placement

Improve pattern precision



Tip-Assisted Dopant Incorporation

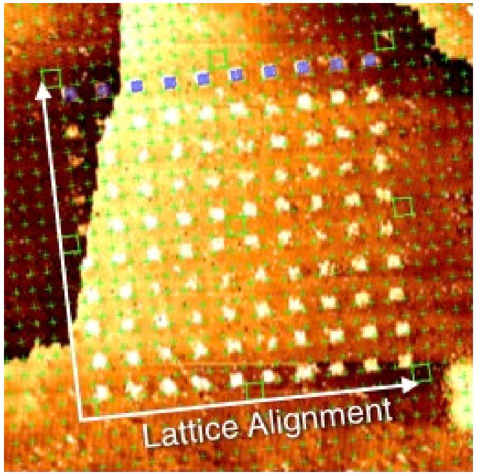


- Current dopant placement process using PH_3 has imprecision of ±1-2 atomic lattice spacings, and only 70% yield at best. For arrays of single dopants, this is inadequate.
- Tip-assisted Dopant Incorporation is one way to raise yield to 100% and reduce position imprecision to 0-1 atomic lattice spacings.
- This requires single-dimer patterns to be created.
- Non-P dopants likely to have different chemistry to PH_3, likely also to require single-dimer patterns.

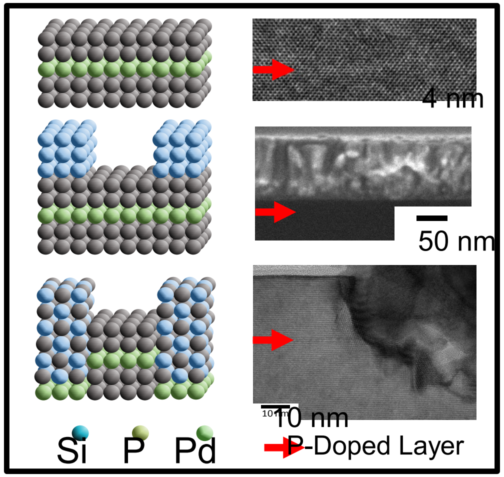
Results and Accomplishments

Year 1: Milestones (as per Continuation Report)

- Achieved BP1 Go/No-Go milestone
- Reported device fabrication process of record, including the ability to image buried structures.
- Reported transport data from many devices, such as Single-Electron Transistors (SET).
- Tightbinding models have been developed.
- Reported the selectivity of Trimethyl Al, ready to test diborane and alane precursors in BP2.
- Demonstrated automated patterning of larger dopant patch arrays, but are still working on improving the yield of arrays of single-dopant patches.

