



# Atomic Precision Advanced Manufacturing for Ultraprecise 2D Bipolar Devices

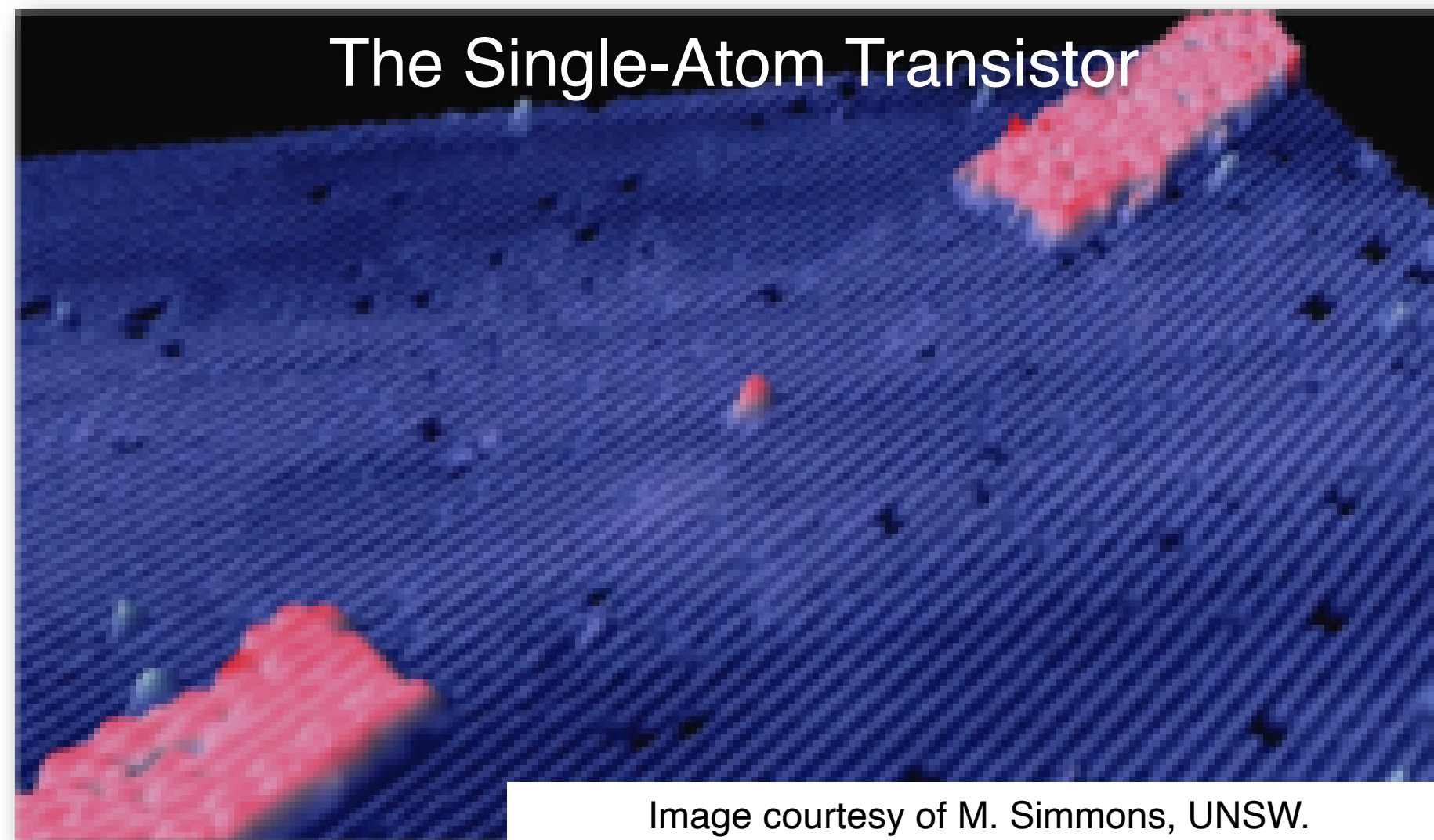
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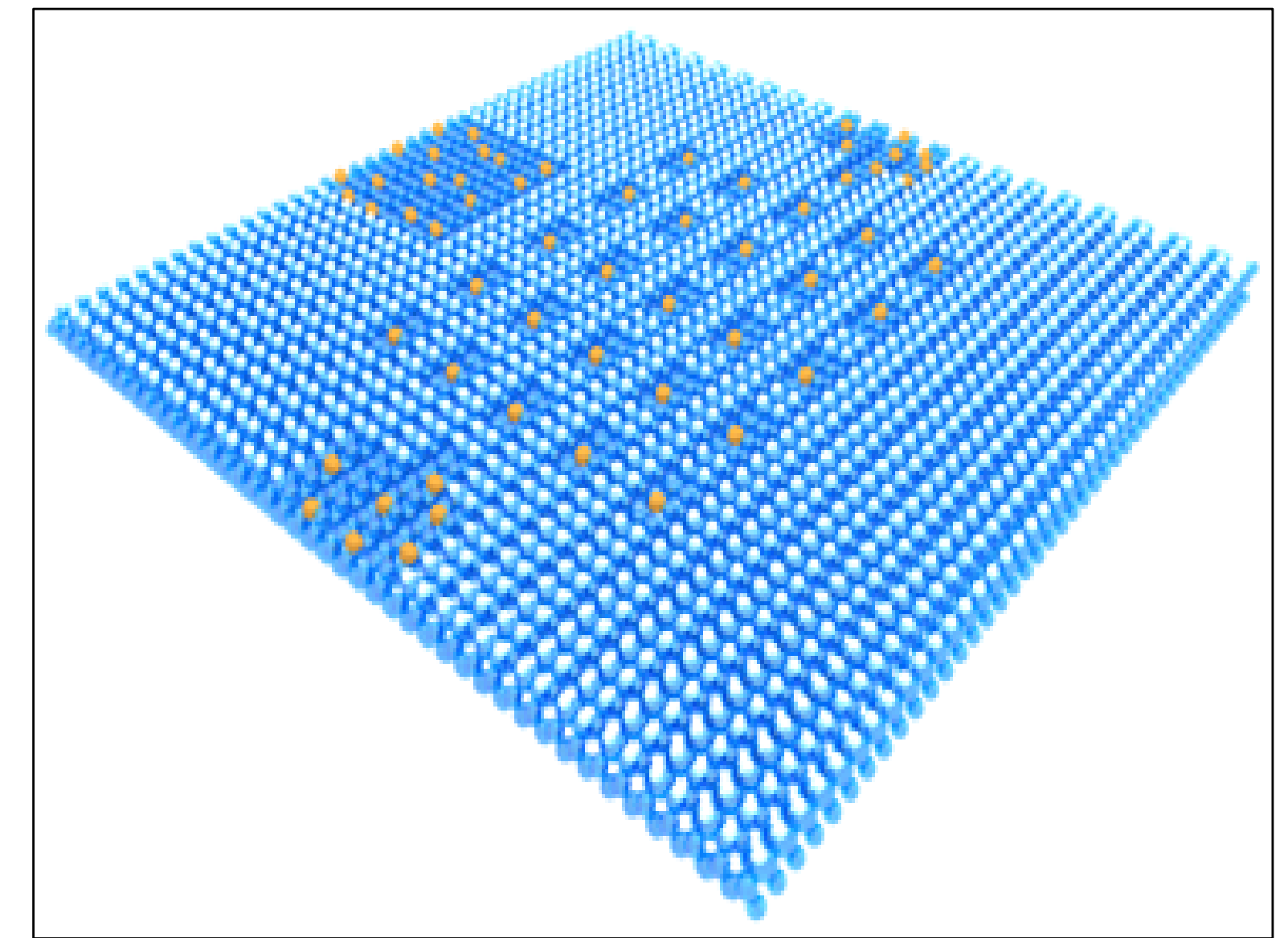
This work was supported by the Advanced Manufacturing Office of the  
DOE through projects DE-EE0008311, DE-SC0020817, DE-SC0020827.

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# Single-Dopant Placement - APAM



Fuechsle *et al.* *Nat Nano* **7** 242-246 (2012) DOI: [10.1038/nnano.2012.21](https://doi.org/10.1038/nnano.2012.21)



HDL has been used for placement of P atoms deposited from  $\text{PH}_3$ , to make P-based spin or charge qubit devices - **quantum computers**.

