U.S. DEPARTMENT OF
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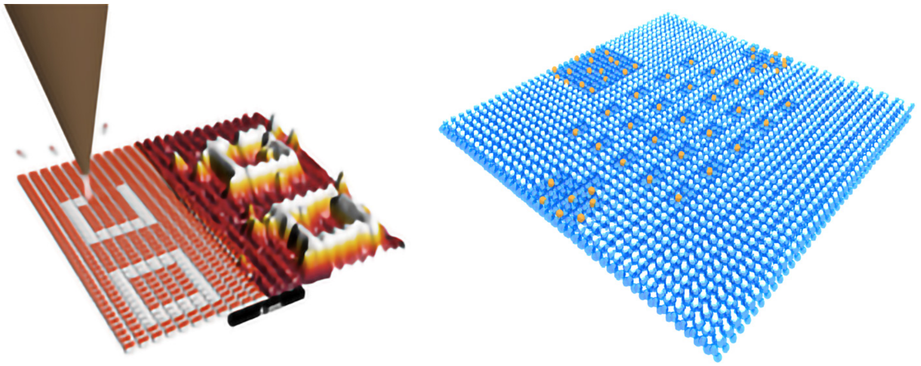
Automated Manufacturing of 2D Atomically Precise and Robust Devices in Silicon Substrates



This project will develop a technology to prepare a crystalline surface so that a scanning tunneling microscope (STM) tip can remove hydrogen atoms from a silicon surface (to make the site reactive) (left diagram) and replace them with dopants. The goal is to develop a first-of-a-kind automated and programmable hydrogen depassivation system—a key step toward fabricating semiconductors with an atomically precise array of individual dopant atoms (right, shown in yellow) in silicon.

Graphic image courtesy of Zyvex Labs

Atomically precise manufacturing (APM) is an emerging disruptive technology that could dramatically reduce energy use and increase performance of materials, structures, devices, and finished goods.

Using APM, every atom is at its specified location relative to the other atoms—there are no defects, missing atoms, extra atoms, or incorrect (impurity) atoms. Like other disruptive technologies, APM will first be commercialized in early premium markets, such as nanoelectronics for quantum computing.

Atomically precise nanoelectronics, a type of APM where atomically precise (AP) features and devices are made at the tiniest scale, is urgently needed so devices such as transistors are smaller and have higher performance. APM is vital for pursuing next-generation technologies as today's electronics industry approaches the limits of Moore's law, the anticipated increase in the density of electronic devices.

This project aims to develop an automated manufacturing process to precisely place individual atoms (known as dopants) to make semiconductors in a two-dimensional (2D) matrix material, typically silicon. The current industrial state-of-the-art for dopant placement—a key step in microchip fabrication—is ion implantation, a method that accelerates dopant atoms into a solid material. The placement accuracy resolution of ion implantation is more than an order of magnitude larger (10 nanometers (nm)) than the atomic spacing (0.23-0.54 nm for various silicone lattices). Thus, ion implantation-based devices are far from atomically precise despite their widespread use in the microelectronics industry.

This project aims to achieve positional control of the dopant atoms to a much higher precision (±0.3 nm), building on recent advances in scanning tunneling microscope (STM) control. However, even the most cutting edge STM-based technique—hydrogen depassivation lithography (HDL)—is far from being a viable manufacturing technology because it is slow, imprecise, and currently only works with phosphorus dopants. Another project is enabling faster, more precise dopant arrays using STMs. This project will develop an automated surface preparation process that works with upgraded STM arrays and allows new dopant atoms, such as boron and aluminum.

Automating and expanding use of HDL would enable the design of materials with tailored electronic and optical characteristics needed for next generation electronics. Eventually, these manufacturing techniques could be used to fabricate materials with physical properties unachievable with existing state-of-the-art manufacturing processes. This project will identify and engineer specific dopants that are needed to realize these material properties and enable the required precision of their placement.

