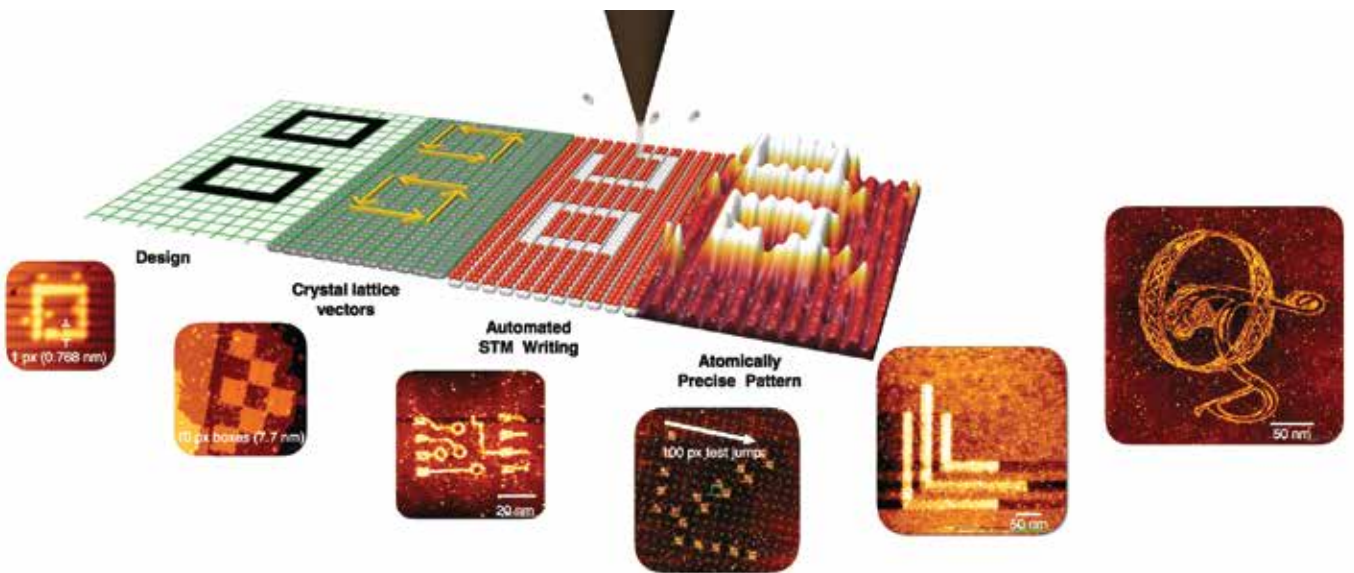


# ZyVector™

STM Control System for Atomically Precise Lithography

*Making Atomic Resolution  
Lithography a reality*

*Distortion-Free Imaging  
Automatic Lattice Alignment  
Digital Vector Lithography  
Built-in Metrology  
Automation and Scripting*



At Zyvex Labs, our vision is to design, construct, and commercialize the world's most precise manufactured products.

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For nearly 20 years, Zyvex Corp, LLC, has been at the forefront of developing tools and processes to create ultraminiaturized systems with atomic precision and unprecedented capability. Sister companies include Zyvex Technologies, the world's leading supplier of carbon nanotube polymers, and Zyvex Instruments, currently owned by ThermoFisher, which is the world leader in nanoprobe testing of integrated circuits.

Zyvex Labs is pursuing research and developing tools for creating quantum computers and other transformational systems that require atomic precision, towards its eventual goal of Atomically Precise Manufacturing. Developed as part of this effort, ZyVector turns the world-class ScientaOmicron VT-STM\* into an STM lithography tool, creating the only complete commercial solution for atomic precision lithography.

*\*Adaptions for other STM systems possible.*



### Digital Vector Lithography

- Takes atomic structure of surface into account
- Sub-nm pixel ( 4 surface atoms)
- Multiple Beam Widths available
- No partial exposure or proximity effects
- Automatic alignment of lattice

### Built-In Metrology

- Nondestructive imaging mode available
- New Patterning can be aligned to old
- Pattern quality can be checked after writing
- Size of developed nanostructures traceable back to original pattern, with atomic precision.

### Automation and Scripting

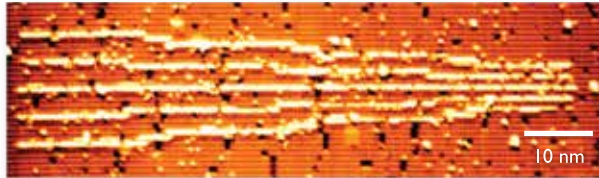
Almost all actions can be automated.  
 Command-line interface for single commands or scripts  
 Script Menu for built-in and user-written scripts  
 Multiple pattern input modes - as geometric shapes, vector lists, black/white bitmaps.