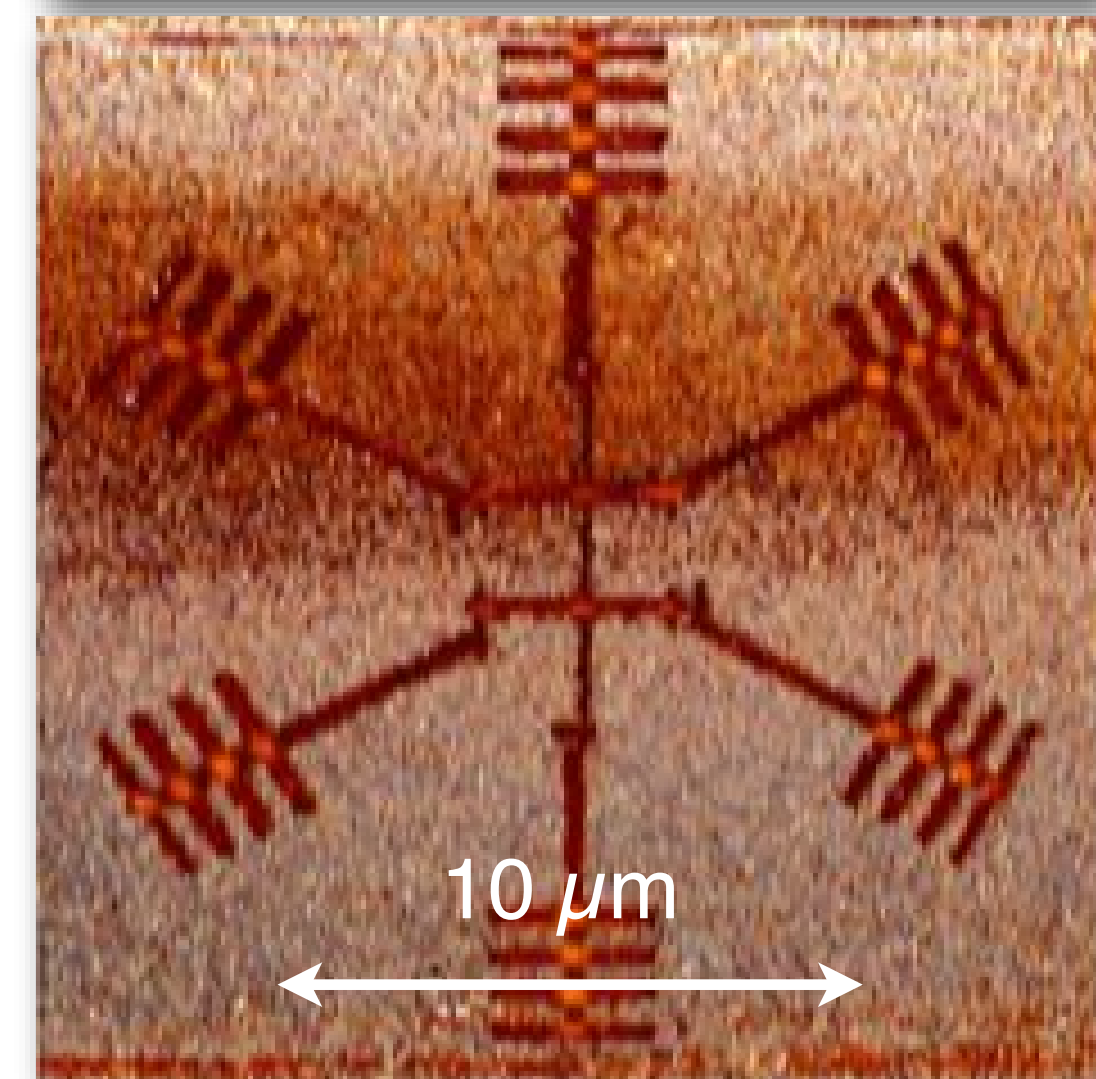
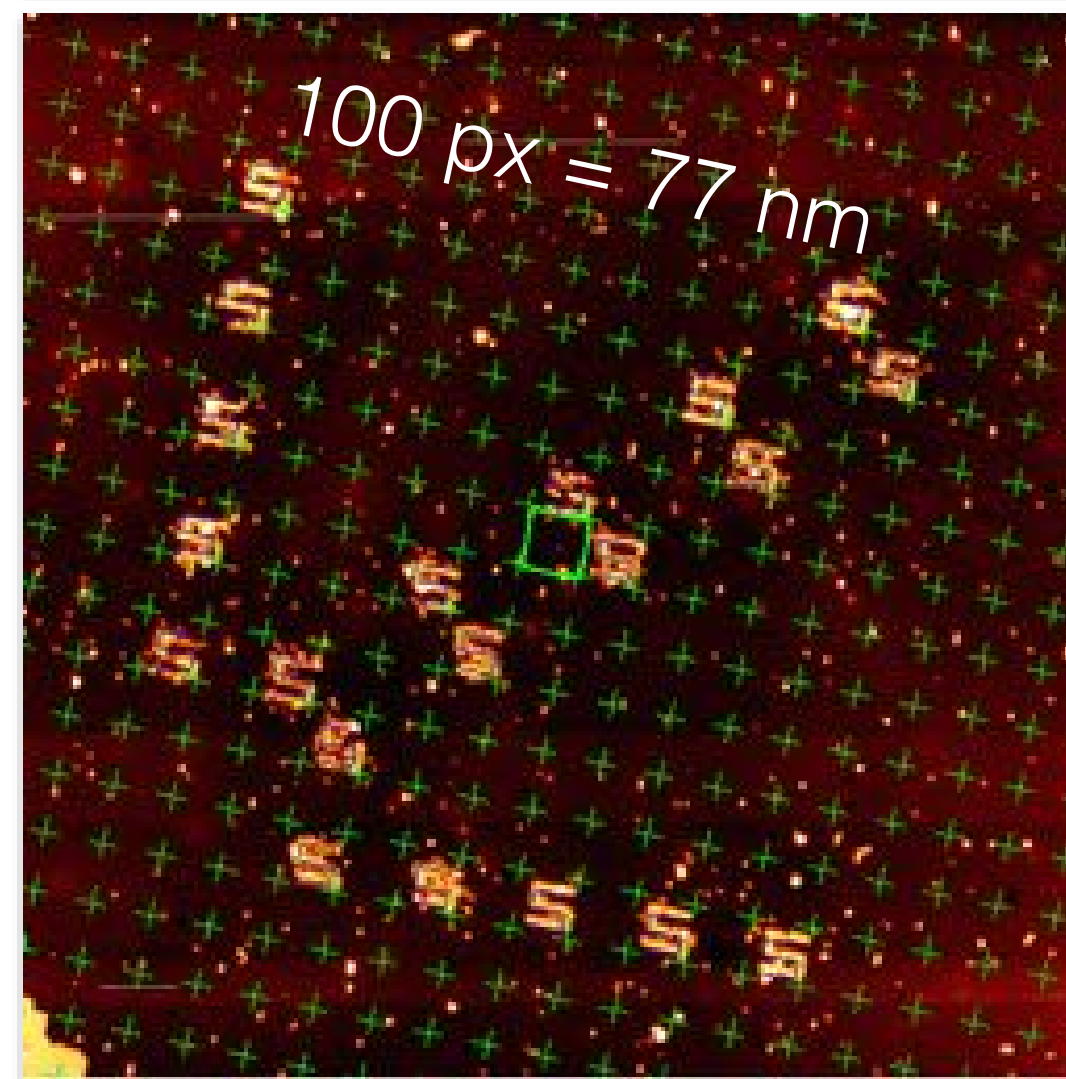
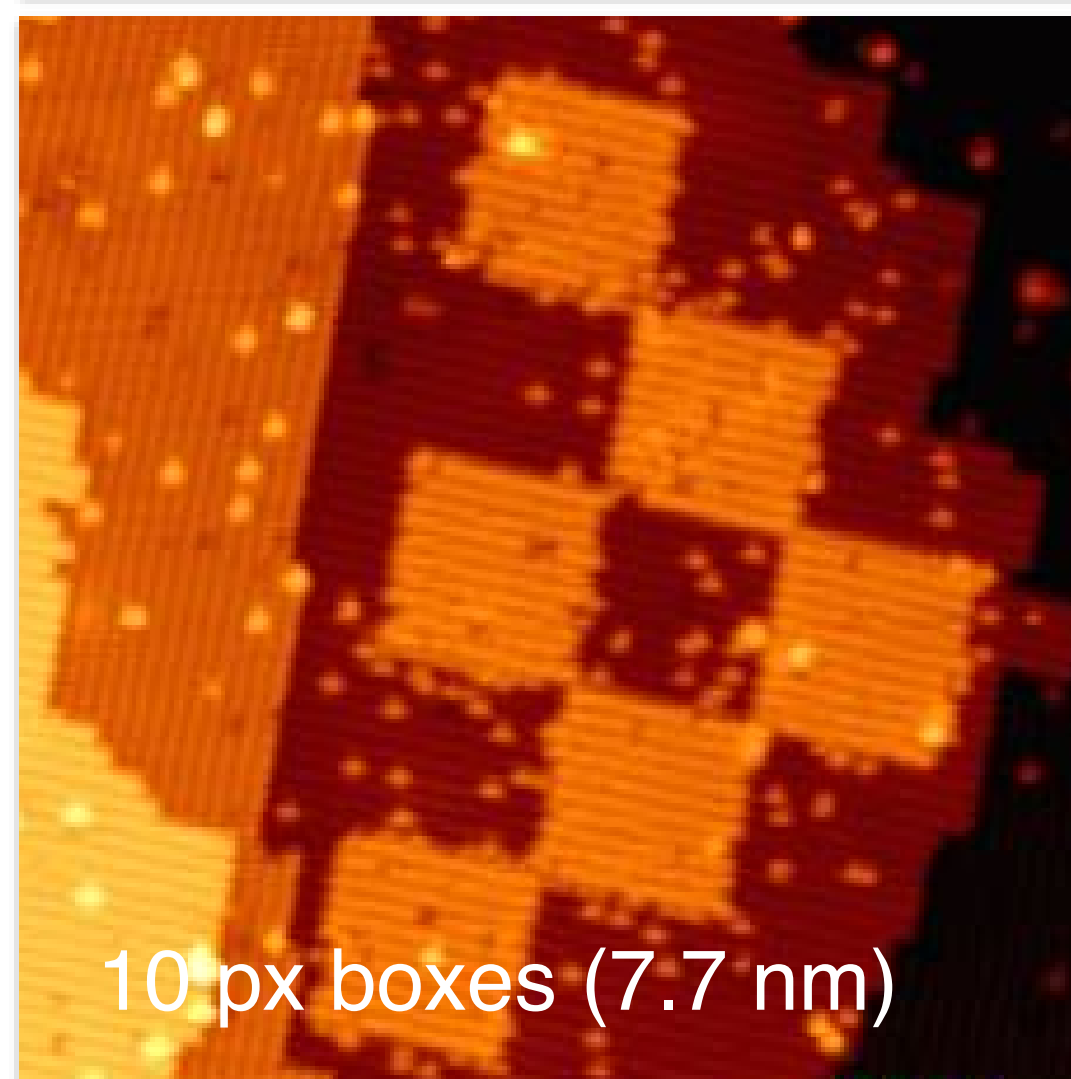
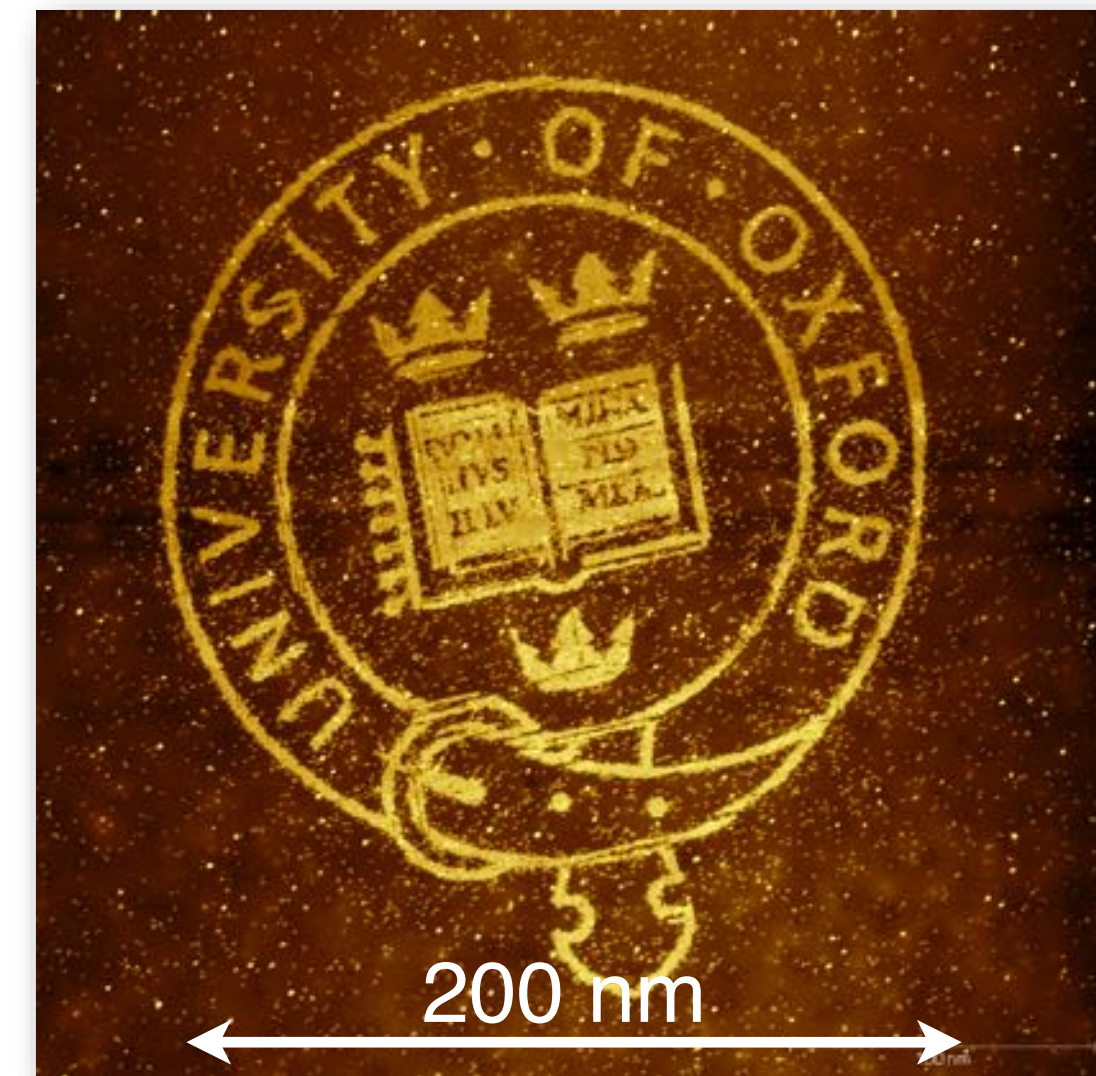
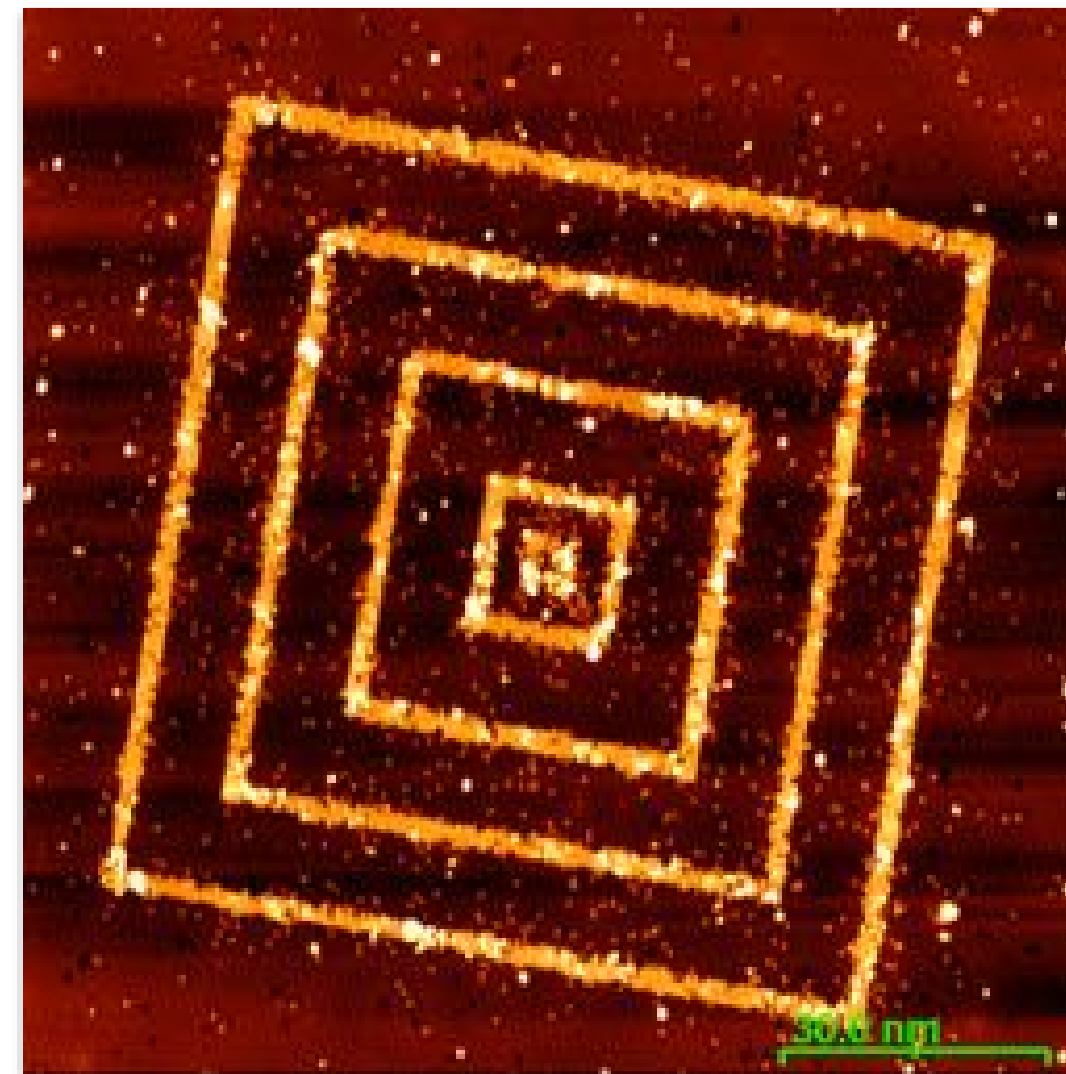
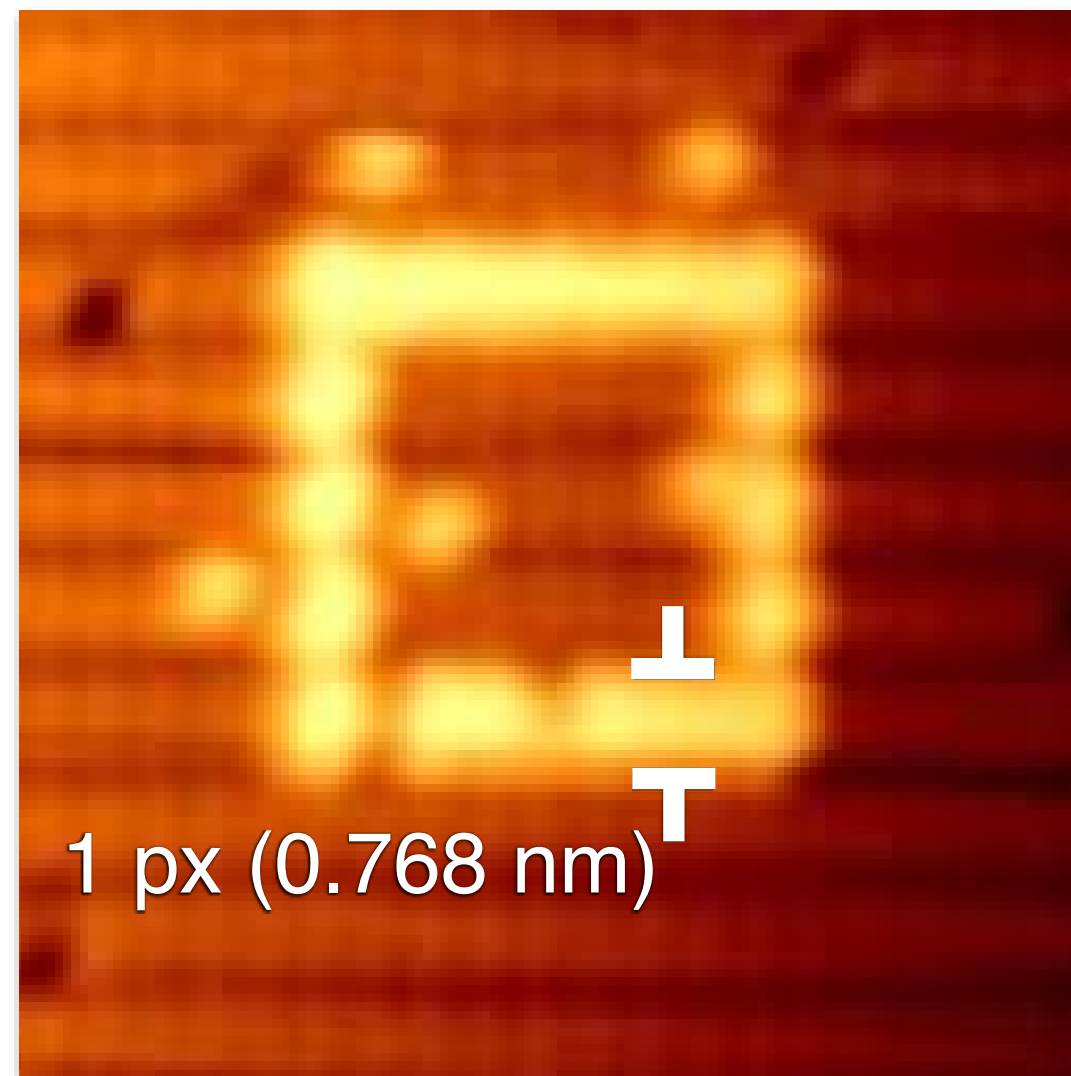
A new type of 2D material, made of arrays of dopant atoms positioned precisely within Si, has been proposed. - **2D Quantum Metamaterials**.