Benefits for Our Industry and Our Nation

Assembly techniques capable of automated sub-atomic-spacing precision will accelerate the development of tools and processes for manufacturing defect-free materials and products that offer new functional qualities and ultra-high performance capabilities—with the potential to dramatically reduce use of energy and materials. These technologies could enable electronic and material properties that are otherwise unobtainable. After an initial focus on early premium markets, these enhanced properties could be vital to national security applications and a broad range of other technologies.

Applications in Our Nation's Industry

AP 2D-designed materials have potential applications in several areas, including nanoelectronics (atomic-scale computer circuits), high-sensitivity sensors, low-noise bipolar analog devices, quantum devices, optical devices, and artificial enzyme-like industrial catalysts. In the longer term, AP materials created through various methods of APM have the potential to revolutionize materials science, providing materials with designed-in specific strength, toughness, or wear resistance, enabling complex and highly reliable systems.

Project Description

The project objective is to develop an automated and programmable method to fabricate 2D semiconductor devices by AP placement of a variety of dopant atoms in a single plane of silicon. Additional surface treatment technologies (molecular beam epitaxy (MBE) encapsulation) will also be developed to ensure these AP solid-state devices are robust, stable, and maintain unique characteristics. These fabricated devices, in turn, will be measured and characterized to determine the impact of atomic precision placement of dopants on the resulting device's material properties.

Placement errors and other imprecisions are known to degrade semiconductor properties. The AP devices being developed are expected to show greater functionality due to a higher level of precision than has been previously achieved. Such materials will have unique and desirable electronic and physical properties. The target level of accuracy in dopant placement will be an orders-of-magnitude improvement over the state-of-the-art. The new technology will also allow much higher doping levels than existing ion implantation techniques. New selective chemistries will be explored to enable the doping of other atoms besides phosphorus, such as aluminum and boron, which will enable PN junctions and much higher energy barriers within devices with no material interfaces.

Barriers

- Achieving ultra-high precision (~0.3 nm) and consistency in the placement of dopants
- Avoiding dopant migration during subsequent processing steps after initial placement
- Successful use of high-quality, low-temperature crystal growth (known as epitaxy) to improve dopant stability

Pathways

STM-based HDL and MBE will be used to fabricate novel nanoelectronics devices, which will be characterized and tested to determine the impact of automated atomic positioning, precision dopant placement, and dopant type on resulting material behavior.

To accomplish this, the first project pathway is to produce a quantum tunnel junction transistor or other device geometry reliably. This device will be used to measure the impact of placing dopant atoms with atomic precision. Improved STMs developed in other projects will be used to prepare the surface of the silicon crystal to accept dopants and provide greater control of dopant placement. Process improvements are expected to: 1) produce the most accurate patterns possible, 2) establish a process for fabrication of an exemplary metrological device for measuring voltage differences, and 3) advance simulation tools.

The second project pathway will identify potential alternative dopants. New selective chemistries developed in this pathway will broaden the range of dopants that can be incorporated into the prepared silicon surface. Research will focus on dopants near phosphorus on the periodic table, such as aluminum and boron, that enable PN junctions. These dopants will be made available to the surface as triethyl aluminum, alanes, and diborane. This pathway will aid understanding of the impact of different dopant atoms in a simple device and enable the development of simulation and design rules for the automated fabrication of complex 2D materials and devices.

Milestones

This three-year project began in 2018.

- Fabricate a model device to enable measurement of the effect of a single dopant atom; down select novel dopant chemistries that enable placement of new dopants (completed)
- Validate capability to place dopants with atomic precision in a crystal; characterize bulk layers for each novel chemical species (2020)
- Fabricate and test 2D designer materials made with two different species and deliver design rules for each dopant (2021)

Technology Transition

By the end of this project, researchers anticipate creating 2D AP structures. Subsequent efforts to move this technology into the marketplace will focus on advancing patterning tools, such as the ZyVector STM lithography control system, which was developed by Zyvex Labs under a previous government program. Eventually, Zyvex Labs expects to create a turnkey nanofabrication tool for the research market, likely in collaboration with its current distribution partners. Zyvex may also become a foundry for these innovative 2D-designed devices.

Project Partners

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