### Precise Tip Positioning and Motion

Real-time creep correction enables atomic-precision motion over limited areas.  
 Automatic alignment to fiducial marks allows for error correction and precise motion over large areas.  
 Distortion-free imaging for precise tip location.

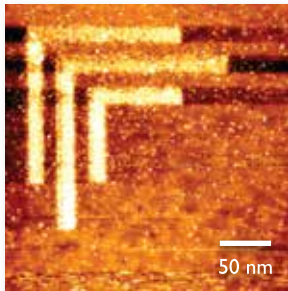
## Applications

*Dangling Bond Patterns, Quantum Dots, Wires.*

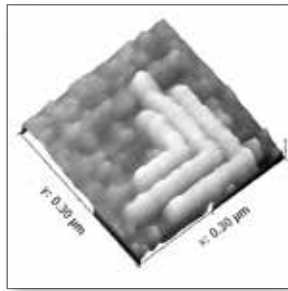


*Sub-nm Lines at 3.8 nm–1.5 nm Pitches*

### NanoImprint Templates



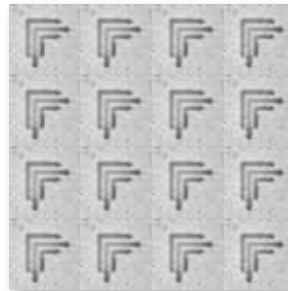
*Patterning*



*Area-Selective ALD*



*Dry Etch*



*NanoImprint (Simulated)*

Patterned ALD of  $\text{TiO}_2$  hard mask in STM pattern  
 RIE of  $\text{TiO}_2$  hard mask to create 3D Si structure  
 Replication of 3D structure using NanoImprint  
 Lithography.

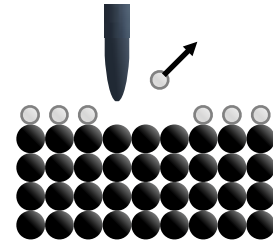
Ballard et al. *J. Vac. Sci. Technol.*  
 B 32 041804 (2014)

### Other Applications

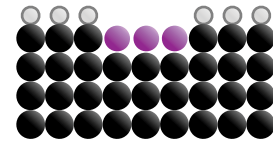
*Patterned ALE of Si, Ge.*

*Selective Placement of many molecules.*

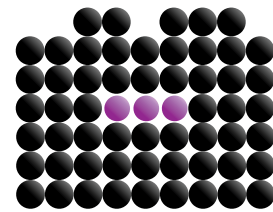
### Dopant-based Electronics



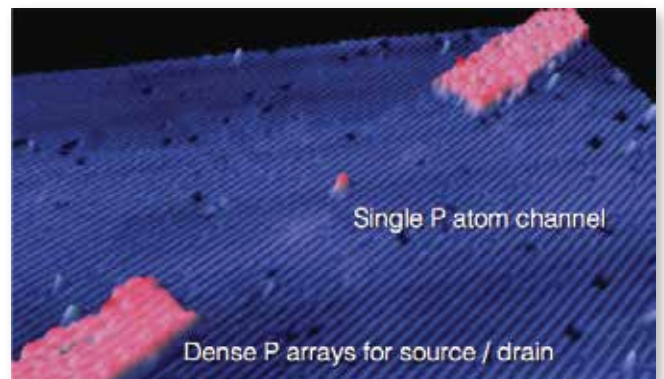
*Hydrogen Depassivation  
 Lithography*



*PH<sub>3</sub> Dose  
 & P incorporation*



*Encapsulation with  
 epitaxial Si*



Deposition of  $\text{PH}_3$  into STM pattern. Overgrowth of P to create embedded dopant layer for quantum computing devices.

Fuechsle et al. *Nat Nano* 7 242-246 (2012),

# Digital Vector Lithography

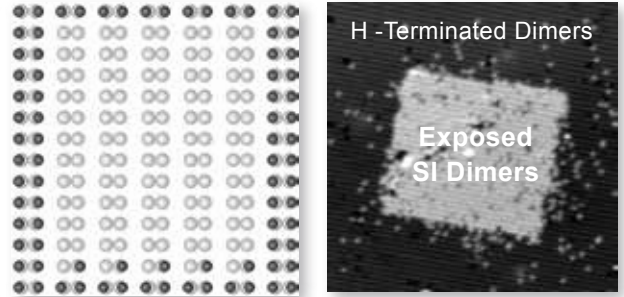
Unlike conventional optical or e-beam lithography, STM lithography takes into account the atomic nature of the surface. In ZyVector, writing is done as vectors, moving along the surface lattice directions, rather than a raster scan across the surface as used for STM imaging.