Other ultraprecise devices, e.g. Tunnel FETs and Bipolar Junction Transistors, have also been proposed. - **Atomically Precise Advanced Manufacturing (APAM)**

Bussmann, E. *et al.* *Atomic - Precision Advanced Manufacturing for Si Quantum Computing*. MRS Bulletin. 2021, **46**, 1–9. DOI: [10.1557/s43577-021-00139-8](https://doi.org/10.1557/s43577-021-00139-8)

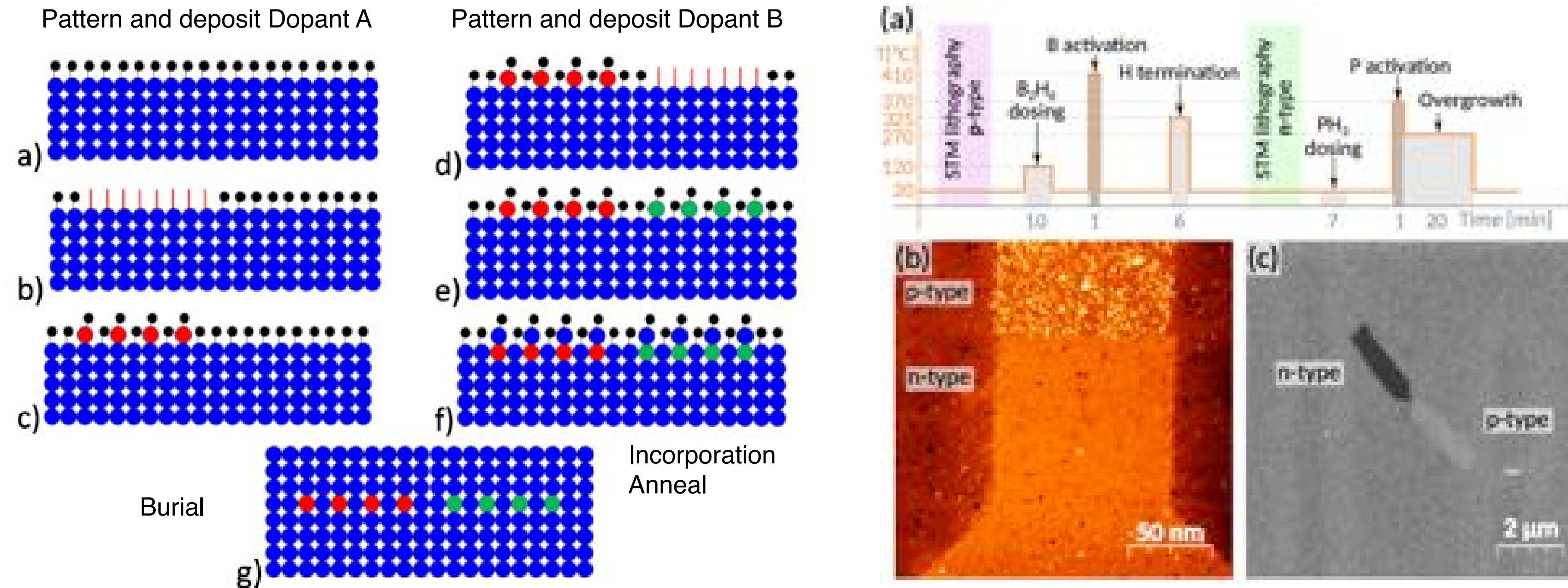


# Automated AP Lattice-Aligned Patterning



Zyvex Labs developed tools for automation of Atomically Precise STM lithography, aligned to the surface lattice.

# Bipolar devices



“Bipolar device fabrication using a scanning tunnelling microscope”  
 T. Škerekň, S.A. Köster, B. Douhard, C. Fleischmann, and A. Fuhrer, Nat. Electron. 1 (2020).

- In order to expand the range of applications of APAM technology, we need precursors for both donor and acceptor dopants.
- Here diborane and phosphine were used to make a p-n junction, depositing B first and then P.

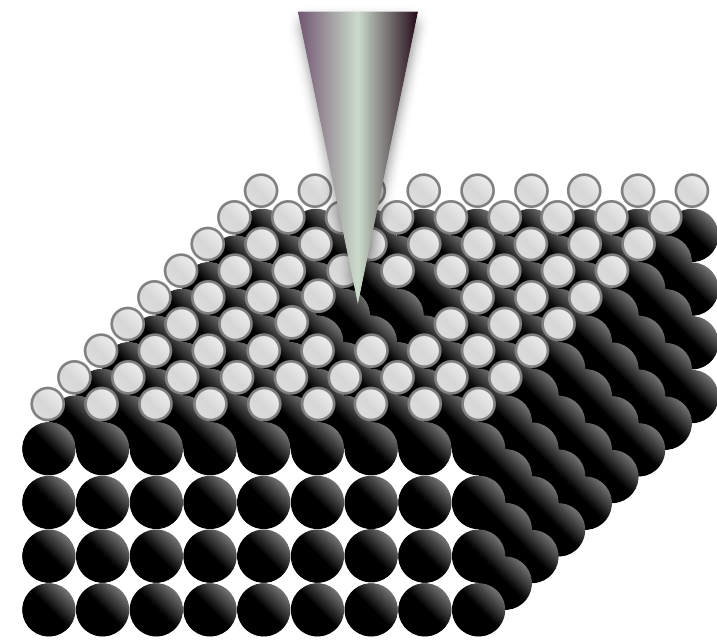


# APAM Precursors for B, Al

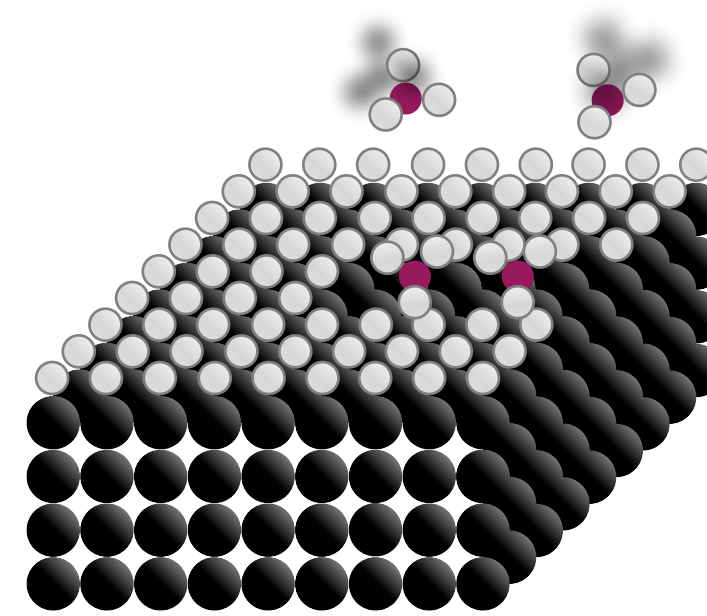
- It is not obvious that diborane can be used to place single B dopants.
- Alanes, analogues of phosphine, are not stable at room temperature.
- In the CVD and ALD worlds, typical Gr. III precursors are alkyls:
  - Trimethyl Al (TMAI), Triethyl Al (TEAI)
  - However, we have found that alkyl precursors show weak selectivity for APAM, due to a strong van der Waals interaction with the H-terminated surface.
  - Owen, J. H. G. *et al. Al-Alkyls as Acceptor Dopant Precursors for Atomic-Scale Devices.* J. Phys. Condens. Matter **33**, 464001 (2021).
- Hence we have moved to halide precursors,  $\text{BCl}_3$  and  $\text{AlCl}_3$ 
  - Dwyer, K. J. *et al. Area-selective deposition and B delta-doping of Si(100) with  $\text{BCl}_3$  ;*
  - Radue, M. S. *et al.  $\text{AlCl}_3$ -dosed Si(100)-2x1: Adsorbates, Chlorinated Al Chains, and Incorporated Al.* arxiv (2021)

