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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Washington, D.C.
July 17-19, 2018

Overview

Timeline

- Award issued April 2018
- Projected End date March 2021
- Project **just started**

Challenges

- High Yield Device Fabrication
- Atomic Precision Lithography
- Single dopant placement
- High-quality, low-temp epitaxy
- Increased range of dopants

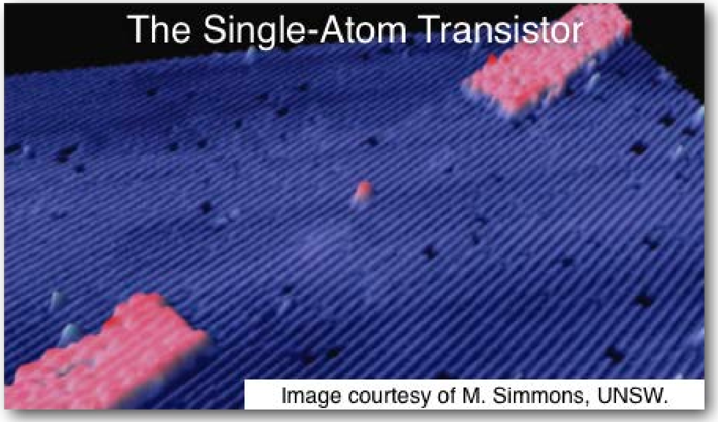
Partners

- Zyvex Labs is joined by two well established collaborators: NIST and 3D Epitaxial Technologies
- NIST will make devices in parallel with Zyvex Labs, and will measure and perform modelling of completed devices.
- 3D Epitaxial Technologies will assist with process development particularly in increasing the range of dopants that can be used.

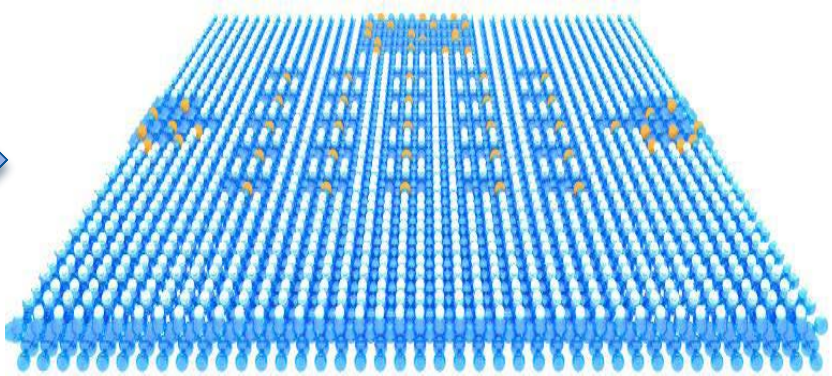
Budget

	FY 18 Costs	FY 19 Costs	FY 20 Costs	Total Planned Funding (FY 18-FY 20)
DOE Funded	802K	832K	823K	$2,457K
Project Cost Share	463K	464K	465K	$1,392K

