# Scalable Atomically Precise Manufacturing

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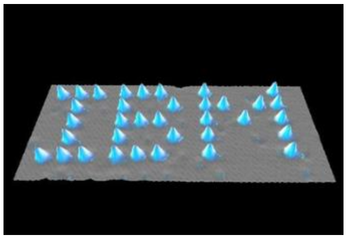
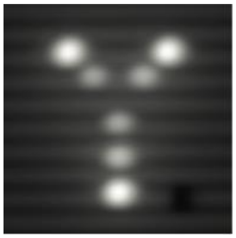
It was in 1989 that Don Eigler at IBM's Almaden Research Center showed how to use a Scanning Probe Microscope (SPM) to position individual atoms. He demonstrated the technique by spelling out "IBM" using 35 Xenon atoms. IBM at the time predicted that the technique might one day be used to build atom-scale transistors that would be faster than what was available then. That singular accomplishment took almost a whole day to position the atoms and the result, remarkable as it was, was stable only at extreme cryogenic temperatures. It set in motion several decades of work aimed at developing atomically precise manufacturing methods. Now, over 30 years later, QSi is leading the world in developing and using atomically precise manufacturing to create electronics that use no transistors, are far faster than their transistor-based equivalent, and consume orders of magnitude less energy.



*35-atom IBM - 1989*

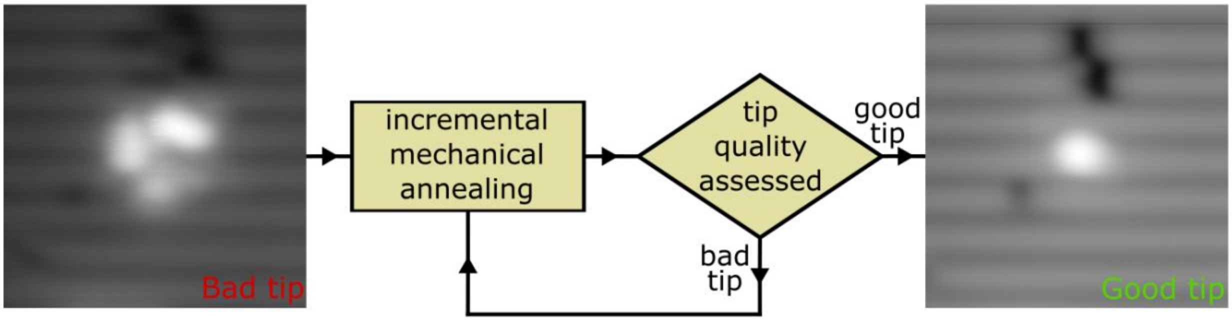
*QSi's 32-atom maple leaf - 2017*



*QSi's atomic OR gate - 2018*

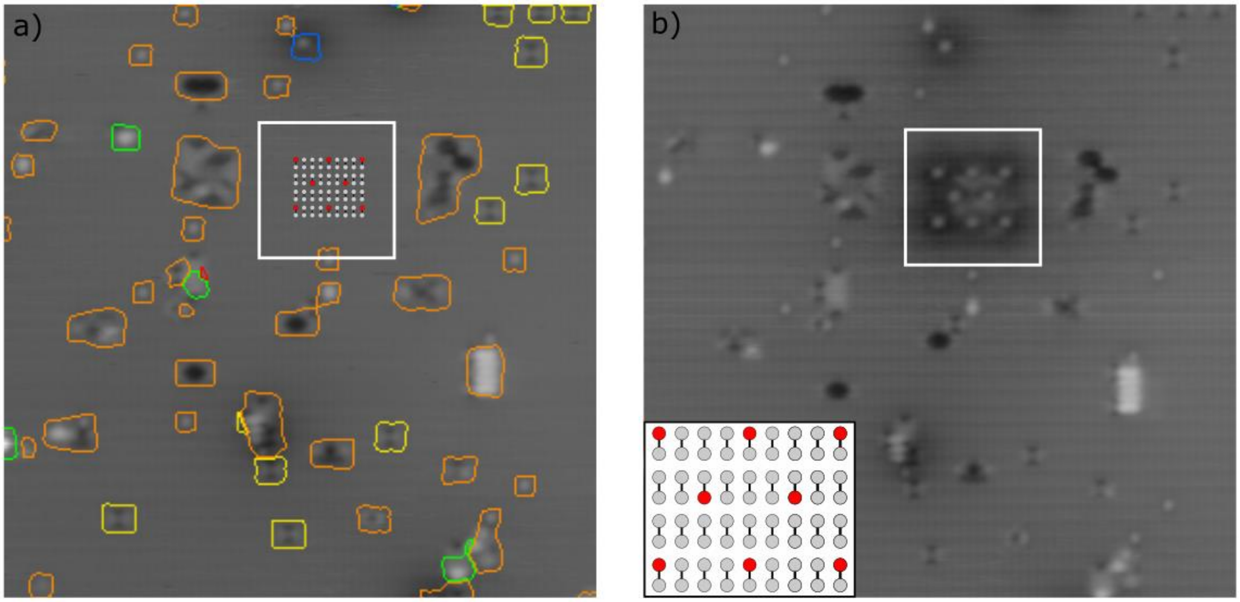
Capable of addressing structures with single atom precision, QSi uses SPMs with our proprietary single-atom tip for atomically precise hydrogen lithography – removal, replacement, and modification of single atoms within more complex systems. Despite the remarkable abilities of SPM systems in fabricating single atom devices, until now the standard fabrication process has remained relatively slow, requiring extensive intervention from highly skilled users. QSi has developed and applied machine learning techniques to automate the process. We use these techniques to enable automated probe tip conditioning, automated substrate defect classification, and automated error correction.