# Bipolar Device Fabrication Process

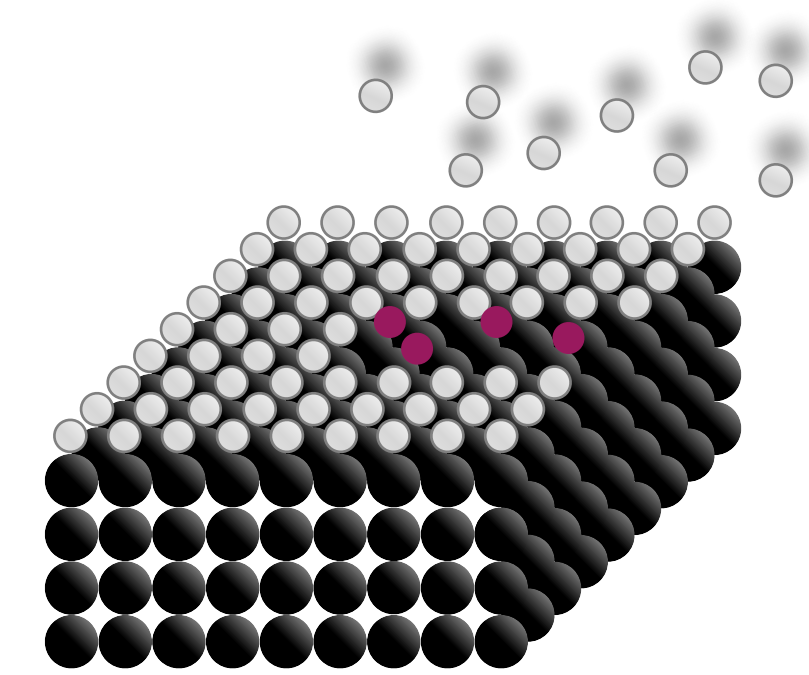
Pattern n-type electrodes



Dose  $\text{PH}_3$



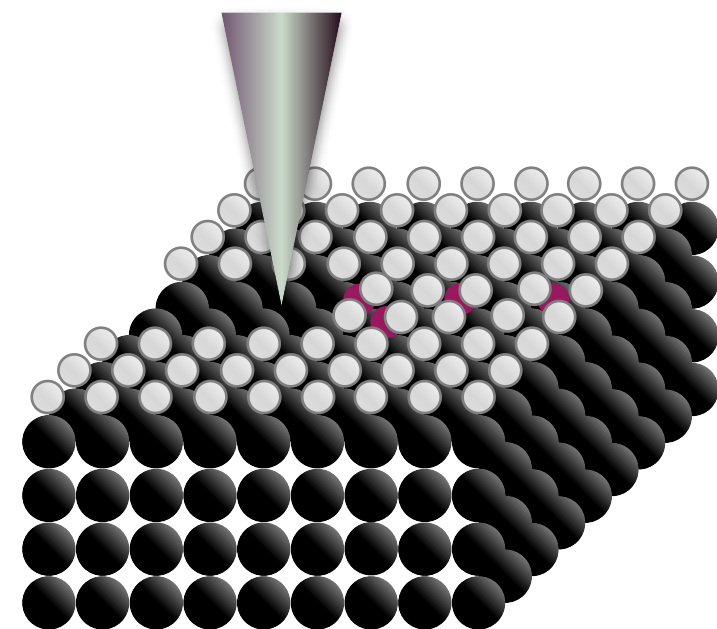
Incorporate and Anneal;  
Repassivate



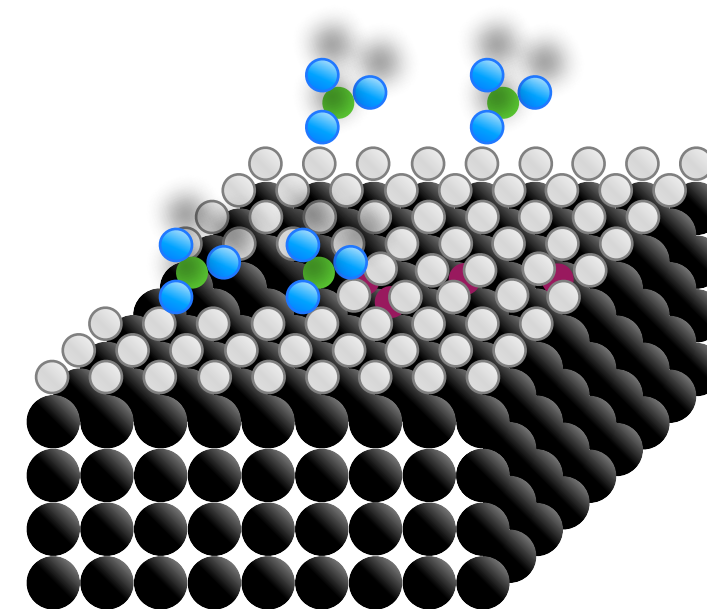
Remove  
to Prep

Relocate pattern in STM

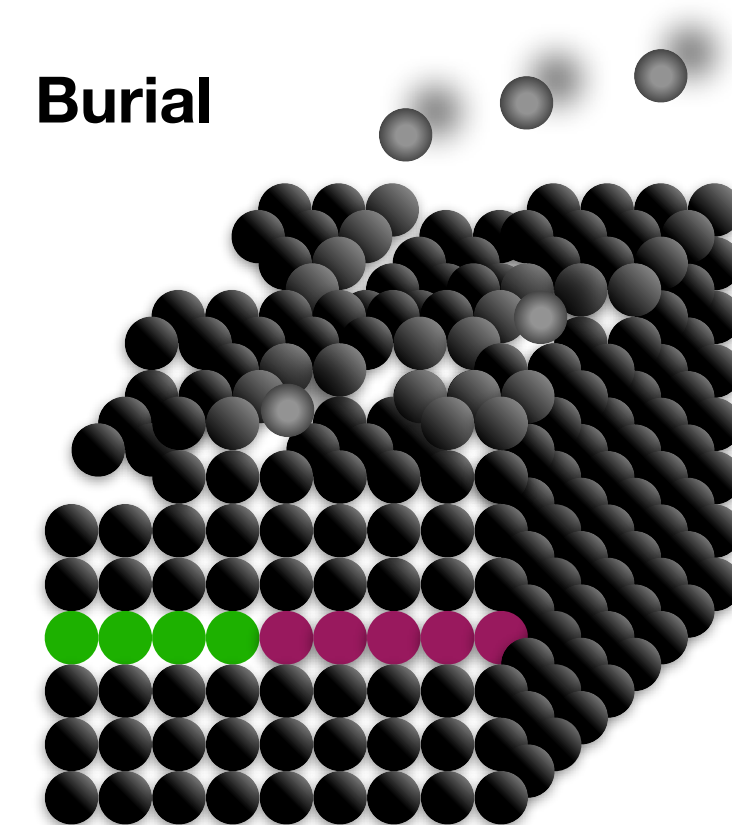
Pattern p-type electrodes



Dose  $\text{BCl}_3$

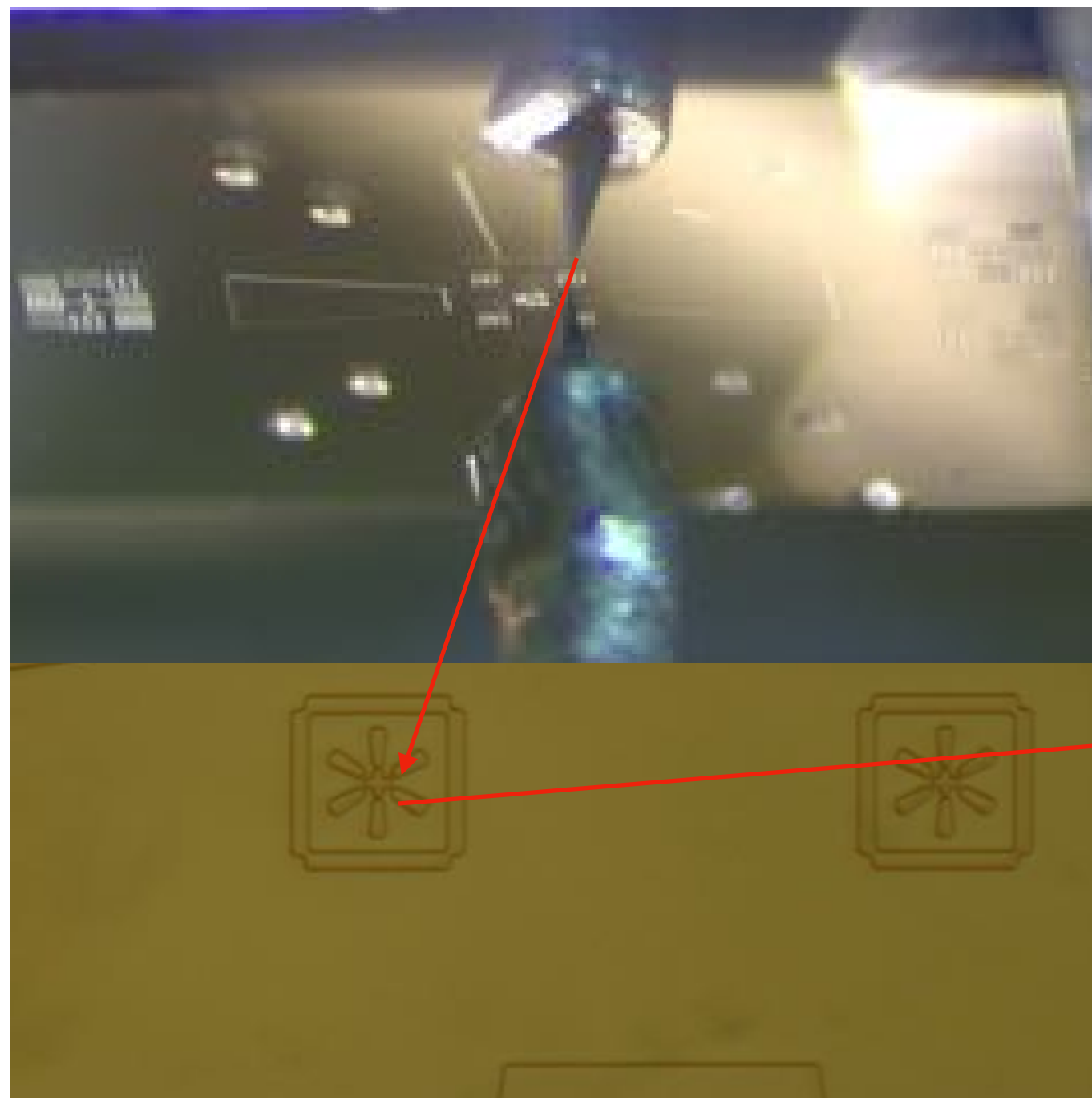


Burial

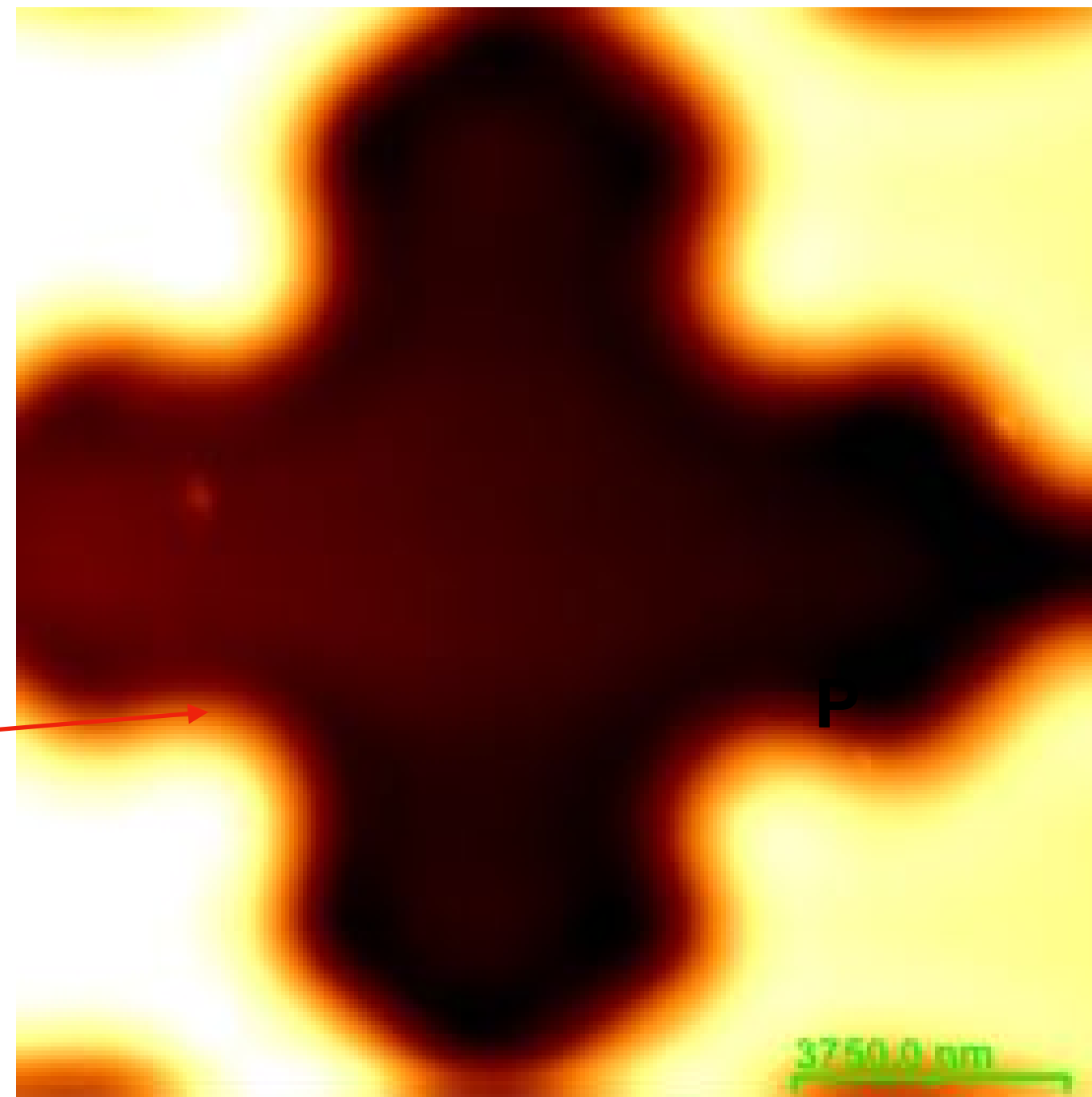


Remove  
to Prep

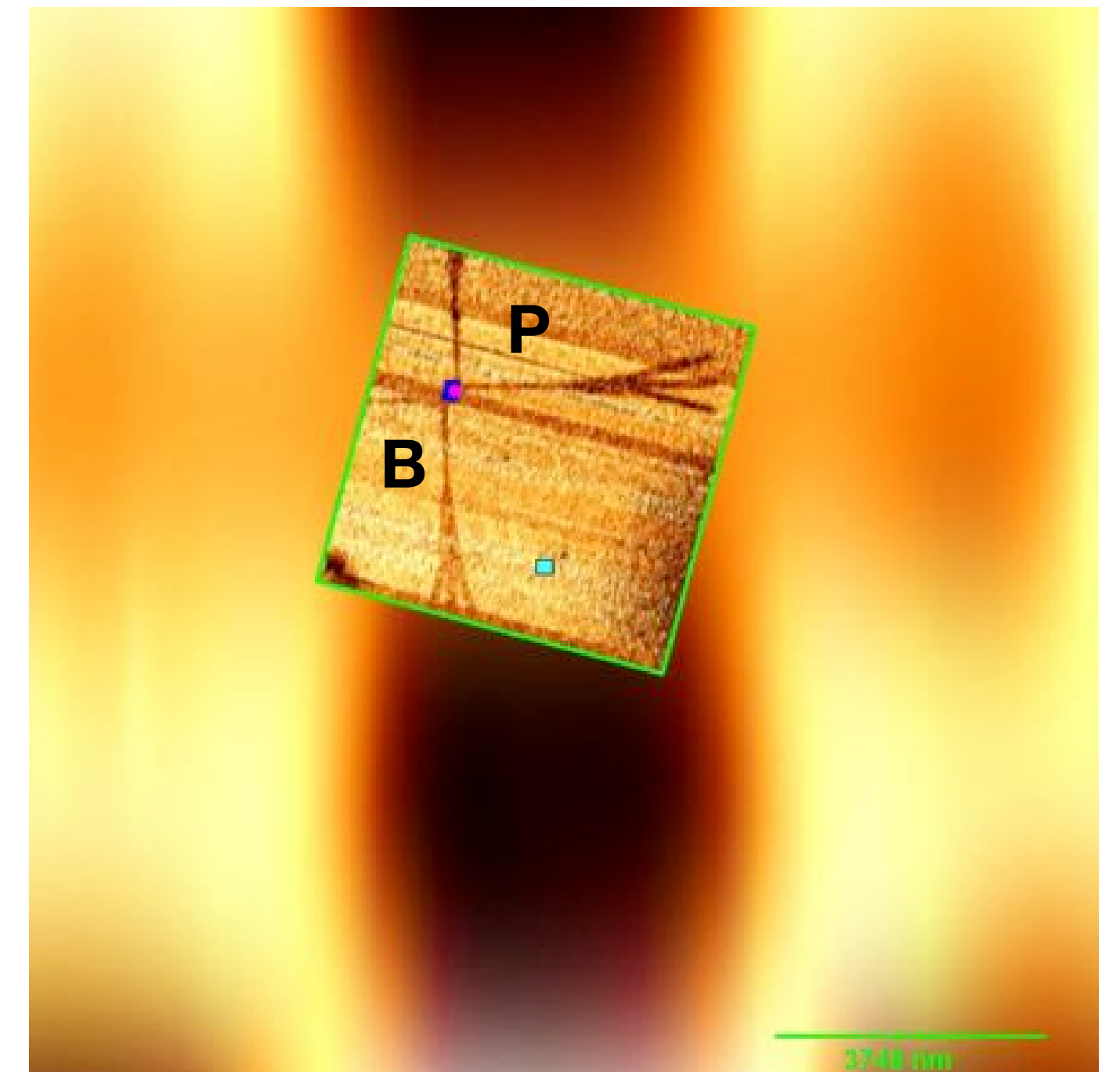
# Locating devices on the substrate



An STM tip landing on the central 20  $\mu\text{m}$  device area defined on a 4x8 mm Si sample in an Omicron VT STM.