Project Objectives



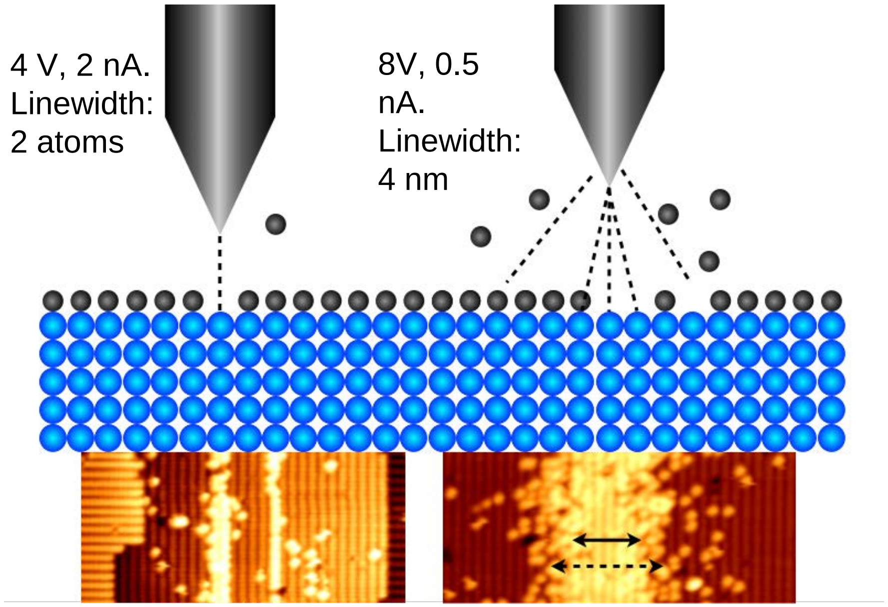
State of the Art



Our Goal

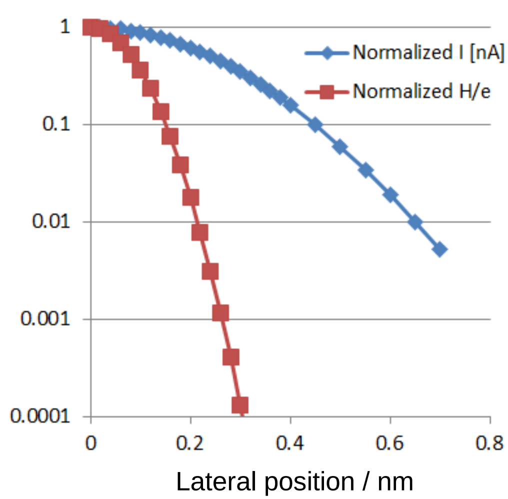
- We will fabricate atomic-scale devices by atomically precise placement of a variety of dopant atoms in a single buried (100) plane of Si. We will develop tools to do this in an automated, programmable way, as cited explicitly in AMO MYPP Target 5.4.
- The difficulties lie in the unprecedented manufacturing precision required (~ 0.1 nm) to place single atoms, and the selective chemistry required for each dopant.
- This project can lead immediately to a dramatic new understanding and exploitation of designer materials, “2D quantum metamaterials”.
- Our program is aligned with AMO’s mission of creating “*foundational energy-related advanced manufacturing technologies*”. The tools developed will enable Atomically Precise Manufacturing, **which does not currently exist.** If successful, our program will have enormous long term impact on energy use and manufacturing efficiency.

Technical Innovation - STM Lithography



STM Lithography Modes

- An STM tip can be used to remove H atoms from a Si(001) surface. Single atoms or wide lines.
- PH_3 adsorbs selectively into these patterns.
- The P can then be buried in epitaxial Si making a 2D device.
- State of the Art is the Single-Atom Transistor, from UNSW.
- Our goal is to create arrays of single dopants, including dopants other than P (B, Al etc.).
- We will increase the yield of dopant incorporation with reduced position error.



Unprecedented Patterning Resolution

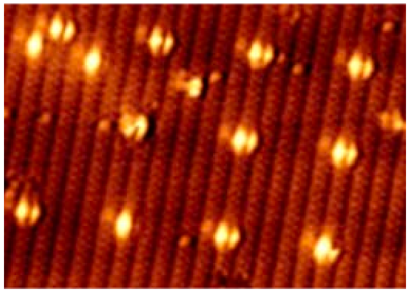
In e-beam lithography, the lateral point spread function intensity drops to about 10^{-2} at about 5 nm.

Minimum pattern size ~6 nm.

For STM lithography, the tunnel current drops off with lateral distance (blue). The H yield scales by $I_t^{\,8}$, giving the overall depassivation yield (red) reduced to <10^{-8} @ 0.5 nm lateral position.