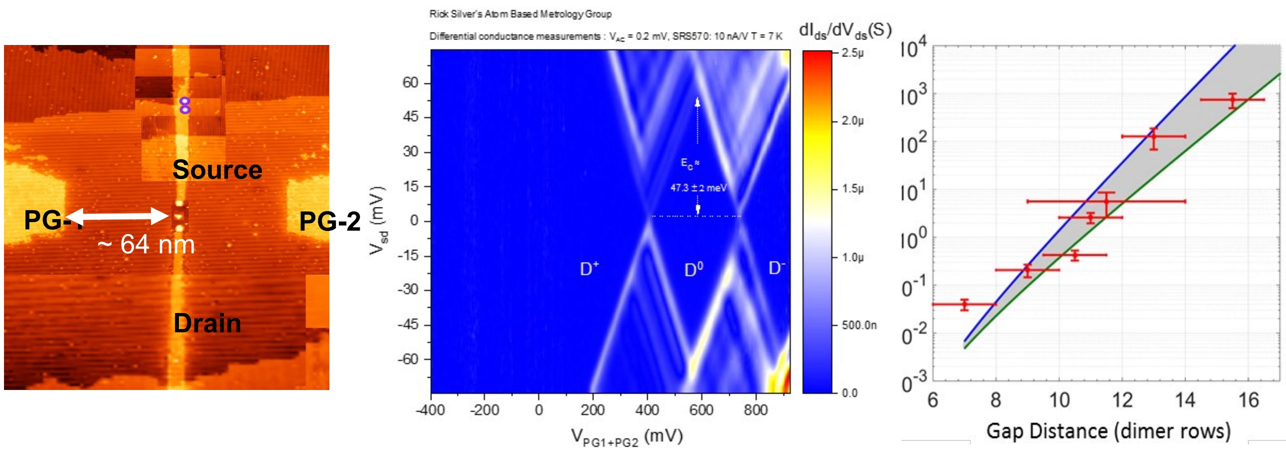


Automated Lithography of 10x10 array of 7px boxes.



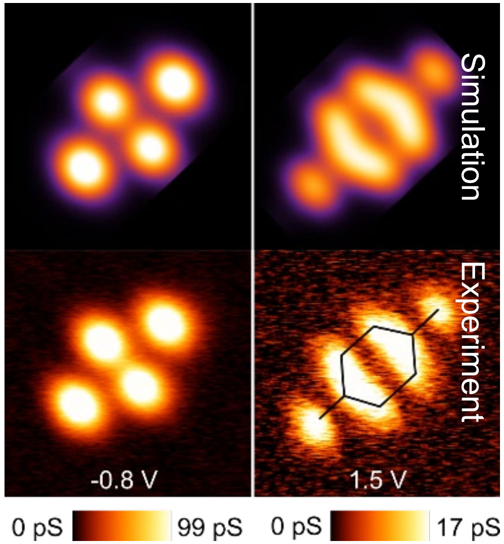
PdSi$_2$ contacts: 99.8% yield.

Go-NoGo Milestone



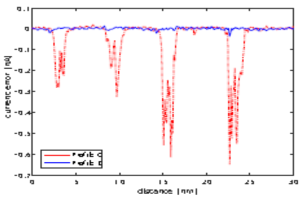
Measuring single-atom SET devices: 5-11 nm gaps, compare with WKB model

J. Wyrick *et al.*, "Atom by Atom Fabrication of Single and Few Dopant Quantum Devices", submitted to special issue on Atom by Atom Fabrication, Advanced Functional Matls., April 2019.



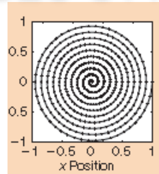
Feedback-controlled lithography

Transition (beyond DOE assistance)