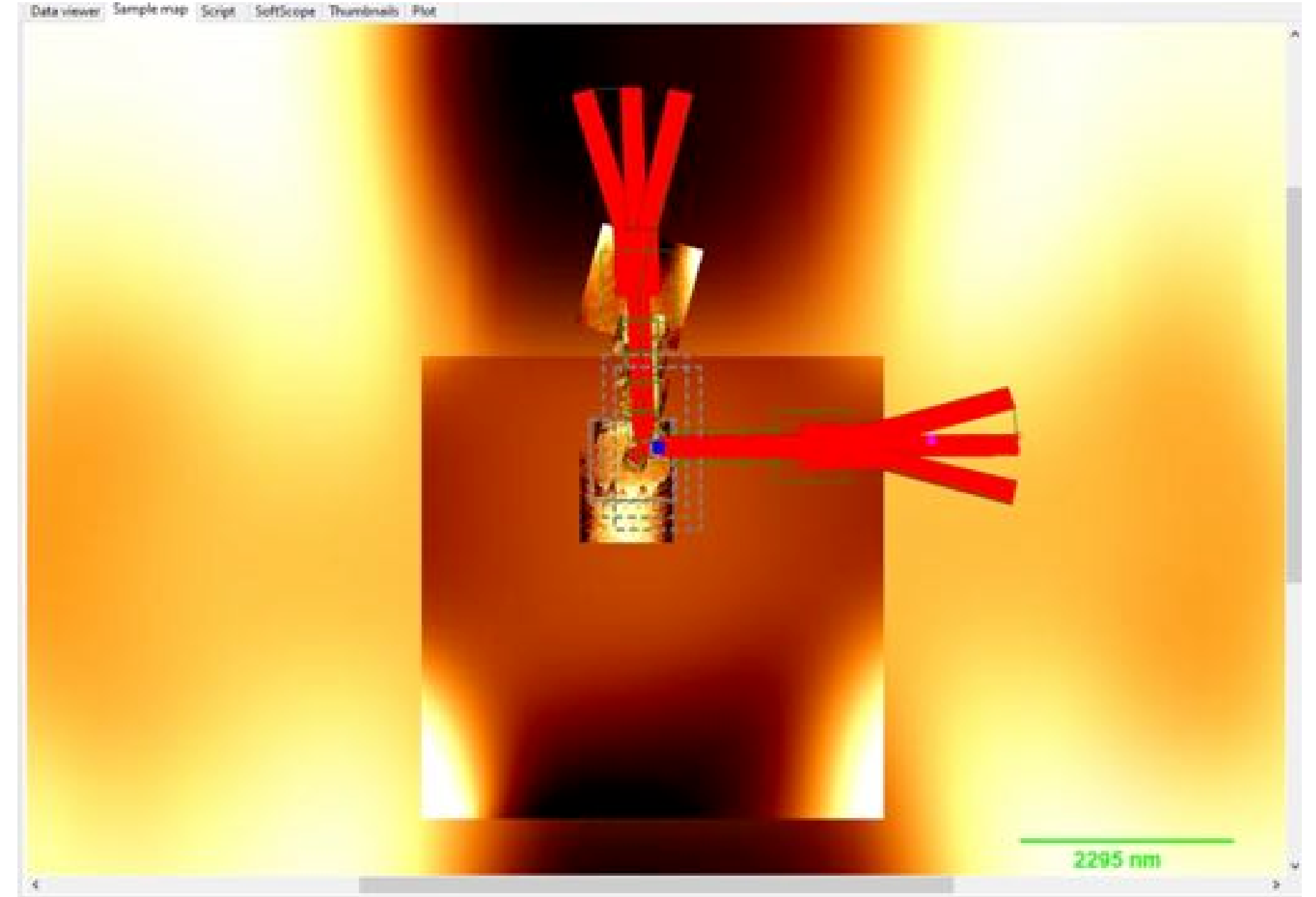
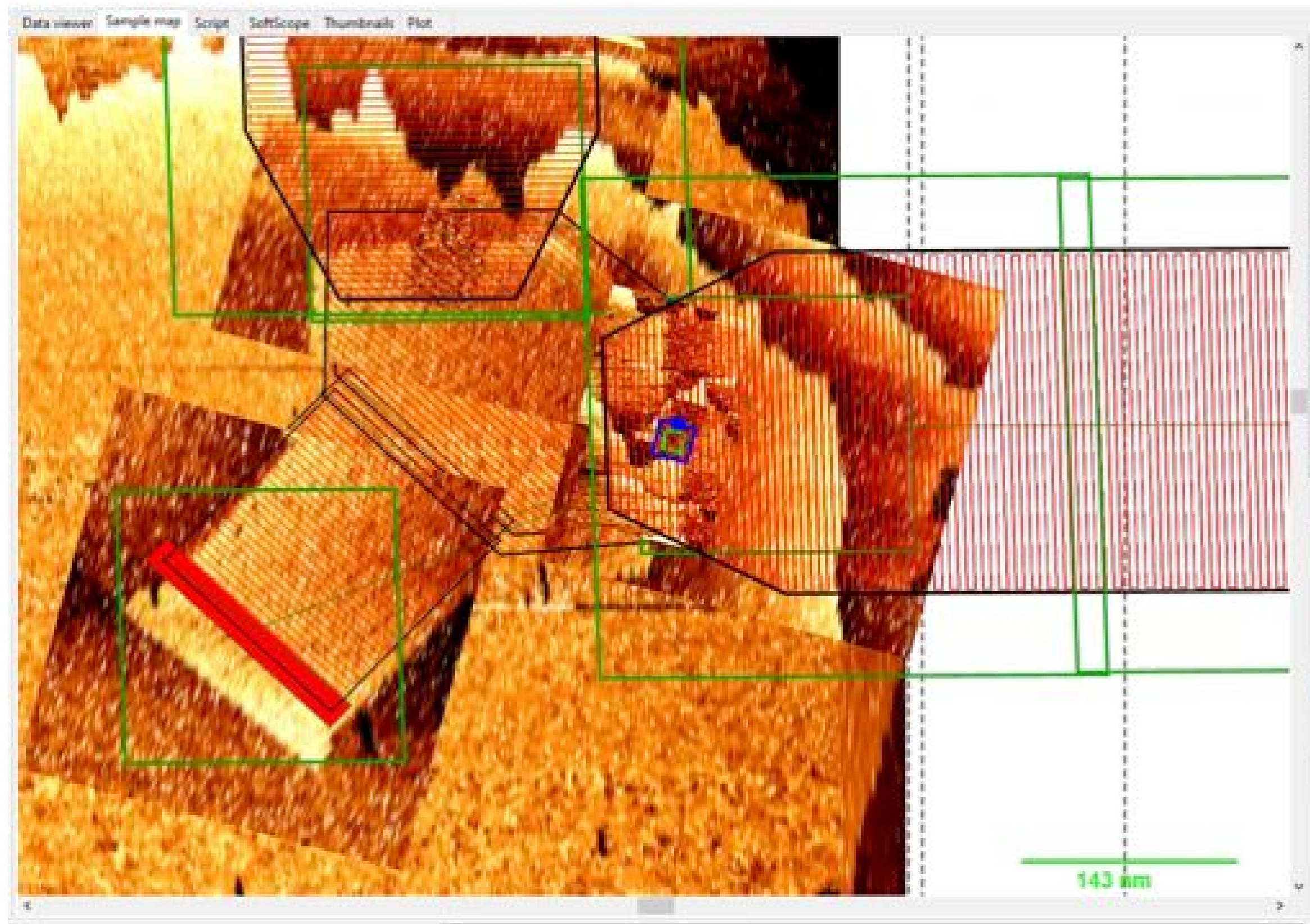
STM image of the central device area, showing 4 lobes for contact pads.



Our ZyVector STM lithography control system allows multiple images to be laid out to show the position of patterns relative to the overall substrate, for easy relocation.

Topography,  $dI/dZ$  and  $dI/dV$  images can also be mixed.

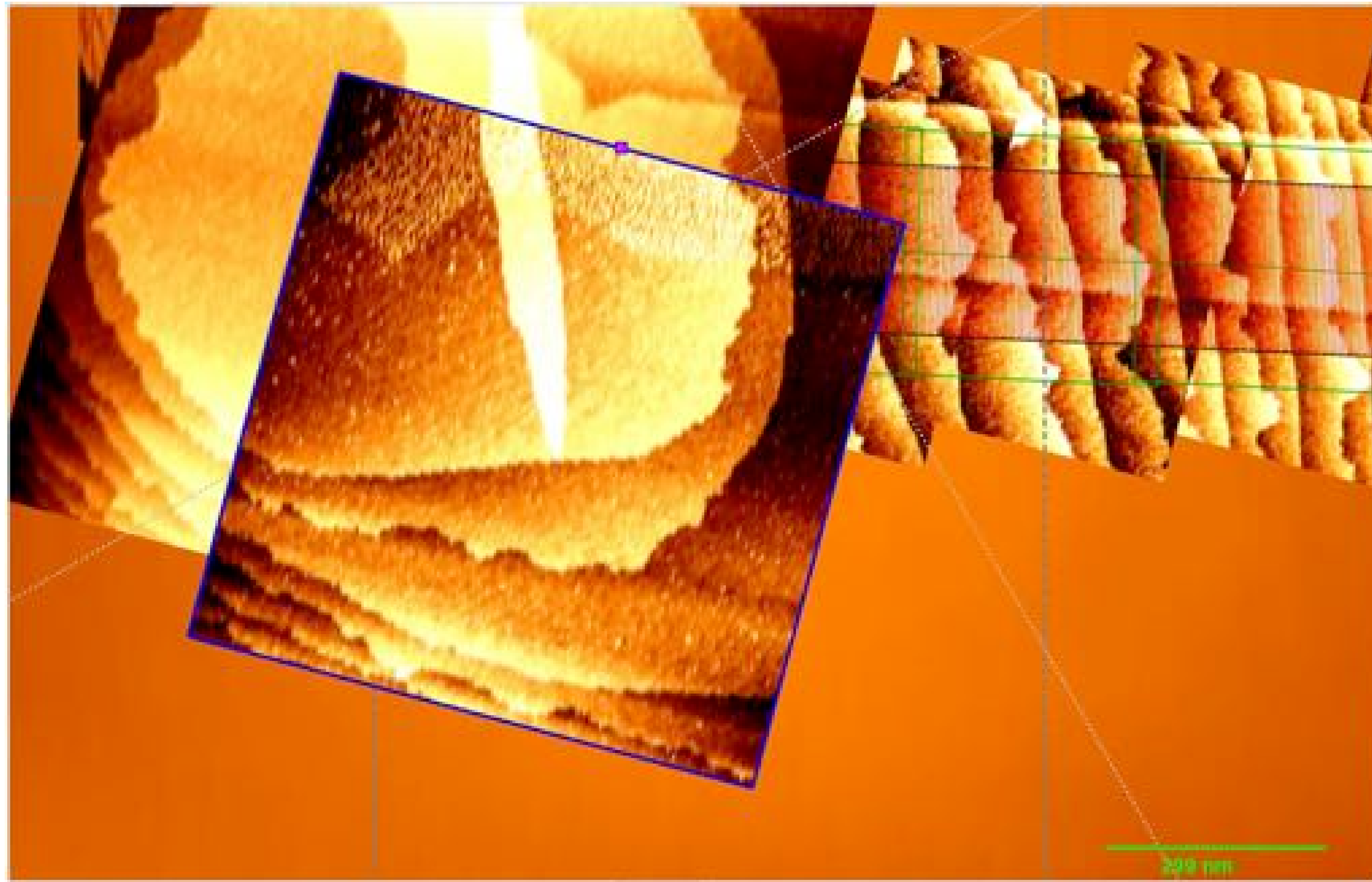
# Writing an atomic-scale pn junction



Sample Map views of P electrode patterns after writing using SVG patterns (red)