Minimum pattern size: 1 atom (0.4 nm)

Technical Innovation

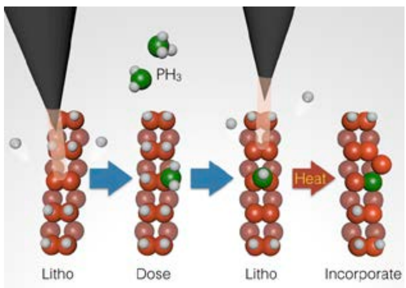


What we do now

- **STM Lithography:**
  - Manual Positioning by Dead Reckoning
  - Constant dose
  - No detection of H atom removal

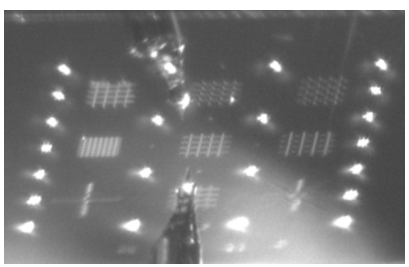
What we will develop

- **Automated STM Lithography**
  - Alignment to lattice
  - Creep and hysteresis correction
  - Improved current feedback loop
  - Digital lithography



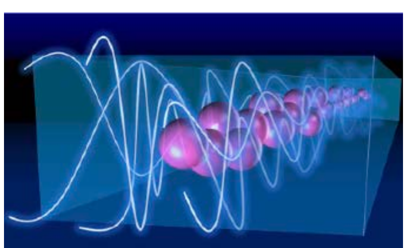
- **Dopant Incorporation:**
  - Ion Implantation: large position uncertainty
  - Thermal Incorporation Process: Precise but Yield 70% at most.

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



- **Sample processing**
  - Al spikes down to a 2D delta layer
  - Device found by reference to optical markers

- **Improved sample processing**
  - E-beam defined alignment marks
  - Kelvin Probe Microscopy used to find buried devices.
  - Low-temp. patterning - improved vacuum, reduced contamination



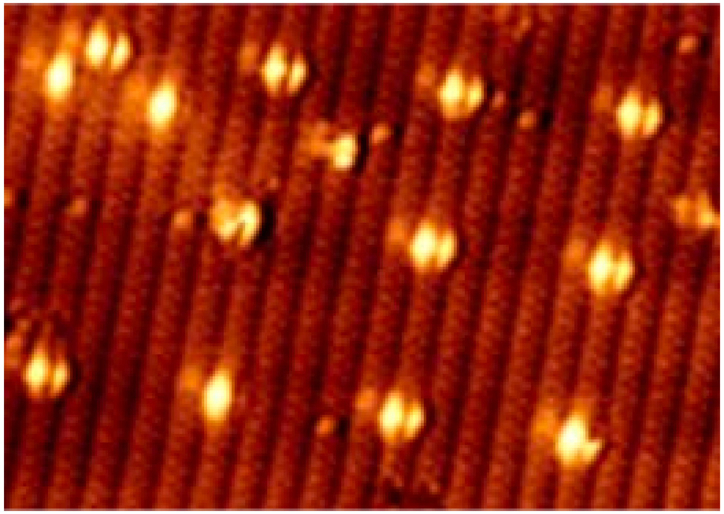
- **1D Quantum Metamaterials**
  - Correlated electron effects found in 1D chain made by ion implantation
  - Only P can be placed by STM

- **2D Quantum Metamaterials**
  - AP fabrication allows for designed quantum properties
  - Wider range of dopants that can be placed with Atomic precision

