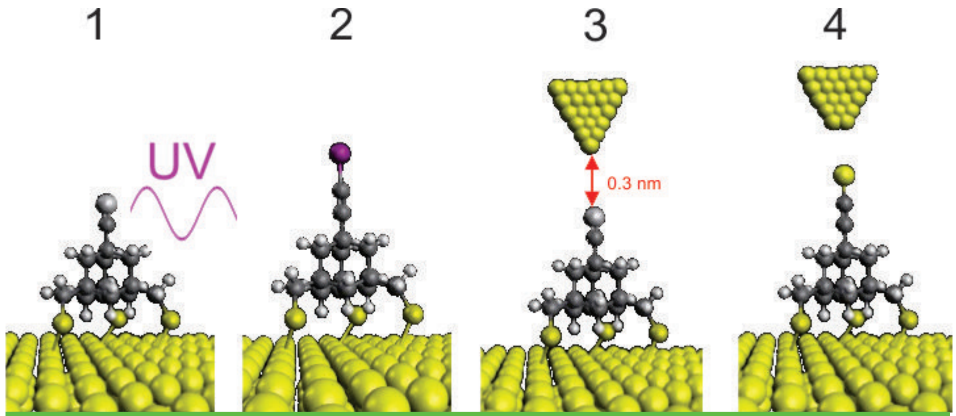
U.S. DEPARTMENT OF ENERGY

Office of ENERGY EFFICIENCY & RENEWABLE ENERGY

A Radical Tool for 3D Atomically Precise Sculpting

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.



Graphic shows the proposed mechanochemical reaction in which a highly reactive radical atom tool is used to remove an atom from the apex of a silicon scanning probe microscopy (SPM) tip (gold atoms on top). Irradiation of a surface-bound molecule with ultraviolet light (1) forms an atomic radical (purple) (2). As the SPM tip approaches the reactive molecule within a few tenths of a nanometer (3), the reactive molecule forms a chemical bond with an atom on the SPM tip and pulls it off (4). *Graphic image courtesy of University of California at Los Angeles.*

The ambitious goal of this project is to mechanosynthesize structures in three dimensions (3D) for the first time. Mechanosynthesis is a radically different manufacturing approach where atomically perfect structures are created (synthesized) by directly moving atoms (mechanically). To control chemical reactions, precision movement in 3D must be controlled in tenths of a nanometer. To date, mechanosynthetic techniques have only been used to make two-dimensional (2D) structures.

In this project, a molecular tool is created that has a highly reactive (radical) atom at its tip. This tool is moved like a lathe, but rather than machining or cutting, it gently transfers atoms sequentially in 3D through a combination of mechanics and special chemistry. The tool is used to pull defect atoms from molecules on the tip of an externally controlled scanning probe microscope (SPM). The structure is being sculpted to make an atomically sharp tip for the SPM, an atomic-scale imaging tool. At each stage of the process, the SPM tip can be used in imaging mode to help detect and remove defects. Unlike a sculpting knife, during this type of mechanosynthesis, the tool is stationary and the SPM tip being sculpted moves in 3D with a precision measured in tenths of a nanometer. This project aims to develop a reproducible proof-of-principle mechanosynthetic approach for fabricating atomically precise SPM tips that is ultimately extendable to making surface bound nano-products. This type of APM method has the potential to become a disruptive technology that is applicable to a broad range of products.

The best SPM tip materials are those that already are close to being atomically precise, such as crystalline materials. The best materials for the molecular sculpting tool are high-energy, reactive atoms on designer molecules that can pull atoms from the lattice of the single crystal SPM tip. Appropriate materials will be designed by a computer and then synthesized. Computational modeling is used to guide the precise trajectory required for the molecules of the SPM tip to approach the reactive molecular tool. The tool will remove defect atoms and the process is repeated until the target structure is created.

Benefits for Our Industry and Our Nation

Assembly techniques capable of atomic-level precision, such as 3D mechanosynthesis, will accelerate the development of tools and processes for manufacturing defect-free materials and products that offer new functional qualities and ultra-high performance—with the potential to dramatically reduce the use of energy and materials. Such potentially groundbreaking technologies could also enable electronic and material properties that are otherwise unobtainable. These enhanced properties could benefit a broad range of applications after entering early premium markets.

Applications in Our Nation's Industry

Some of the most promising applications of atomically precise technology include clean energy, water purification, next-generation computing and data storage, and cybersecurity. Applications with high potential for scaling-up commercial use in the near-term include catalysts with specific structures for a desired catalytic activity, membranes with greater selectivity and durability, and sensors to detect the presence of chemical and biological trace molecules. These products are expected to include new mechanical, photonic, electronic, quantum, and sensory capabilities as well as other enhanced properties.

Project Description

This project aims to demonstrate the use of mechanosynthesis to produce an atomically precise SPM tip by sequentially removing defect atoms via externally controlled 3D movement of the tip around a molecular tool anchored on a surface. First, specific identified reactants will be designed, synthesized, and utilized to control and selectively extract atoms from the SPM tip, re-shaping it to a predefined crystalline form. If proven, radical tool chemistry with atomically precise (picometer) control of SPM tip's movement will enable the fabrication of other atomically precise 3D structures on surfaces with designer functionality guided by computer simulation. Since lack of atomically precise SPM tips is a challenge for many APM processes, tips produced in this project would also be an important enabling technology for more widespread use of APM.

Barriers

- Identifying tip materials of sufficient hardness and standardized surface chemistry for strongly reactant molecules for the tool
- Demonstrating a low-temperature SPM with simultaneous scanning tunneling microscope (STM) and frequency-modulation atomic force microscopy (AFM) imaging capabilities
- Developing a chemical synthesis route for the reactant precursor materials and scaling their production, first on the microscale and eventually in gram quantities
- Demonstrating and characterizing single atom transfer
- Sequentially removing several atoms from the SPM tip

Pathways

Today, scientists use SPMs to positionally assemble novel, laboratory-scale, atomically precise structures only in 2D. In this work, major challenges include the inability to make atomically precise microscope tips, tip crashes, thermal drift, achieving positional repeatability, and the need for tenths of a nanometer accuracy. To overcome these challenges, a synergy of computational design modeling efforts, advanced instrument and method development, as well as validated experimental implementation of SPM-based atomic manipulation will be leveraged throughout this project. The project is organized into three highly integrated and collaborative pathway areas: 1) computational modeling and simulation to better understand both tip and surface chemistry to produce surface-bound reactants for atomic abstraction; 2) instrument and method development to enable enhanced accuracy in tip positioning and throughput; and 3) proof-of-concept experimental implementation of SPM-based atomic manipulation.

Milestones

This two-year project began in July 2018:

- Achieve formation of activated, surface-bound reactants by SPM (2019)
- Demonstrate ability to use the selected reactant as a probe to image the SPM tip (2020)
- Successful removal of atoms from the tip through reactant-driven abstraction (2020)

Technology Transition

After successful demonstration of the tip-based atom removal process, the eventual goal is to develop atomically precise assembly systems with multiple tips operating in parallel at the physical limits of atomic and nanoscale fabrication and measurements. In the short term, this project will enable the SPM scientific community to work with tips of known structure. In the medium term, the developed technology can enable the manufacture of 3D structures using known tips as well as have groundbreaking applications in metrology applicable to energy technologies.
If these technical approaches are successfully developed further, they could eventually lead to very fast assembly systems with multiple tips focusing on covalently bonded structures, which could broaden the commercial application of APM.

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