**Automated Probe Conditioning**: When fabricating atomic scale devices, it is necessary to ensure that the probe tip remain atomically sharp during the fabrication process. It is possible however for the probe tip to become dull and require a mechanical annealing step to return it to a desirable shape. Previously, this step required extensive interaction by the probe operator to recover the tip. Now, by using machine vision, we have replaced the operator with a machine learning algorithm that continually checks the condition of the probe and identifies when the probe tip is not atomically sharp and requires mechanical annealing. The algorithm monitors the annealing process, and continually checks the state of the probe. Annealing continues in this fashion until the tip is returned to an optimal condition as detected by the machine learning algorithm and the tip-based manufacturing continues.



*Automated Probe Tip Conditioning. The probe tip is observed in a "bad" tip state by the machine learning algorithm. Incremental mechanical annealing is executed autonomously until the tip is in a "good" tip state as indicated by the sharp, symmetric shape of the bright feature in the image.*

**Automated Defect Detection**: The fabrication of atomic logic devices using hydrogen lithography is a relatively simple process in which bias pulses from the probe tip selectively remove hydrogen from the surface. Automating this process is complicated by the need to identify and distinguish defects on the silicon substrate. These defects not only affect the ability to fabricate the logic devices, they also interfere with the operation of the devices. Unfortunately, these defects are a common part of the substrate used. The concentration of these defects can be reduced by optimizing substrate preparation techniques, but it is impossible to remove them completely. By using machine vision and semantic segmentation, we use a machine learning algorithm to identify the types and locations of defects on the surface, thus removing the need for a human user to manually prescreen the substrate for unwanted defects.

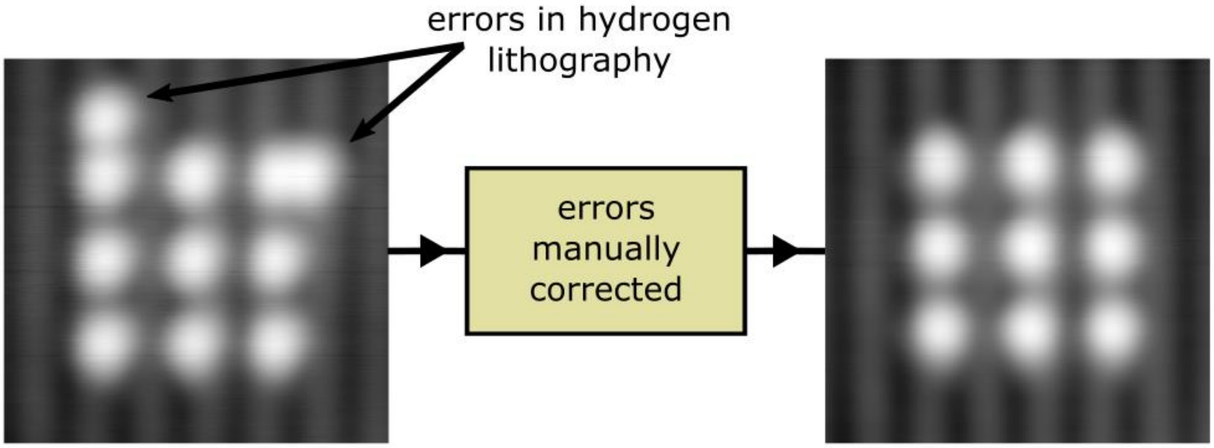


*Automated Defect Segmentation and Device Fabrication. The machine learning algorithm can locate and distinguish between defects found on the surface. The different colours represent different types of defects. Given a predefined atomic scale device pattern, the most viable area on the surface away from unwanted defects is determined. The probe tip then executes an automated fabrication procedure until patterning is complete.*