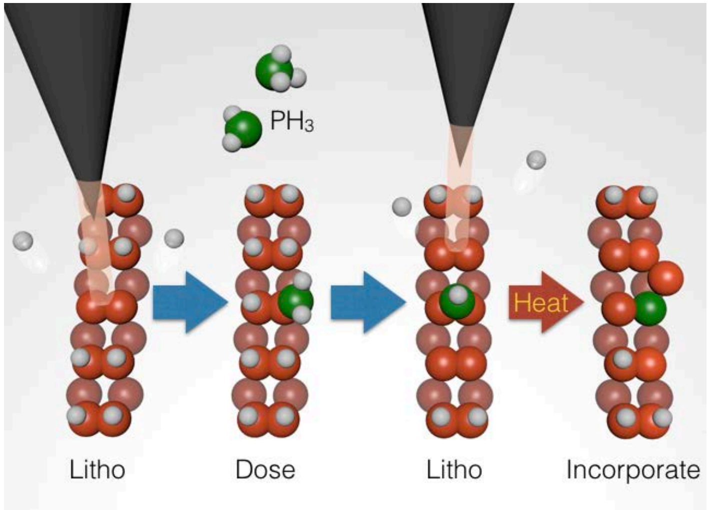
Technical Approach

4 Steps for fabrication of 2D Quantum MetaMaterials

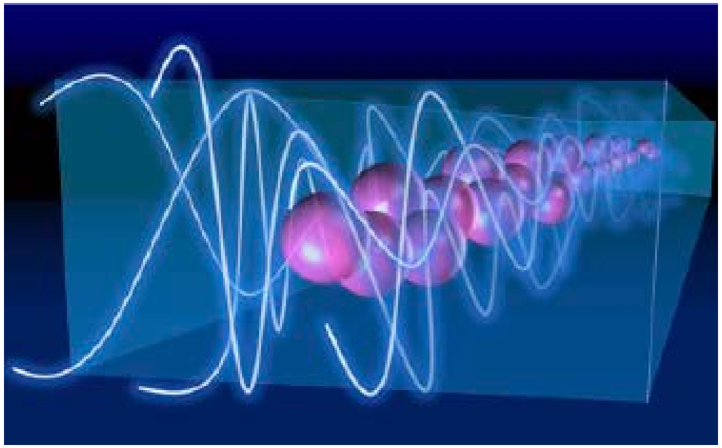
Improve STM Lithography



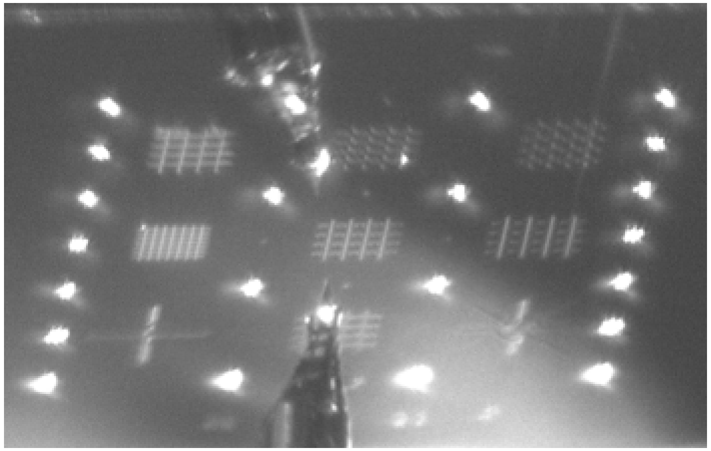
High-Yield Dopant Incorporation



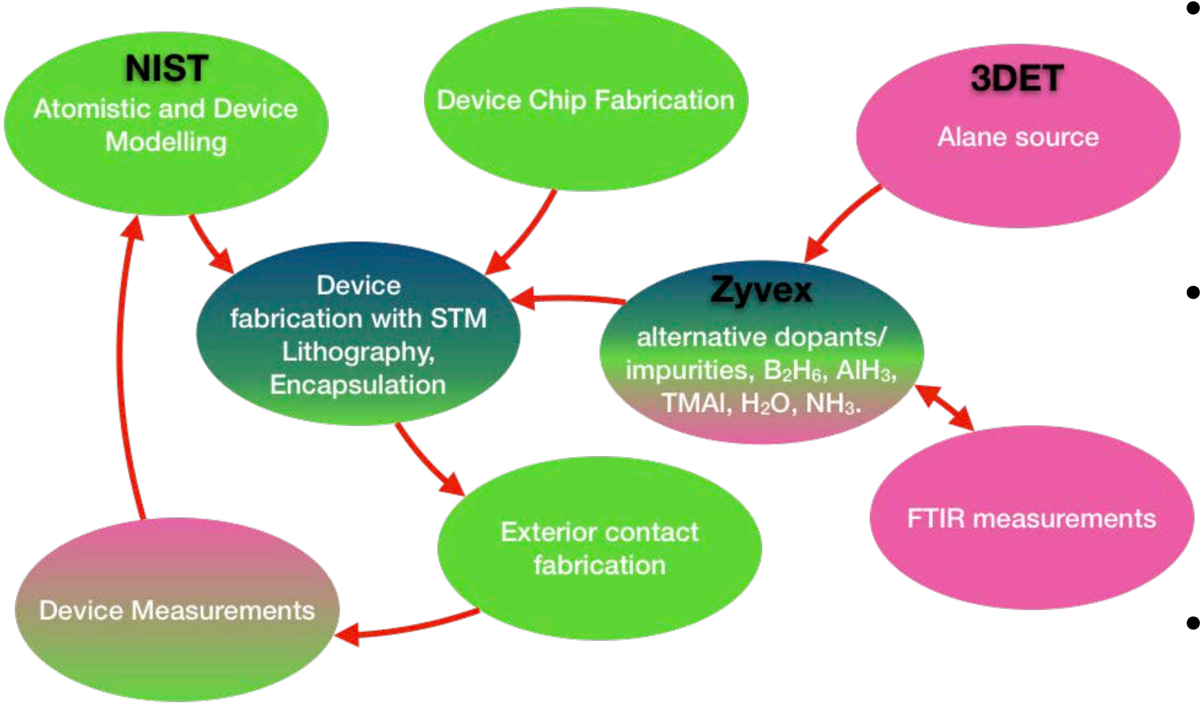
Designed Quantum Metamaterials



High-Yield Device Fabrication



Technical Approach



Project Risks

- The single-dopant placement process has not been proven. Consistent lithography on this scale will be difficult.
- Similar designer quantum materials can be made using larger patches, each containing several dopants, as proposed by Sandia National Lab.
- Selective chemistry has only been demonstrated for P thus far. Each dopant precursor must be tested.