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## Hydrogen Depassivation Lithography (HDL)

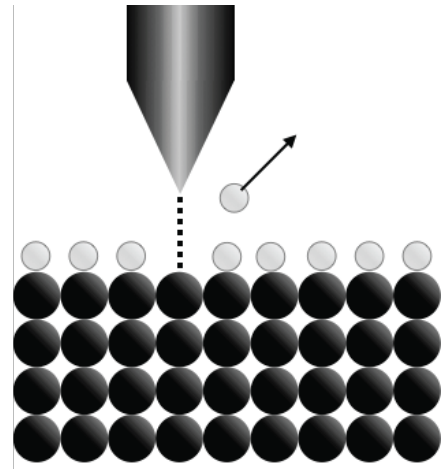
Lyding et al.\* first showed that at a positive sample bias, an STM tip can be used to inject electrons into a surface Si-H bond, until the bond breaks, exposing a chemically reactive Si dangling bond. Other materials are then selectively reacted with the dangling bonds, forming atomically precise nanostructures.

\*Applied Physics Letters 64 2010-2012 (1994)



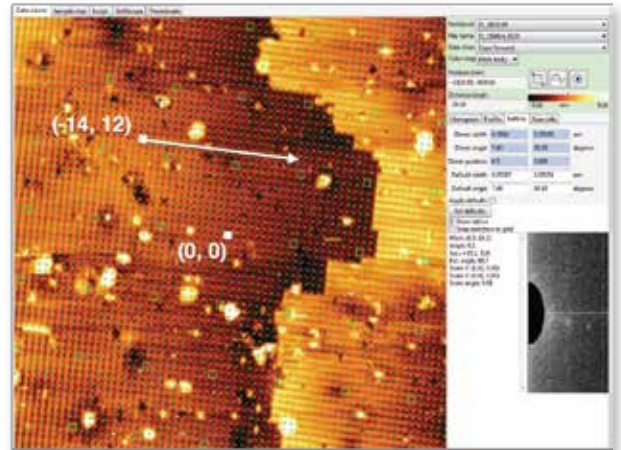
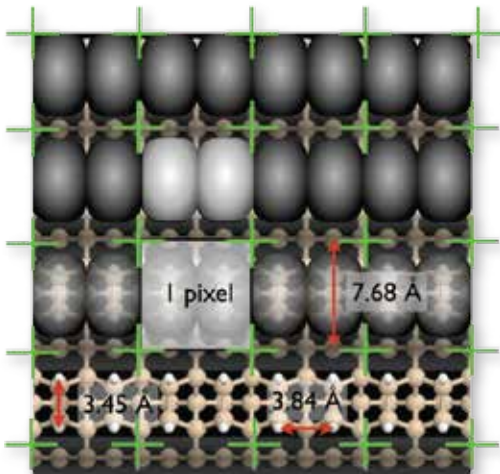
## Atomic-scale lithography pixel

For the Si(001): H surface, we use a standard pixel size of 2 dimers on a single dimer row, giving a lithography pixel size of 0.768 nm. Patterns are typically generated from integral numbers of pixels, although for some special cases, such as the 3-dimer pattern used to place single P dopant atoms, half-pixels can be used.



## Writing to the lattice

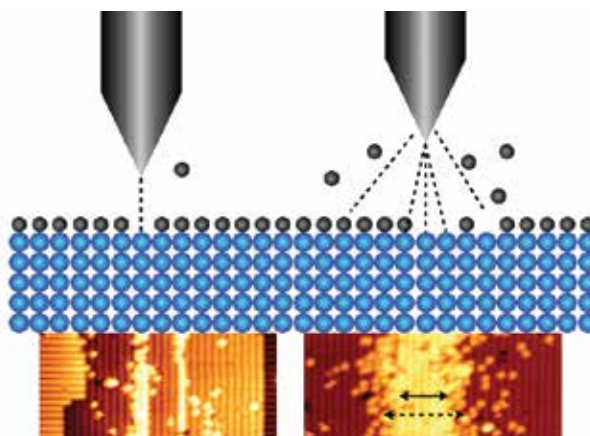
In order to write atomically-precise patterns, the location of the surface dimer rows are identified from the Fourier Transform of an STM image, and a pixel grid is overlaid onto the image. To perform lithography, the tip is then instructed to move to a particular pixel, change to lithography conditions, and write a line along or across the dimer rows of the desired length.



