Profile of Ellen D. Williams

Modern electronic circuits, like those used in computers and cell phones, rely on stability. The atomic-level structure of the electronics in these devices, down to the semiconductors, is vital for their proper function.

New nanoelectronic materials in development, however, have a far greater level of complexity and present a higher possibility for molecular malfunction than their older, larger forebears. Physical and thermal fluctuations can alter the behavior of these forthcoming devices, which poses unique challenges for physicists and material scientists.

Over the course of her scientific career, University of Maryland (College Park, MD) physics professor Ellen D. Williams has investigated the atomic-scale interactions on the surfaces of materials. Her research group in experimental surface science explores fundamental issues in statistical mechanics and their practical applications in the growing field of nanotechnology. Her work may help guide and usher in an era of more stable nanodevices.

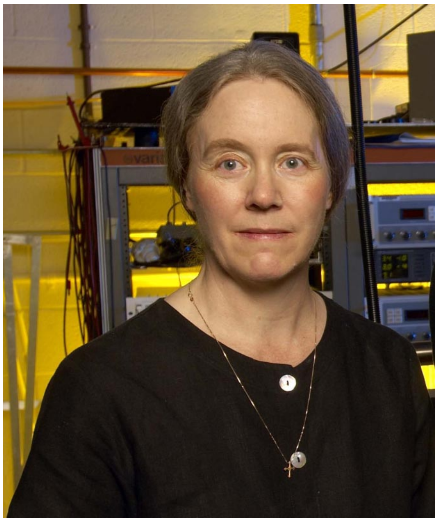
For her contributions in the field of physics, Williams was elected in 2005 to the National Academy of Sciences. In her Inaugural Article in the current issue of PNAS (1), Williams focused on organic electronic materials. Such organics can be incorporated into plastics and nontraditional electronics more readily than commonly used silicon-based materials.

In the article, Williams and colleagues used scanning tunneling microscopy to examine the dynamic properties of an organic thin film called acridine-9-carboxylic acid, or ACA. The researchers found that the film's molecular properties fluctuated at room temperature, although its physical characteristics acted independently of these boundaries. Her group then explored the nature of ACA's internal interactions and developed a new molecular basis for predicting thin film morphology (2).

"This is a very exciting area," Williams says. "There is a huge amount of interest right now in looking at organic molecules that have semiconducting properties. And organics allow for a quick turnaround time when developing a new electronic device."

A Chemist by Training

Born in Wisconsin, Williams' family moved to Livonia, Michigan, a sprawling suburb northwest of Detroit, during her childhood. Like many of their neighbors, her father worked for the Ford Motor



Ellen D. Williams

Company. An engineer, he discouraged his daughter from studying the subject. Instead, the elder Williams encouraged Ellen to study computers and computer programming, a prescient observation for the early 1970s.

"He was a young engineer in the 1930s, and engineers then were on the production floor dealing with tough guys," Williams recalls. "From his perspective, it was no life for a woman."

Williams attended Franklin High School in Livonia and found an after-school course to explore computer programming. With the help of outstanding high school teacher David Danes, she developed a strong interest in chemistry. "[He] helped me see a logical train of argument in the reactions."

Williams traveled to college in East Lansing, home of Michigan State University, where she majored in chemistry. Her advisor, Frederick Horne, who is now an emeritus professor of analytical chemistry at Oregon State University (Corvallis, OR), taught her the fundamentals of the statistical analysis of spectroscopic signals. "I learned some computer instrumentation, interfacing with experiments, which was pretty crude back in those days," she says.

Horne encouraged Williams to take a graduate-level statistical mechanics class as an undergraduate. In that class, she explored the physical basis for the laws of thermodynamics, including the effects of entropy. She found the course compelling, and the experimental tenets of "stat mech," as the field is called by its practitioners, have formed the basis of her research ever since.

"Analyzing distributions of behaviors to try to pull out fundamental understandings was just something that I really enjoyed the minute I started playing with it," Williams says. "When I was a little kid, I remember groaning to my mother about how unfair it was that when left out, my soup got cold and my milk got warm. But that's the basis of stat mech, which is that we don't go to the most energetically preferred configuration because of entropy. There's always a tendency to maximize disorder, which is in direct competition with the 'good energy' situation where atoms are very well ordered."

Order and Disorder

Williams continued her education at the California Institute of Technology (Caltech, Pasadena, CA), pursuing a graduate degree in chemistry. She arrived at the university in 1976, only a few years after women were allowed admittance as undergraduates. "Caltech had not formally forbidden women graduate students previously, but they were just opening up the idea of regularly accepting woman students on the whole," she says.