- Multiple candidates for acceptor dopants will be tested, and the most promising will go forward to device fabrication in the third year.

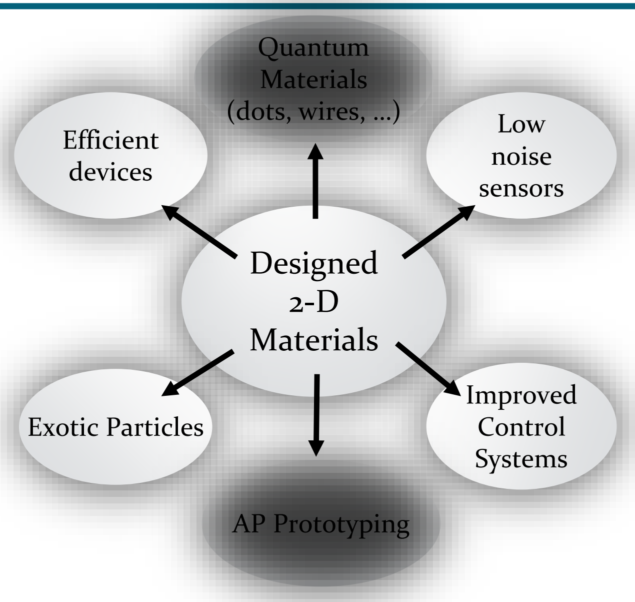
- Zyvex Labs leads the world in the development of STM lithography, in particular its ZyVector automated STM lithography tool. It will lead in exploring new dopant incorporation processes.
- The NIST “single atom devices” program has significant expertise in creating atomic scale devices, and external contacts to them. They will make devices in parallel with Zyvex Labs, and will measure devices.
- NIST will model planned devices, to compare with and guide the experimental results
- 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 is developing an in-situ Al precursor dosing system and will assist with increasing the range of dopants.