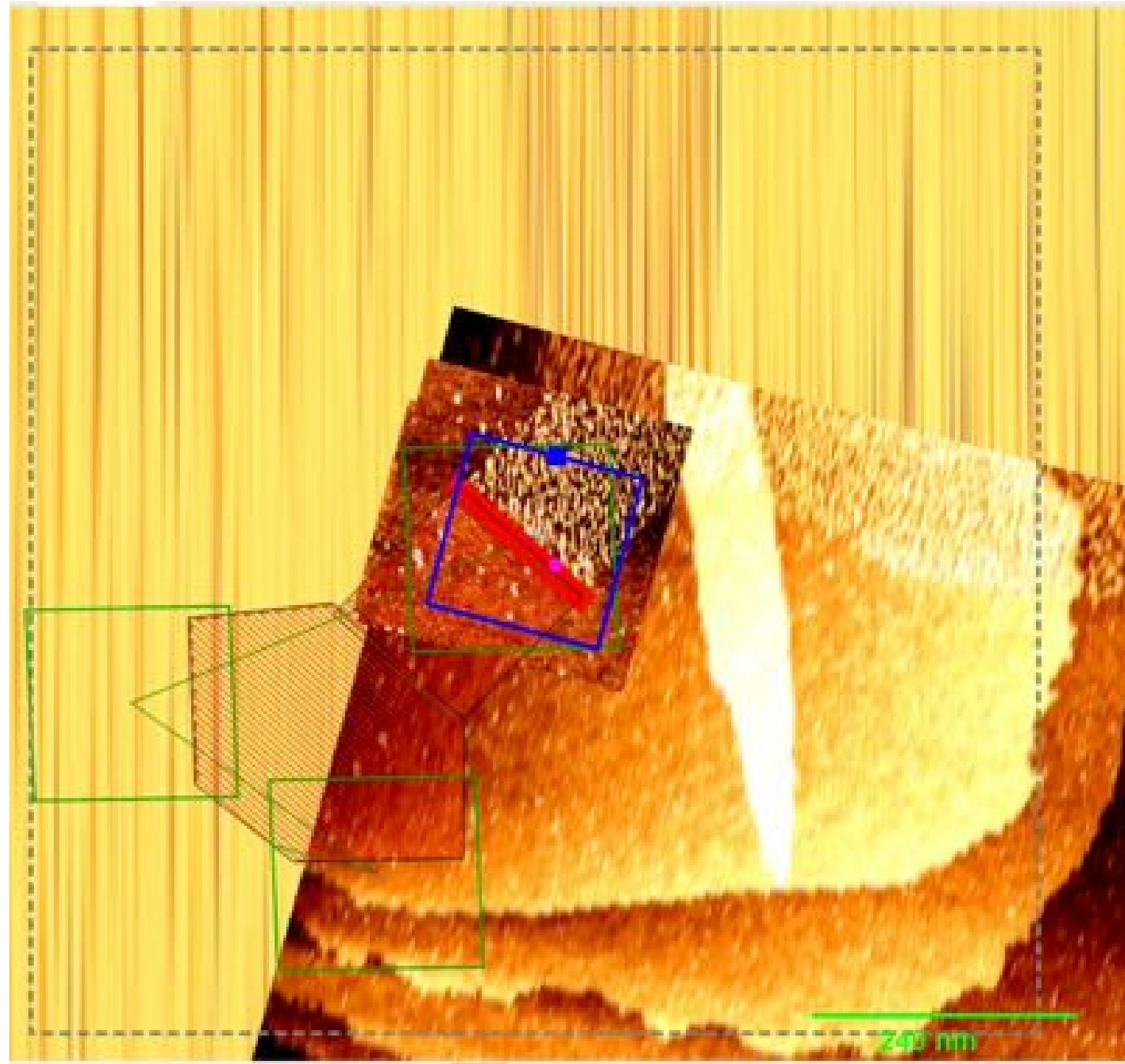


# Writing an atomic-scale pn junction



Realignment to device (blue edged image) after P dosing and incorporation

# Writing an atomic-scale pn junction

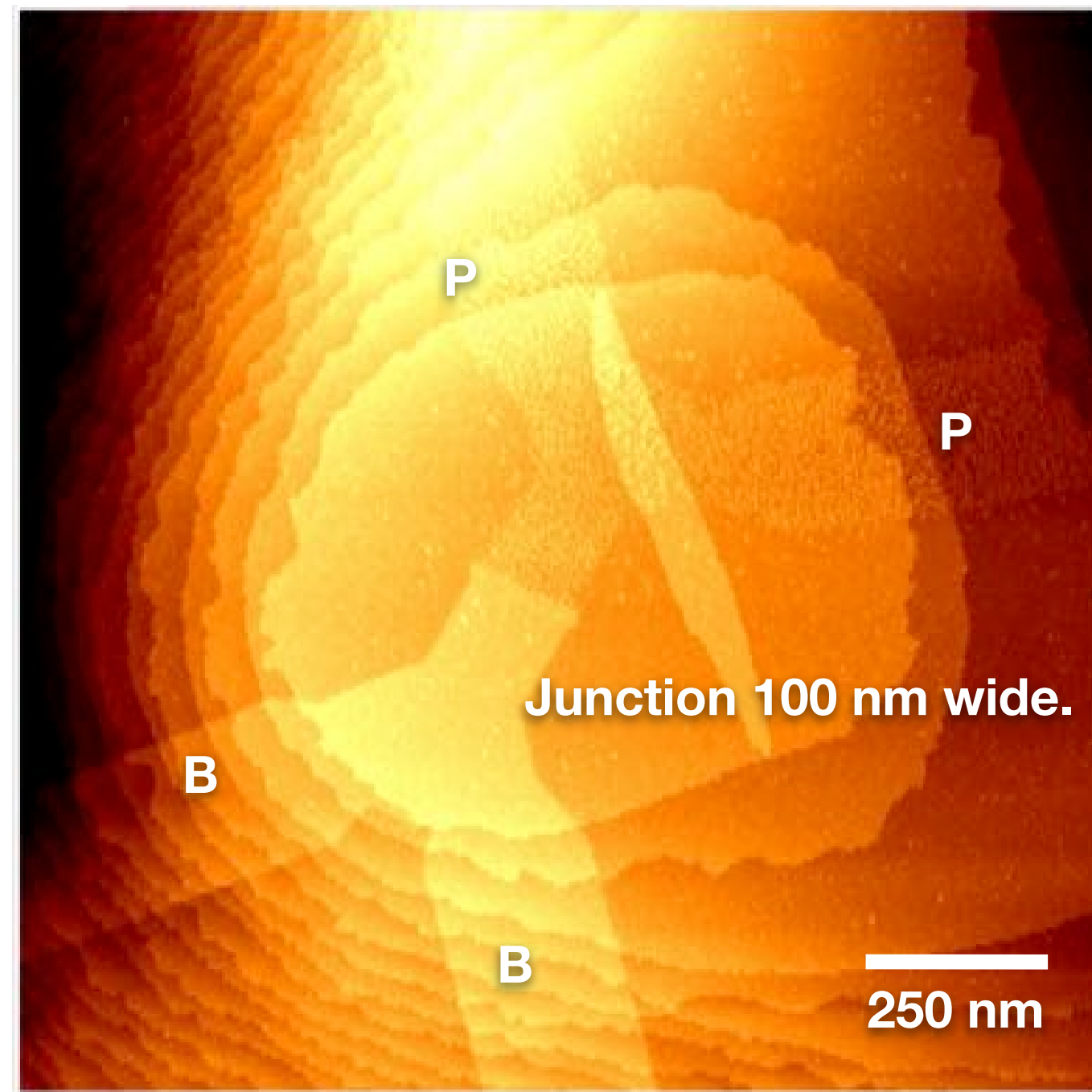


Aligning B pattern to incorporated P

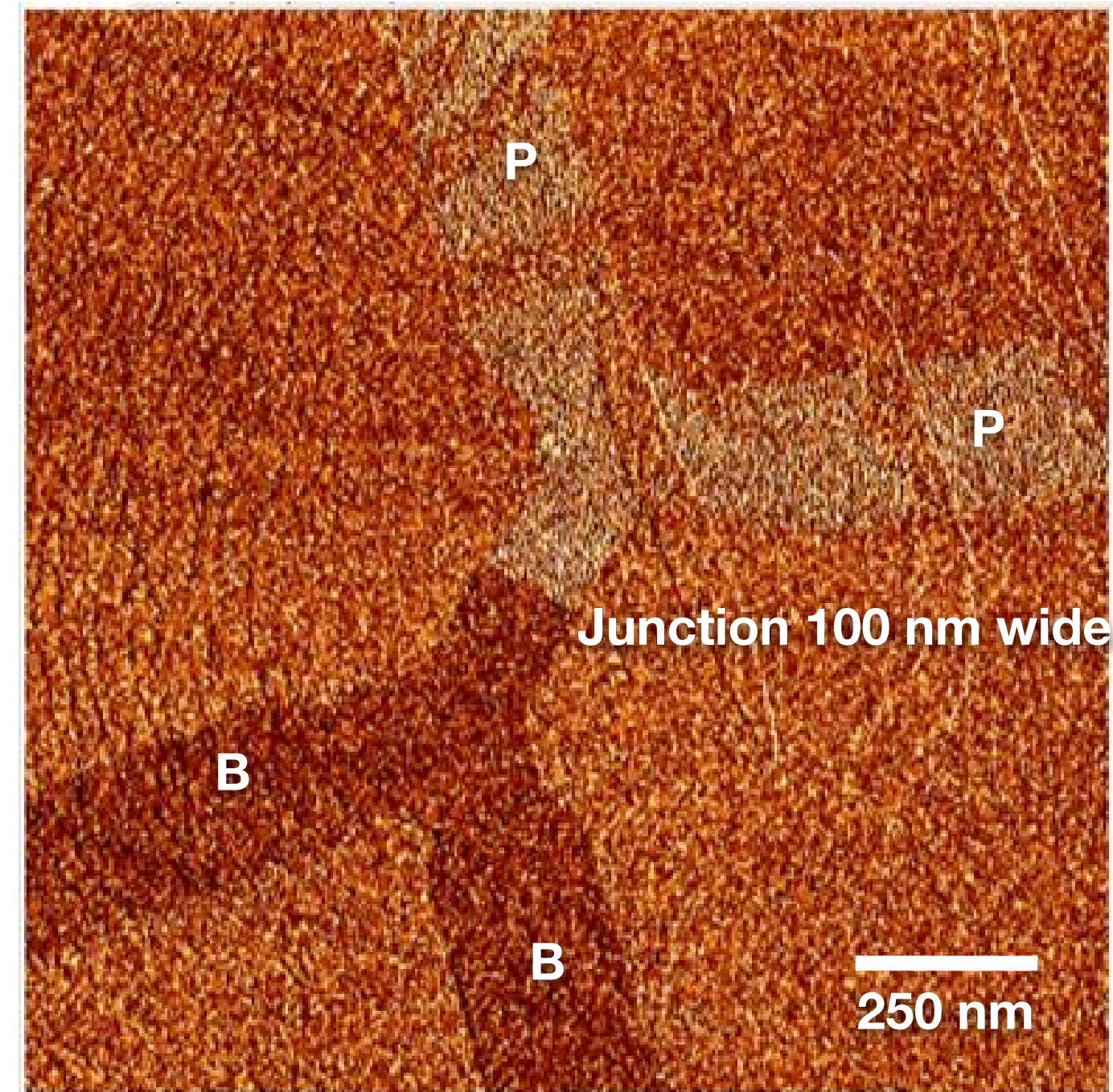


B pattern with zero gap to incorporated P

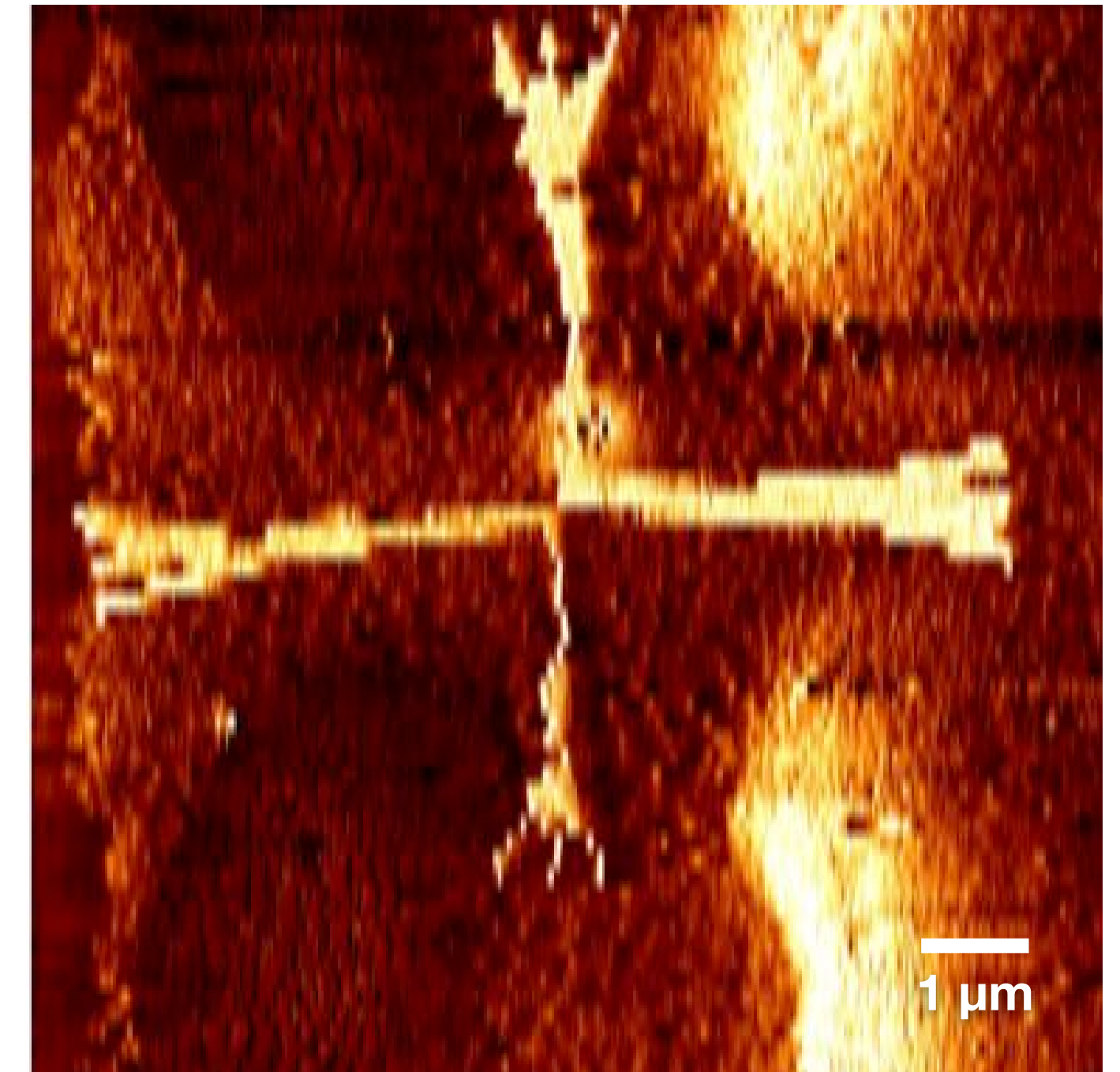
# Multivariant Imaging for Device Metrology