Combining automated probe tip conditioning and defect classification has resulted in a fully autonomous atom scale fabrication system. Given a predefined atomic scale device design, the SPM can fabricate it with no additional user interaction. The software will first ensure the tip is in a good fabricating condition and correct it if not. Then, the substrate is scanned for nearby defects. When a viable area of the substrate that will support the desired pattern is found, the SPM begins fabricating the components via hydrogen lithography with atomic precision. Fabrication then continues until the entire pattern is completed with the option for additional tip conditioning if needed.

**Automated Error Detection and Correction**: While most atomic logic devices are fabricated without any errors, it is still possible that some errors may occur during hydrogen lithography. Fabrication errors during hydrogen lithography are generally caused by two main factors. The first is unwanted probe tip changes during bias pulsing. The second is drift in the motors used to control the position of the tip. The first cannot be prevented and depends on the random motion of the atoms that make up the probe. But as discussed above, it is now routine to fix the probe tip if it is damaged during the fabrication process and correct any mistakes made in fabrication.

These errors take the form of a misplaced logic component and require selective hydrogen repassivation. We have developed several techniques for error correction that use either the probe tip or ambient hydrogen molecules. In the first, the scanning probe tip can be functionalized with additional hydrogen from the substrate. The tip is then brought within atomic distance of the error allowing a hydrogen from the tip to selectively bond to the substrate, erasing the error. The second method requires less involvement from the tip and takes advantage of a unique reaction specific to our surface. Removing another hydrogen right next to an error creates a chemically reactive site that will spontaneously react to ambient molecular hydrogen in the SPM system, erasing the error. This second method has proven very useful since the erasure does not require any additional time to functionalize and position the tip for hydrogen transfer, and the rate at which molecular hydrogen reacts with the surface can be almost instantaneous by adjusting the background concentration in the SPM system.



*Error Correction Using Hydrogen Repassivation. Two errors emerged during patterning in the form of incorrectly removed hydrogen atoms. Once the errors are identified, a user can manually remove the mistakes leaving the desired pattern.*

Moving the probe is controlled by a piezo electric motor. When scanning across the substrate, the piezo motors instill a slight delay in the motion of the tip, meaning that once the tip has been moved to a certain area, the piezo motors will continue to “creep” across the substrate in correlation to the probe’s previous velocity. We are developing a creep-free piezo motor to position our tips, but until that project is complete, we will continue to use reinforcement learning to learn and apply a creep correction factor. In this way, any errors in fabrication due to unwanted probe tip motion are eliminated, thus reducing the number of errors in need of correction.

**Atomic Scale Design Tools**: With the fully automated error correction procedures incorporated, the automated fabrication system will be capable of completely user-free fabrication. We continue to develop refinements to the fabrication system to further automate circuit design and fabrication. We have developed a unique design tool which we call SiQAD. It makes possible a thorough exploration of device configurations with a multitude of functionalities and applications. By using reinforcement learning, these potential new designs can be explored much more quickly and with much more rigor than could be done in person, enabling the continued refinement and improved operation of QSi's atomic silicon devices. This automated circuit design will also be coupled to the defect identification algorithms which will be used to ensure that device operation is consistent across different areas of the surface which may have different concentrations and types of defects.

Overall, the application of machine learning to the automated fabrication of atomic silicon devices has resulted in huge improvements in the overall fabrication time due primarily to the major reduction in needed user interaction with the SPM. Probe tip conditioning and defect identification for atomic device fabrication have resulted in marked advancement through the incorporation of machine vision. We are continually improving these processes with the inclusion of reinforcement learning. In both the probe tip conditioning and the hydrogen lithography, probe parameters are incrementally increased until the desired event, either a good tip state or a successful hydrogen lithography event is observed. By using reinforcement learning, it will allow an agent to learn a more ideal action path resulting in either event occurring more quickly, eliminating the need to change parameters incrementally, again increasing the overall fabrication speed.

A combination of machine learning tools already incorporated as well as some still in development will rapidly increase the throughput of device fabrication. A fully automated system will require very little to no user interaction allowing for the parallelization of many probes. Through this parallelization, the device throughput will drastically improve allowing a framework to produce enough components for commercially viable devices.

For more information, please contact

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