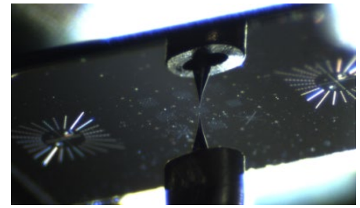


Never Crash A Tip
Better control loop
Cleaner samples
Improved vacuums

BES-STTR



Faster Imaging
Non-Raster Scanning
Better control system
AI Image recognition

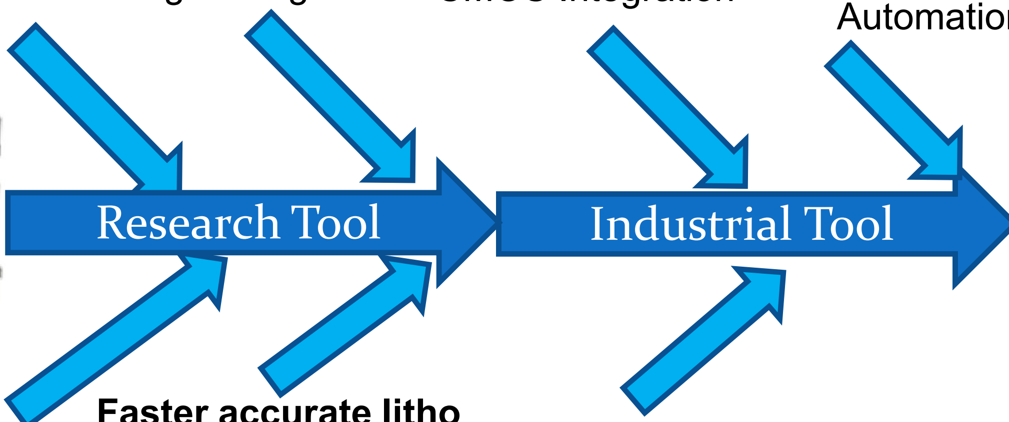


Standard Samples
Alignment marks
Pre-implanted contacts
CMOS Integration

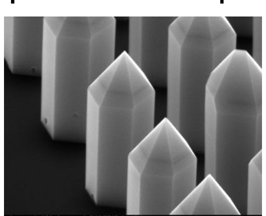
FOA-MEMS

AMO/BES-STTR

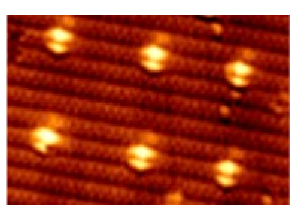
Productivity Gains
MEMS STM
Large Parallelism
Automation



Reliable Tips
Covalently Bonded
Consistent, optimized shape



Faster accurate litho
Perfect litho
Tip induced incorporation
Px-by-px litho
Error Correction



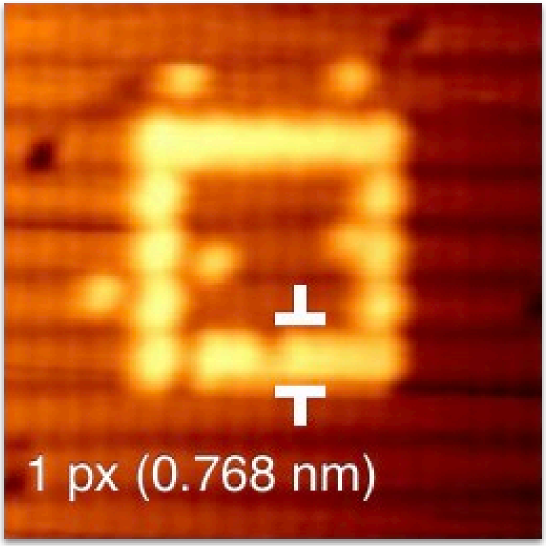
UHV System Design
Better vacuum
Integrate MEMS STM
Sample Prep, MBE,
Gas handling,

