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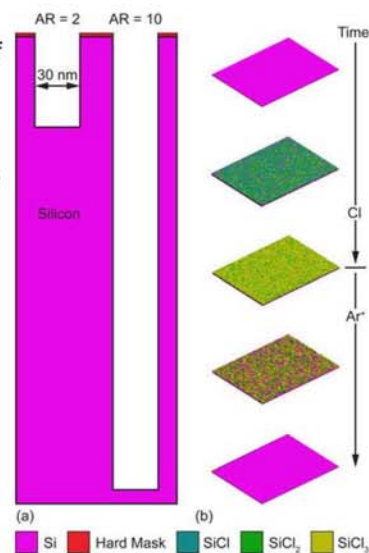
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Computational Models Show Paths to More Efficient Atomic Layer Etching

[Atomic layer etching of 3D structures in silicon: Self-limiting and nonideal reactions](#) C.M. Huard, Y. Zhang, S. Sriraman, A. Peterson, K.J. Kanarik and M.J. Kushner [Journal of Vacuum Science and Technology A, Vol. 35, No. 3 \(May/June 2017\)](#)

Imagine drilling an oil well and having to stop the drill-bit with a precision of a single grain of sand. Manufacturers of microelectronics devices face such a challenge when carving out the tiny, deep and narrow features that serve as transistors in state-of-the-art microprocessors. In this case, however, they must stop with a resolution of a single atom.

To meet this challenge, manufacturers are increasingly turning to atomic layer plasma etching (ALE), an anisotropic fabrication process where material is added and removed from a substrate in the vertical direction rather than horizontal to create small features with atomic-level resolution. Now, researchers at the University of Michigan and California's Lam Research Corp. have developed computational models that enable them to predict how sensitive ALE is to non-ideal conditions and suggest strategies that will optimize the process, even in those situations.



The researchers detail their work in a recent issue of the *Journal of Vacuum Science and Technology A (JVST A)*.

Conventional plasma etching will remove materials from a silicon wafer as long as power is applied to the plasma, so it is difficult to stop etching in one region of a feature under construction while continuing in another. ALE solves this problem by separating the process into two parts. First, a passivation step where radical atoms (such as chlorine) coat the top layer of silicon atoms on a substrate followed by an etching step where the passivated silicon atoms are removed by ions (such as argon) having precisely controlled energies. These "self-limited" steps will naturally stop after a single layer of atoms has been etched and not affect other portions of the feature already fabricated.

"ALE enables extremely clean and sharp etching that is nearly independent of the feature's geometry and will stop when only the desired material is removed," said Mark J. Kushner, a professor of electrical and computer engineering at the University of Michigan and corresponding author on the *JVST A* paper.

In ideal conditions, Kushner said, passivation and etching would be totally distinct, so that the chlorine atoms and argon ions are not striking the wafer at the same time.

"If the passivation and etching steps are not decoupled, continuous etching can occur," he explains. "In continuous etching, it is very difficult to control the fluxes of both radicals to the wafer with enough precision to remove only a single layer of atoms."

To better understand the nature of non-ideal conditions and devise ways to avoid them, Kushner and his colleagues use computer models in which nanoscale features are virtually fabricated.

In models developed by University of Michigan graduate student Chad Huard and colleague Yiting Zhang at Lam Research, computational particles are launched toward the surface of the wafer that represent the radicals used in the passivation step and the etching ions produced by the plasma. Numerical techniques are then used to determine what happens to the surface when the radicals and ions hit the wafer, answering questions such as "Do materials get removed or added?" and "Does the incident particle get reflected or implanted?"

These fabrication simulations provide insights into preventing another etching challenge known as aspect ratio dependent etching, or ARDE.

The aspect ratio is the ratio of the depth or height of a feature divided by its diameter, and wider features have a smaller aspect ratio than narrow ones. If there is continuous etching—where the passivation and etching steps are not decoupled—small aspect ratio features will etch faster, which can be problematic if features with many different aspect ratios are to be fabricated."

Kushner said that the simulations that he and his colleagues are performing have begun yielding benefits.

"Based on our computations, we are identifying strategies for producing the desired single layer control of ALE even if the operating conditions are non-ideal," he said. "These predictions enable a larger 'process window' for factors, such as controlling power or ion energy, that will help obtain ALE-like results."