## Variable Spotsize Lithography

STM lithography is digital because it causes the breaking of a Si-H chemical bond by electron excitation. There is no equivalent of partial exposure, because either the bond is broken or it is not. Likewise, there are no proximity effects.

Similar to e-beam lithography, with different settings of bias voltage and tunnel current, multiple line widths are available, from 1 px width up to several nm. Under low-voltage lithography conditions, around +4 V, 4 nA, with a dose of 4 mC/cm, the line width of STM lithography is one dimer row. This is known as Atomically Precise or AP mode. Above about 6 V, the tip moves out of tunneling range into Field Emission (FE) mode with much wider line widths, but also with rough edges to the lines. Use of the FE mode is useful to minimize write time for larger patterns, particularly where there is less need for absolute precision. For large patterns which do require precise edges, the modes can even be mixed within a single pattern, writing slowly around the perimeter, and quickly filling in the centre.



AP mode:  
4.5 V, 4 nA,  
2 mC/cm  
20 nm/s  
Linewidth: 1 px  
26 px/s

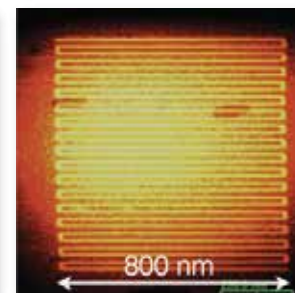
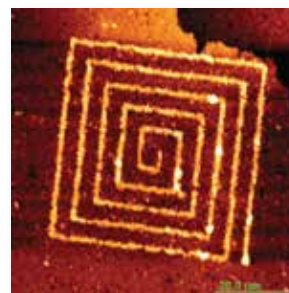
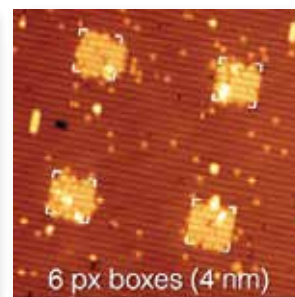
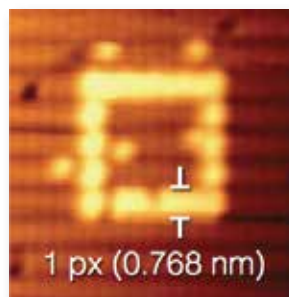
FE mode:  
8 V, 1 nA,  
0.1 mC/cm  
100 nm/s  
Linewidth: 4 px  
520 px/s

## Writing Simple Patterns

Simple shapes can be selected in the Litho Pattern tab and written with just one or two clicks.

In the Script Menu tab, geometric patterns can also be called, with editable parameters, such as dimensions and angles. Here, alignment to the lattice can be turned on and off as required.

Current, voltage and electron dose parameters are selected in the Litho Settings tab. Preset groups of parameters giving different linewidths can be saved, and quickly selected.



## Precise Tip Positioning and Motion

Unlike commercial STM systems designed for imaging, in ZyVector we wish to have the tip move arbitrarily across the surface with atomic precision. Therefore we must achieve real-time accuracy and precision in the tip position, so that STM images are undistorted, and lithography vectors follow their desired path.

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### Piezo Creep Correction

Piezoelectric elements used in commercial STM systems suffer from time-dependent errors called creep. In typical commercial STM control systems, this creep goes uncorrected, because for typically imaging tasks, a distorted image is good enough. The offset between the forward and backward scan while imaging is also due to creep.

In ZyVector, we correct these creep errors in real time. First, the creep characteristics of each piezo scanner must be calibrated.

A large jump is made, and then the tip scans a single linescan repeatedly. As the tip position creeps, the position of the dimer rows drifts, in a curve. The curvature of the dimer rows is parameterized, and used to correct the motion of the piezo scanner.

### Distortion-Free Imaging

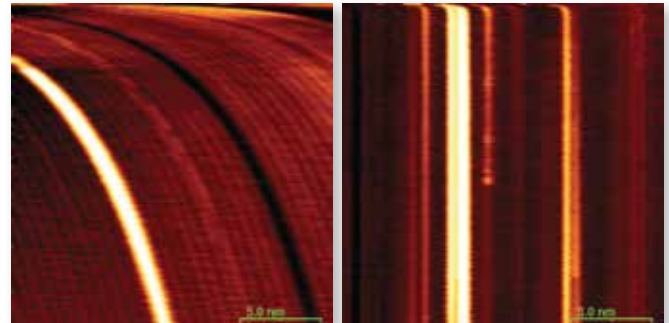
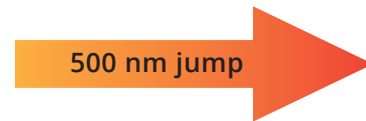
Creep also occurs on a millisecond timescale, and causes an offset between the forward and backward scans. This means that the tip is never really where it appears to be. With creep correction applied, the forward and backward scans overlap exactly, making precise tip positioning over a dimer row or other feature possible.