**Topo**



**dI/dZ**

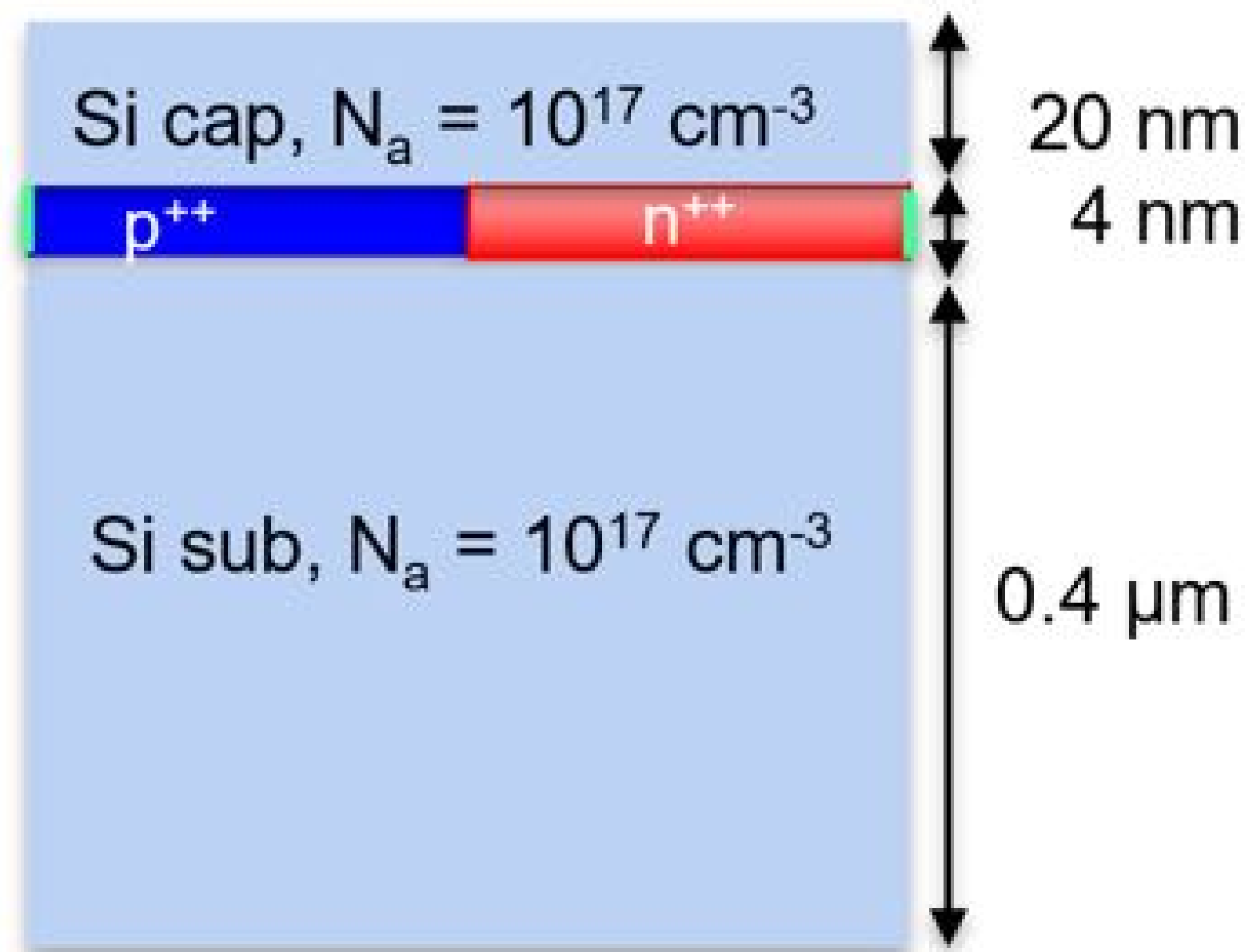


**dI/dV**

- Trials of bipolar device patterning; alignment of B to P.
- dI/dZ imaging gives good contrast for surface features, such as patterns of bare Si, and surface dopant patches. Here, with dI/dZ imaging, the contrast of the B patch is much clearer, and the pattern for the P electrode can be aligned to the existing B patch with dimer row resolution.
- dI/dV imaging allows buried devices to be imaged, to confirm their presence after the overgrowth process.



# Simulation-Experiment Comparison for p-n delta layers

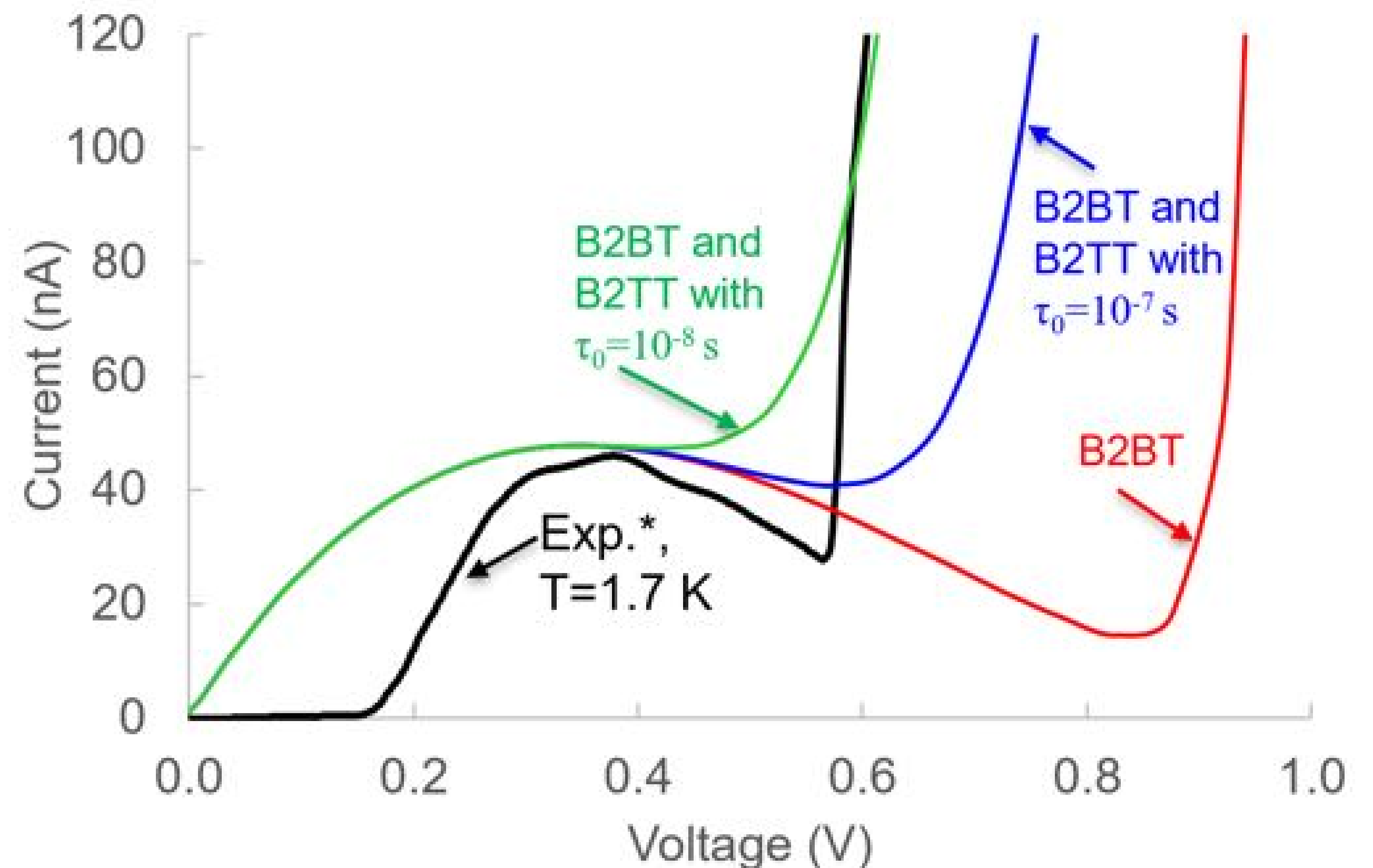


Simulations were done using Charon, an open-source device modelling code developed at Sandia National Labs.



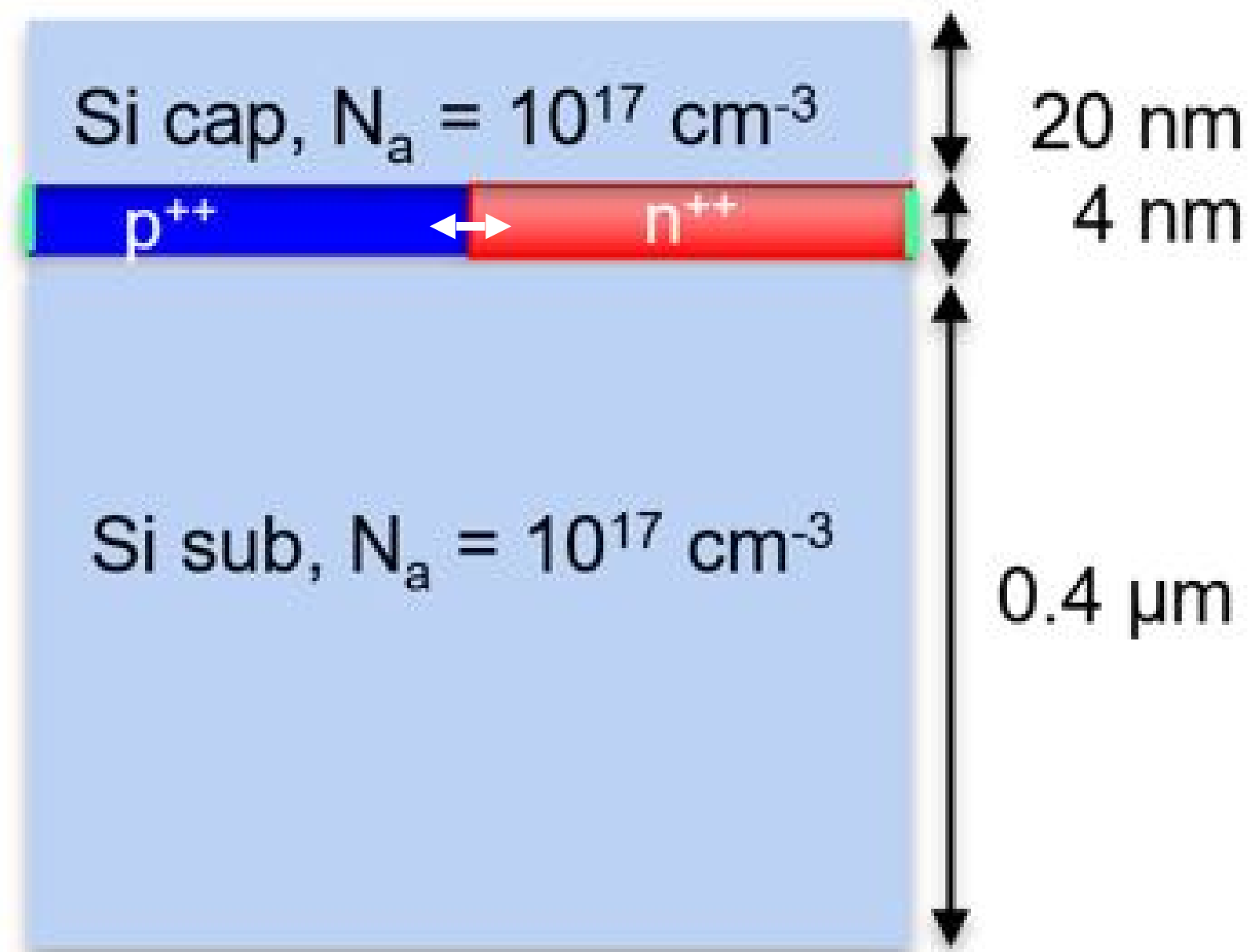
B2BT = Band-to-band tunneling  
B2TT = Band-to-trap tunneling

**With B2BT and B2TT, simulation results are in decent agreement with the experimental data except for voltages less than 0.2 Volts.**



\* T. Škerek et al. Nat. Electron., vol. 3, pp. 524–530, 2020.