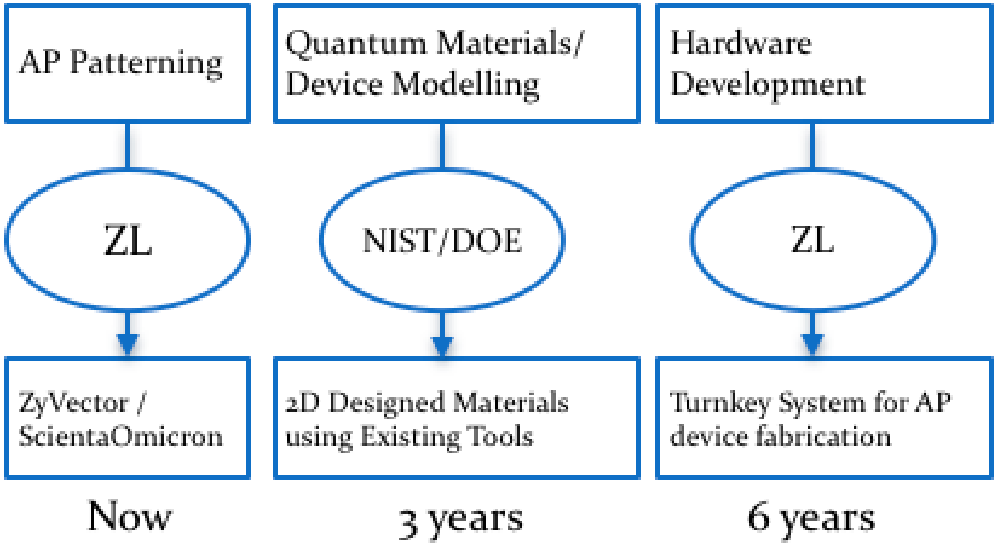
Results and Accomplishments

New Project:

Task/Subtask	Year 1 (BPA) 1	2	3	4	Year 2 (BPB) 5	6	7	8	Year 3 (BPC) 9	10	11	12
Task 1: Tool Development												
1.1: Improve AP Yield			1.1a				1.1b					
1.2: Dopant Incorporation Site Examination				1.2a						1.2b		
Task 2: Exemplary Device Development												
2.1: Process Development	2.1a			2.1b								
2.2: Device Measurement Statistics				2.2a								
2.3: Measurement of Device with Impurities									2.3a			2.3b
Task 3: Novel Selective Chemistries												
3.0 Novel Selective Chemistries				3.0a				3.0b				3.0c
3.1 Water		3.1a		3.1b								
3.2 Ammonia		3.2a		3.2b								
3.3 Diborane				3.3a		3.3b		3.3c				
3.4 Alane				3.4a		3.4b		3.4c				
3.5 TMAl				3.5a		3.5b		3.5c				
3.6 Survey other materials								3.6a				
Task 4: Materials Processing for Device Development												
4.1 Determine Positions for Species in Device								4.1a				
4.2 Minimize Contamination by Ligands								4.2a				
4.3 Determine Impact of Contamination on Devices												4.3a
Task 5: Theory and Simulation												
5.1: Develop Tightbinding Parameters				5.1a								
5.2: Develop test structure models								5.2a				
5.3: Develop designed 2D materials												5.3a
Task 6: Designed 2D Materials												
6.1: Designed 2D material with P								6.1a				
6.2: Designed 2D materials with >2 species												6.2a

Transition (beyond DOE assistance)





- By the end of this program, we expect to have be able to create 2D atomically precise structures. Eventually, we would like to create a turnkey nanofabrication tool for the research market, probably in collaboration with our current distribution partners, ScientaOmicron. We may also become a foundry for these devices.
- The proposed work uses a single STM tip, and so is a slow serial process. In the future, scaling up throughput will require a multi-tip solution, and we are pleased that the AMO is also funding work towards that requirement with our collaborators at UT Dallas.
- Designed materials will have initial impact in several areas, including atomic-scale computer circuits, high-sensitivity sensors, low-noise bipolar analog devices, and Analog Quantum Simulators.
- Over time, an 'Inverse Moore's Law' will take effect, so that the volume of material which can be made with atomic precision will increase, to encompass larger and larger objects.
- In the long term, AP designed materials created through various methods for APM, including STM lithography, have the potential to revolutionise materials science, providing materials with, for example, designed-in specific strength, toughness or wear resistance, thus enabling complex, highly reliable systems.

Questions?