### The effect of Creep on Lithography Precision

We use test lithography patterns to measure the effectiveness of the creep correction. The test pattern shown is a set of concentric boxes, which is defined using two bitmaps, one for the left half of the pattern, and one for the right half.

Without creep correction, the rectangles are not concentric, are not square, and the pairs of lines are not adjacent. There is also an offset between the two half patterns.

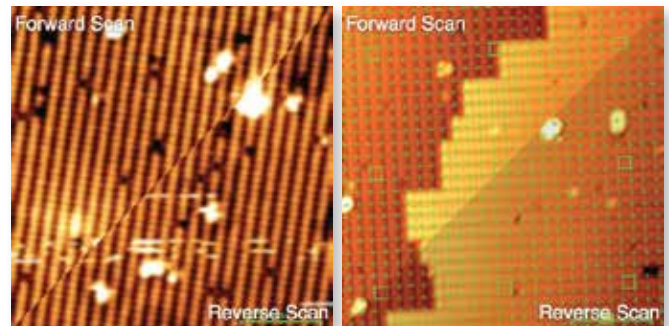
By running this and other test patterns, repeated many times, we can obtain quantitative data for the precision of the motion. The table shown below gives the precision of the tip motion for two different systems, after 10 repetitions of the test patterns.



First 200 s after 500 nm jump

Uncorrected creep

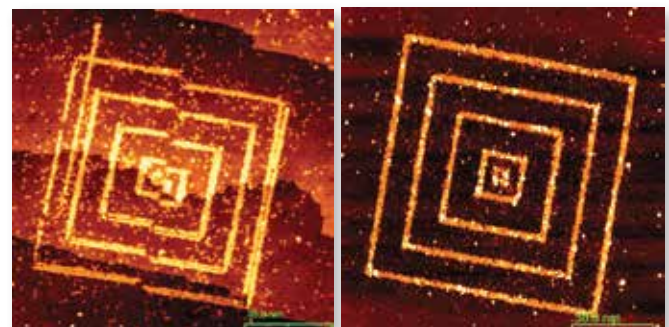
Creep Corrected



Distortion-free Imaging

Creep Correction Off

Creep Correction On



Lithography Test Pattern

Creep Correction Off

Creep Correction On

## Built-In Metrology

Unlike conventional optical or e-beam lithography, the surface can be imaged in the STM without affecting the resist layer, and using the same probe as used for writing. This allows for pattern alignment

Hydrogen removal occurs during exposure at positive sample bias, with the tip moving very slowly across the surface. During imaging, the STM tip is set to negative sample bias, and moves much faster across the surface, so that the Si-H bonds are not affected.

Thus the surface can be imaged prior to writing, allowing alignment of the write vectors to the atomic lattice of the surface, and alignment to fiducial marks or to areas of previous patterning, for stitching between write fields.

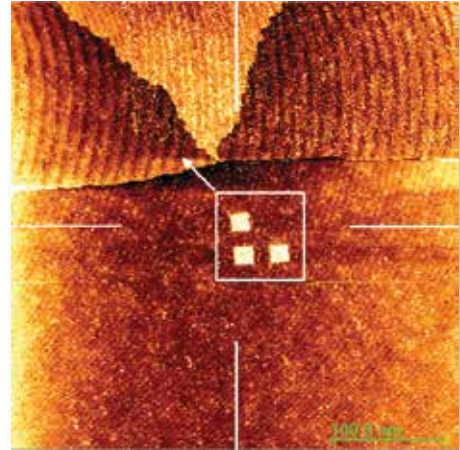
By imaging the pattern after writing, the quality of the lithography can be checked, enabling some error correction, and as the actual written pattern including any errors can be imaged with atomic precision, the actual dimensions of developed nanostructures can be referred back to the original pattern.