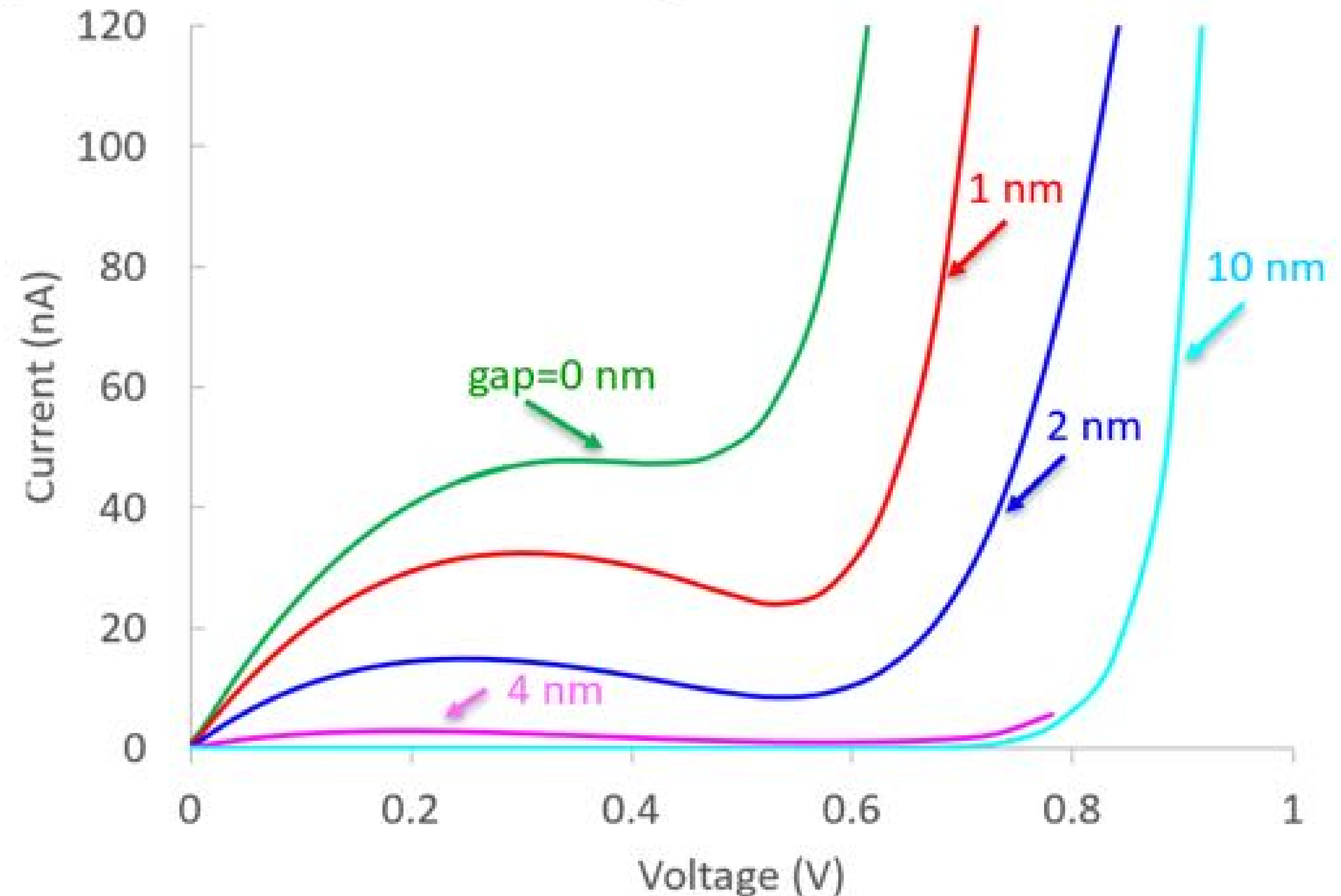
# Simulated I-V dependence on p-i-n gap width



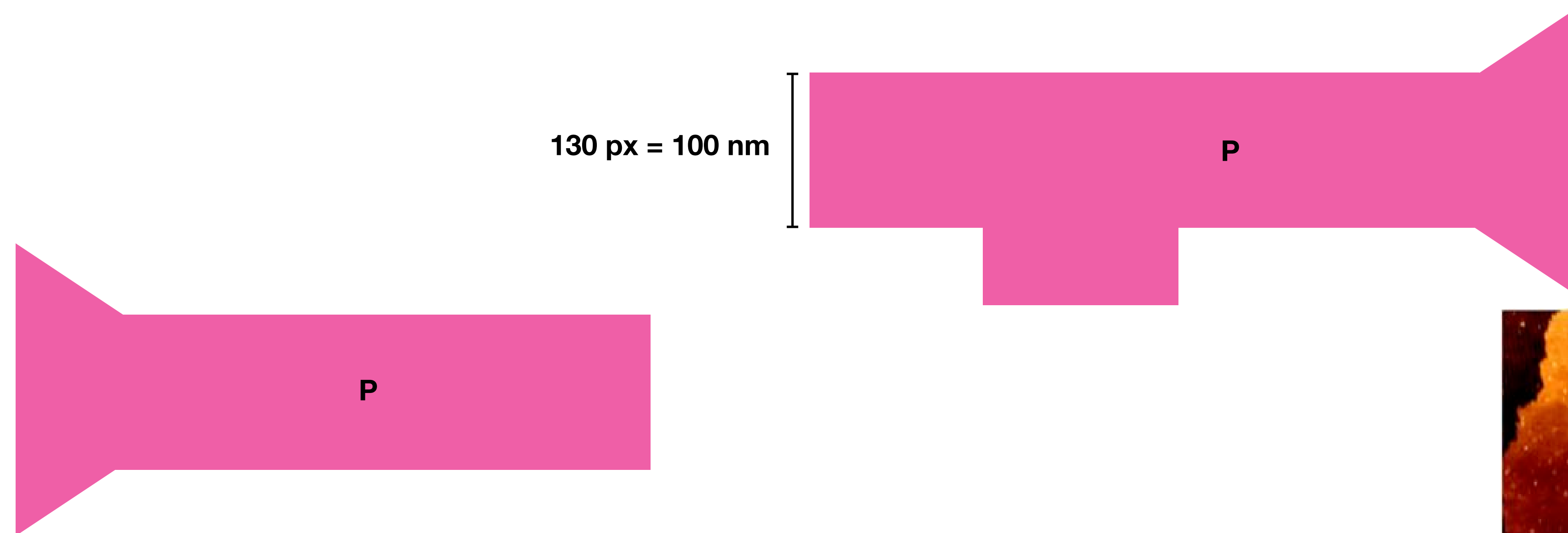
The distance between the two delta layers is varied.

**When the gap is 4 nm or bigger, the negative differential conductance (NDC) behavior is diminished.**

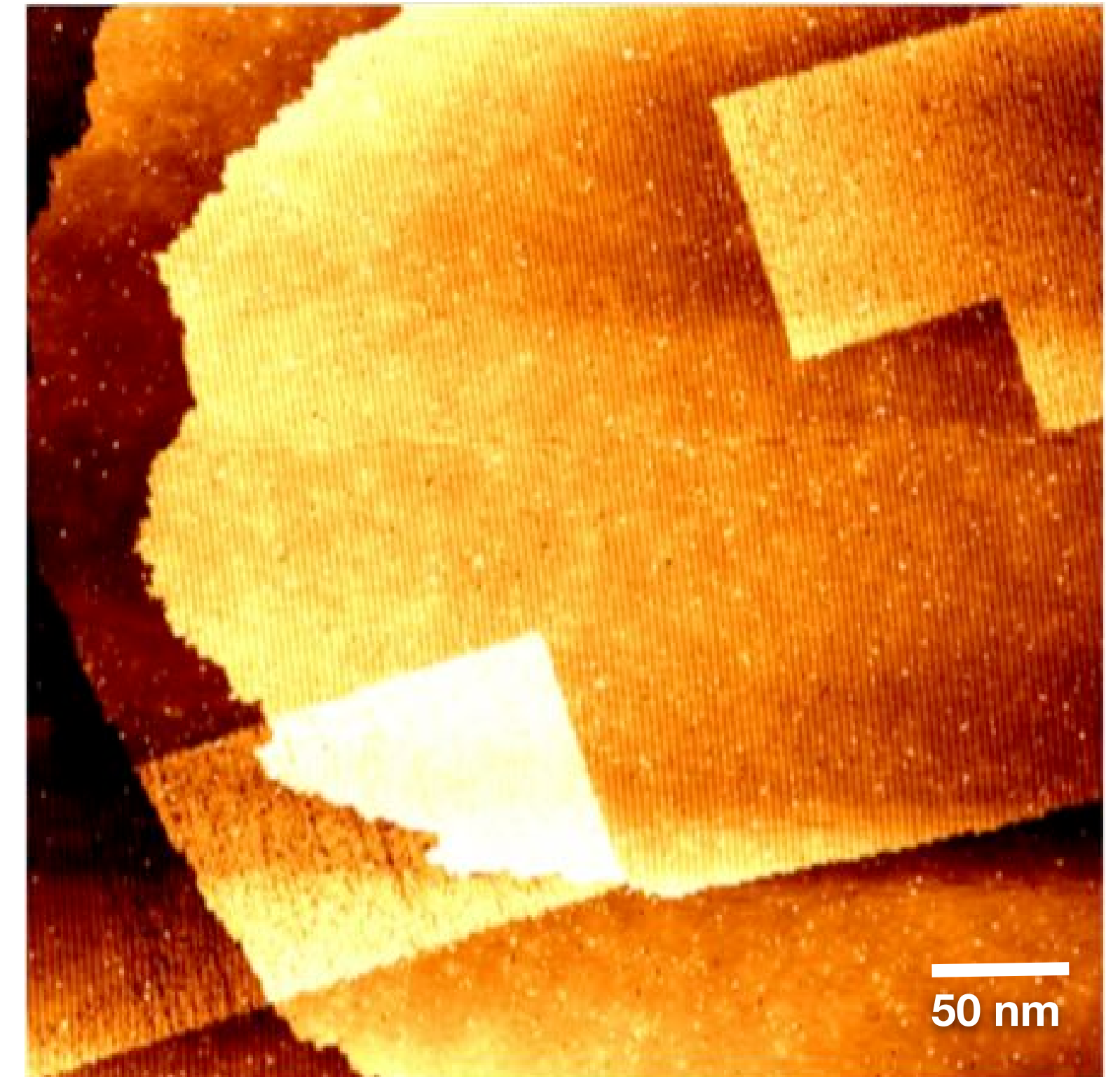
**We are exploring this experimentally.**



# Fabrication of devices with variable gap widths

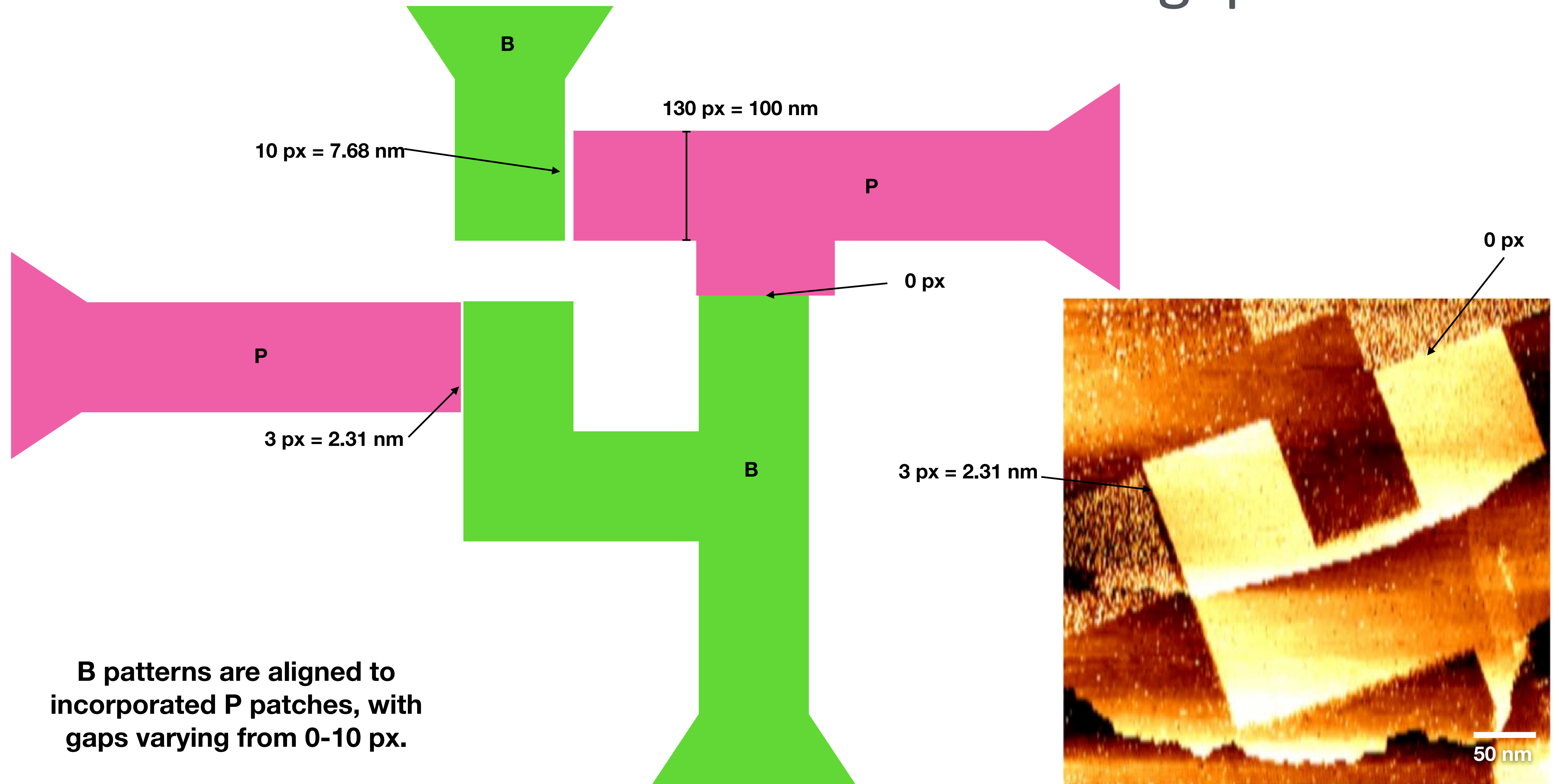


**P** patterns are drawn first, and saturated with  $\text{PH}_3$ . An incorporation anneal is used to activate the **P** dopants.





# Fabrication of devices with variable gap widths



- We are developing STM Lithography for Atomically Precise Advanced Manufacturing.
- Patterns can be drawn with atomic precision from the single-pixel scale, up to the full range of the STM scanner.
- Creep, hysteresis and thermal drift position errors are corrected in real-time in our ZyVector™ controller to achieve near-perfect positioning.
- For bipolar devices, the n-type patterns are written first, dosed with  $\text{PH}_3$ , and the P incorporated. The p-type patterns are aligned to the P patches to provide atomic-precision gaps between p and n electrodes.
- $\text{dI/dZ}$  and  $\text{dI/dV}$  imaging simultaneous with topographic imaging provide extra electronic contrast of patterns and incorporated dopants, to make alignment of patterns easier.
- p-i-n junction device simulations indicate that the device behaviour is strongly dependent upon the gap width. A set of junctions of varying width (0, 3, 10 px) have been fabricated to test this prediction.
- The next step will be to measure the electrical properties of these devices, compare to the modelling, and test these predictions.