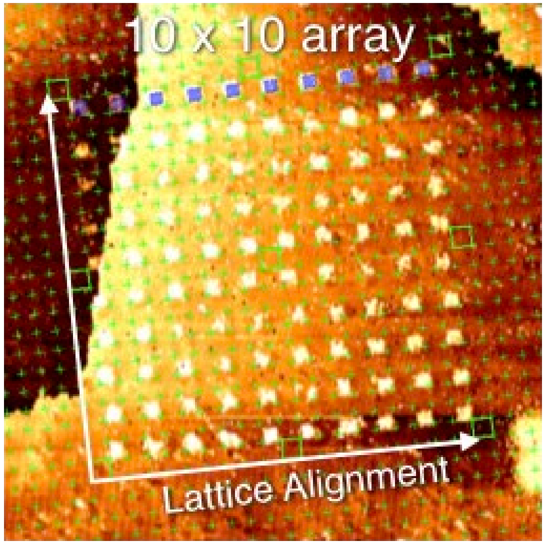
scientaomicron

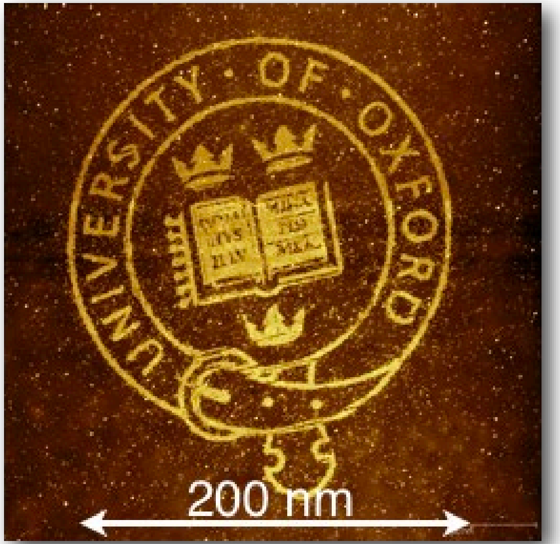
Industrial HDL Tool

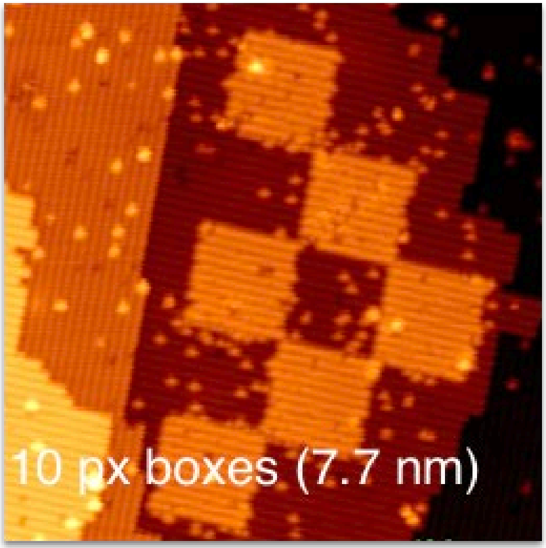
- **Totally automated processing control and sample handling**
- **Integrated sample prep, dosing, incorporation, and epitaxy**
- **XHV and control of mobile surface molecules**
- **APM Device Foundry**

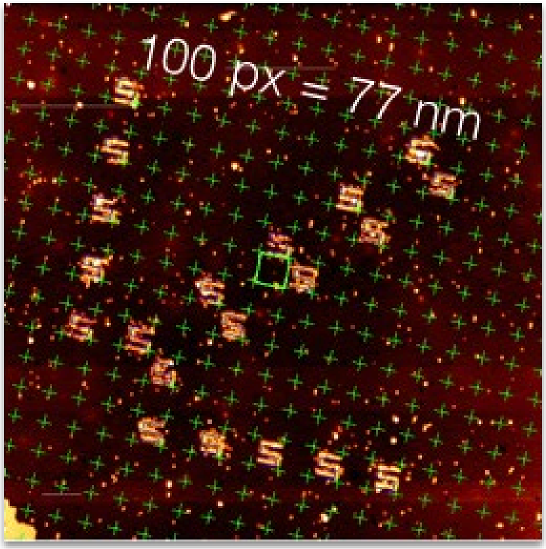
Questions?

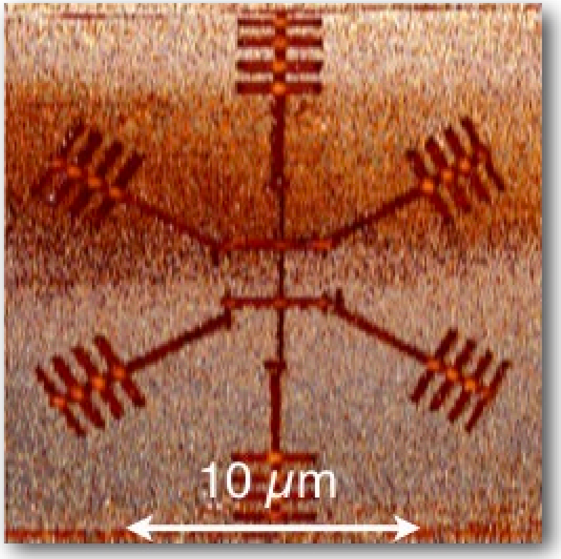

1 px (0.768 nm)


10 x 10 array
Lattice Alignment


UNIVERSITY · OF · OXFORD
200 nm


10 px boxes (7.7 nm)


100 px = 77 nm


10 μm