### Automated Fiducial Mark Alignment

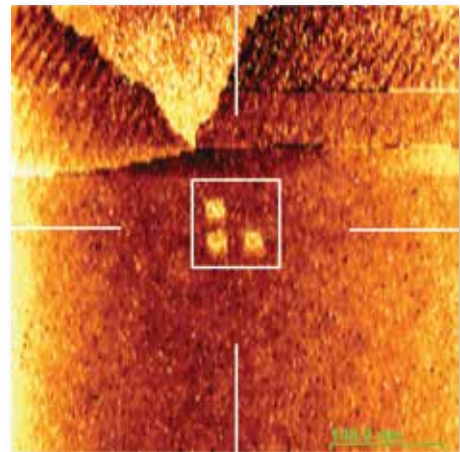
Over larger distances, effects such as hysteresis, thermal drift and uncorrected creep can still cause errors in the tip position.

In particular, hysteresis errors increase quadratically with jump size. For a movement of several  $\mu\text{m}$ , the hysteresis errors can be hundreds of nm.

Therefore, Scanz has the capability to search for, identify, and automatically align to fiducial marks on the surface, so that accumulated position errors can be zeroed. A fiducial realignment step can be included in a larger script, so that operator intervention is not required.



*A fiducial mark is located, by comparison to a previous image of the mark taken after writing.*



*The scan centre is relocated to the fiducial mark, even using low resolution, fast imaging.*

### Summary of Lithography Test Data

	System 1	System 2
CD control	0.1 nm $\pm$ 0.74 nm	1.7 nm $\pm$ 0.38 nm
Positioning	-0.22 nm $\pm$ 1.18 nm	1.9 nm $\pm$ 2.39 nm
Stitching	0.43 nm $\pm$ 0.61 nm	0.25 nm $\pm$ 0.48 nm

# Automation and Scripting

The ZyVector software, Scanz, enables automation and user scripting of almost every part of the software, including imaging, movement across the surface, and writing.

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The simplest form of automation is the queuing of commands in the user interface. A series of actions can be queued up, and are shown in the Info Panel at the bottom of the Scanz window. Individual items can be cancelled with the 'x' button, or the whole queue is cancelled with the Cancel action button.

To extend the capabilities of ZyVector, users can write their own scripts, typically in a text editor outside Scanz, and then uploaded to the software.

Scripts for ZyVector are written in a Python-based script language and can be a simple list of commands all the way to a complex set of instructions describing all the moving, imaging, writing, and other tasks required for generating a pattern for a whole device.

Many built-in scripts are provided, to perform tasks such as calibration of the default lattice parameter, determination of lithography parameters, writing simple shapes, etc.

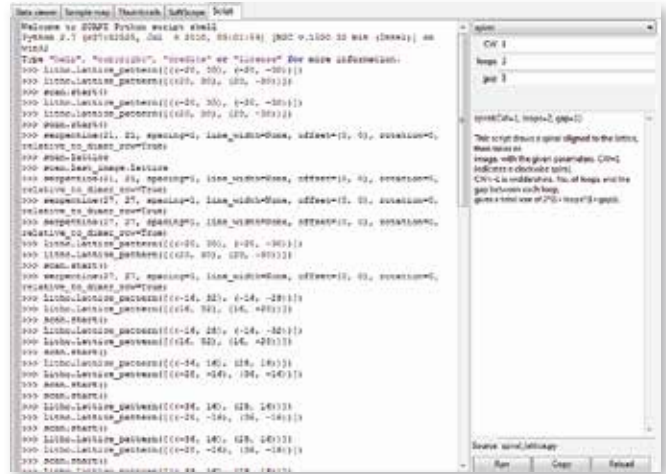
The Script view tab provides both a command line interface to commands and scripts, and also a Script Menu to provide a GUI to easily find and run scripts. Many scripts have various input parameters, such as dimensions, rotation angles, etc. and the Script Menu tab provides a convenient way to edit the desired values for these parameters.

## Bitmap Input

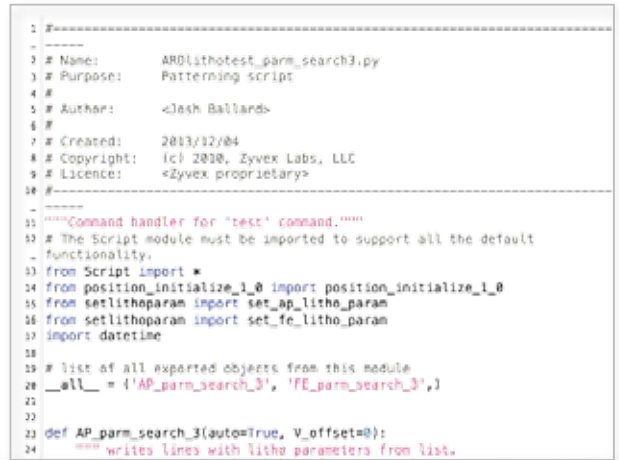
Any arbitrary pattern can be input as a black and white bitmap. The white pixels will be written with one bitmap pixel corresponding to the standard 0.768 nm lithography pixel.

The Multimode\_VectorGen script parses the bitmap, producing a list of tip vectors organized in the order of writing. For large patterns, both AP mode and FE mode vectors are used to achieve an optimal write time. The edges are written using AP to achieve atomic precision. The larger patterns are filled in quickly with FE mode vectors. The pattern can then be written.

All of these standalone methods for writing patterns can also be incorporated into a script. Thus ZyVector is capable of very sophisticated automated patterning tasks.



The Script tab, showing the command line interface, and the script menu panel.



A ZyVector script



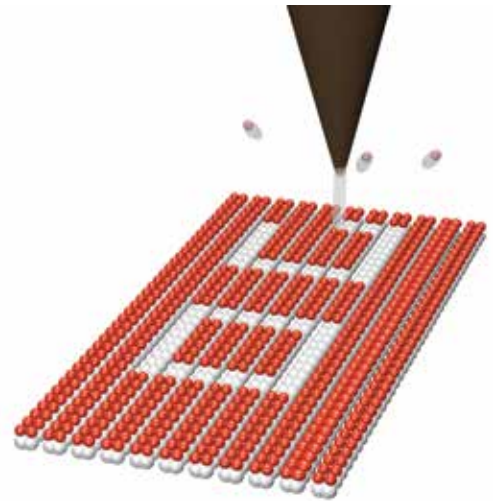
Queued actions in the Info panel



ZyVector has great flexibility in the methods for pattern definition; either as geometric shapes, or as arbitrary bitmaps. There is a special script, Multimode\_VectorGen, which reads bitmaps and writes them out as patterns.



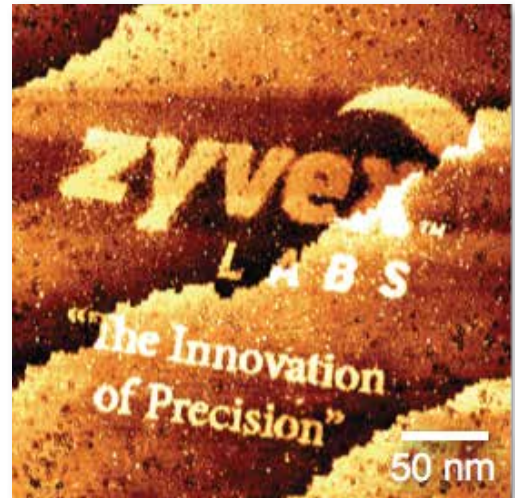
1. Pattern File comprises black-and-white bitmap input file.



3. STM tip moves along the write vectors removing H atoms.



2. ZyVector converts the pattern file into write vectors, following the Si(001) lattice.



4. The final atomic-resolution pattern of exposed Si dangling bonds.

# Scanz User Interface

The Scanz software that controls ZyVector provides the fundamental functionality for STM imaging, but its true strength lies in the ability to automate almost all aspects of operation in order to perform atomically precise lithography most efficiently.

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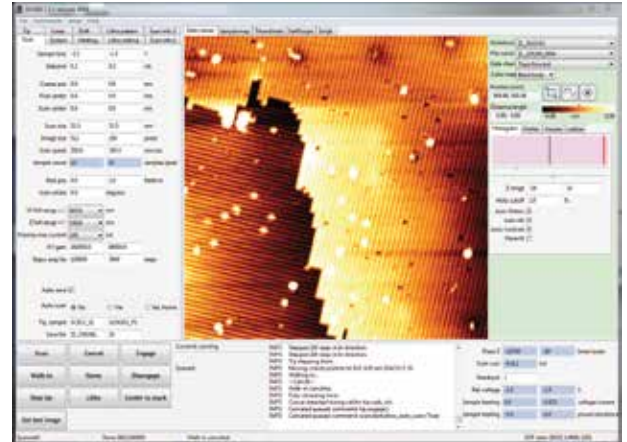
Scanz is contained within a single window - to the left are the Control Panels where settings are changed, and to the right are the View tabs, where STM images are viewed, and analysed, and from where scripts can be run.

## Control Panel Tabs

For routine imaging, the user will mostly make use of the Scan Tab, allowing for movement across the surface in x and y, settings for scanning such as image size and pixel resolution, and scan speed. The feedback control loop sensitivity is also set here.

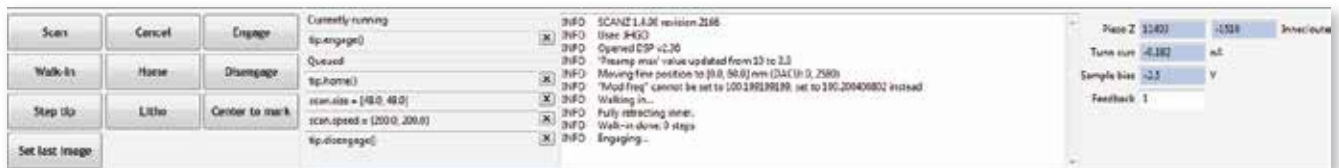
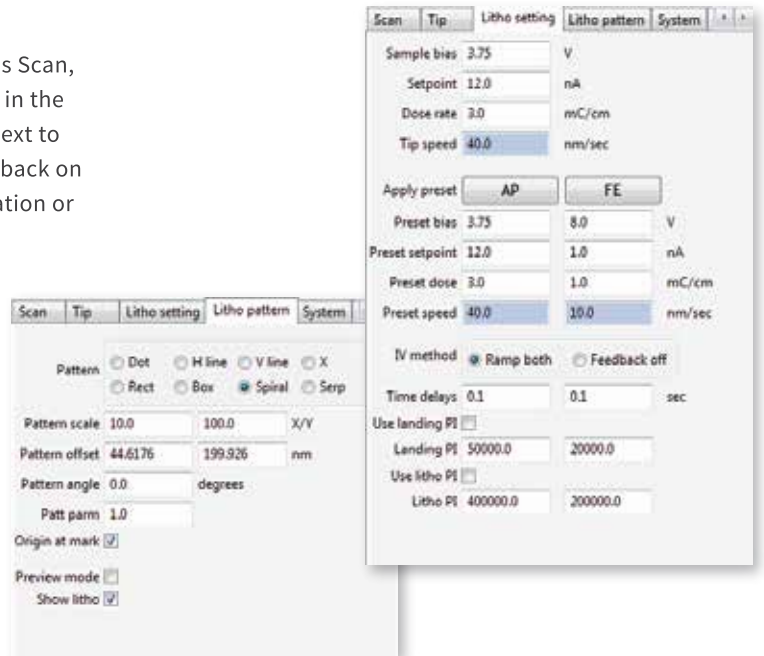
Simple lithography tasks can be set up in the Litho tabs, one of which allows the user to set up voltage, current and electron dose settings for performing lithography, and another has a menu of shapes to be written.

Below the Control Panels, are the Action Buttons, such as Scan, Litho and Cancel. Actions which are pending will appear in the Queue, from where they can be cancelled individually. Next to the Queue is the Information Panel, which provides feedback on the status, such as movements across the surface, activation or completion of commands etc.



The ZyVector software, Scanz, showing the main Scan control tab and the Data Viewer tab.

The Litho Settings and Pattern tabs, for performing simple STM lithography.



The Action Buttons, Queue and Information Panel



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## Technical Specifications:

### ZyVector Hardware Controller

Provides:

- 4 fine x/y channels ( $\pm 135$  V)
- 1 fine z channel ( $\pm 135$  V)
- 3 coarse xyz channels ( $\pm 200$  V)
- 1 tip bias channel ( $\pm 10$  V)
- Pre-amp gain control, for Omicron preamp
- Pre-amp bias range control for Omicron preamp amplified current input
- Fits Omicron VT STM preamp and PIC cabling.

### 20-bit Digital Control Box

Provides real-time control of the tunneling feedback loop, and voltage control for creep-corrected motion across the surface.

### Scanning

- xy ranges depend on nm/V calibration.
- For Omicron VT system: 9500 nm.
- Z-range 1.3  $\mu$ m
- Minimum scan bit size: 10 pm.
- Minimum vertical bit size: 1 pm.
- Fast scan direction arbitrarily defined between 0-359.9° relative to piezo tube axes.

### Advanced Position Controls

- Local piezo tube calibration based on lattice recognition, including determination of lattice angle relative to piezo tube axes.
- Lattice phase recognition for precise lithography positioning.
- Linear creep correction in xy
- Initial optimization of creep over central portion of scan range. (Fine optimization by user required periodically.)

### Hydrogen Depassivation Lithography (HDL)

Two spot size modes available

- AP mode ( single-dimer-row line width)
- FE mode ( wide line width, rough edges)

### Advanced Scripting Capabilities

- We provide scripts based on Python for test HDL patterns, creep correction calibration, lithography parameter calibration, etc.
- User-written scripts can be easily incorporated and run using command line interface or drop-down menu.