Happily for her, a large fraction of the entering graduate students in chemistry were female. Far from feeling out-of-place or intimidated, Williams says that, "being a woman [at Caltech] really was not a big deal. It was all about what you could do, rather than anything else."

During her graduate career, she worked in the laboratory of her thesis advisor, surface chemist W. Henry Weinberg, studying the atomic-scale mechanisms important to catalysts. She remembers developing calluses on her hands from cranking down the bolts that sealed shut the ultra-high vacuum chamber used in her electron diffraction studies, designed to measure the atomic structure of well-ordered surfaces.

"Surface chemistry was a hot, breaking field because the experimental technology was just maturing at that time," Williams says.

Williams' first paper, published while she worked in Weinberg's lab, combined her interest in then-emerging computational capabilities with the mechanics of order and disorder. Using Monte Carlo simulation, a mathematical algorithm for introducing randomness into a system,

This is a Profile of a recently elected member of the National Academy of Sciences to accompany the member's Inaugural Article on page 16418.

she developed models to describe the interaction energies that govern how oxygen atoms arrange themselves on tungsten surfaces (2). She applied her model to an original surface chemistry model: the interactions between oxygen and tungsten in light bulbs (3).

Williams' fascination with symmetry and order led her to investigate the structures formed by chemical adsorbates on reactive metal surfaces during her graduate career (3, 4).

"By observing order-disorder transitions, we can find out the basic atomic properties that govern surface reactions," she explains. "You need to know how atoms are arranged, and how they interact with their neighbors. Do they like the way they are, or are they random and disordered? If they are disordered, another molecule could slip right in and start an unforeseen chemical reaction."

At Caltech, Williams also met her husband, astrophysicist Neil A. Gehrels. He now works at NASA's Goddard Space Flight Center (Greenbelt, MD) and like Williams, was elected to the American Academy of Arts and Sciences. She counts him as "one of the most influential people in [her] scientific career." Williams says that "it's phenomenal interacting with someone at home who is also actively pursuing fundamental scientific questions."

Maryland Microscopy

After completing her Ph.D. in 1981, Williams left California and drove across the country for a postdoctoral fellowship at the University of Maryland at College Park. Here, she ascended from postdoc to physics professor to the university's Institute for Physical Science and Technology.

On her arrival in College Park, she worked in Robert L. Park's lab studying surface phase transitions with the electron diffraction techniques she learned at Caltech. Williams investigated silicon surfaces and found their symmetries to be exciting sources of new experimental systems (5).

In 1981, the same year that Williams launched her career in the thermodynamics of surface chemistry, the field of surface physics took a quantum leap forward with the development of the scanning tunneling microscope. The microscope almost immediately became the enabling technique for her subsequent work in experimental statistical mechanics.

The scanning tunneling microscope works similarly to the Braille alphabet. "If you traced your fingertip across your desk and could record the peaks and valleys of what you felt, you'd develop a map of the surface," Williams says. "What we're doing with scanning microscopy is similar, but we don't actually bring a needle down to touch the surface molecules. Instead, we use a miracle of quantum mechanics—electron tunneling—to serve as our sense of touch."

"Everything that we were able to determine indirectly with electron diffraction, you instantly could see more directly with this instrumentation, including every aspect of disorder on surfaces," Williams says. "The implications were so huge that I was filled with scientific lust—I immediately needed to build such a microscope for my lab," she adds.

"Analyzing distributions of behavior was just something I really enjoyed the minute I started playing with it."

In her own laboratory, Williams transitioned from chemically oriented to physically oriented problems. She applied electron diffraction and the new capabilities of scanning tunneling microscopy to study silicon (6) and electronic materials, instead of metals and catalysts (7).

Later, in conjunction with Theodore L. Einstein and his student Norman C. Bartelt, Williams demonstrated the feasibility of combining breakthrough imaging techniques and statistical mechanics to study the underlying thermodynamics of silicon surfaces as they underwent a new kind of phase transition, reversible faceting. She calls this development "orientational thermodynamics" (8, 9).

During this time, she focused on a specific type of surface defect called a "step," a commonly seen one-atom-wide ledge on a seemingly flat surface. Steps can appear on nearly any material and play a crucial role in surface stability.

"A surface on a diamond, for example, looks planar," Williams explains. "But, the gemstone would not truly be flat on the scale of individual atoms. There would be little boundaries where the height on the surface would change. These are steps, one-dimensional linear boundaries."

Steps also provide scientists with a way to manipulate material on surfaces, allowing for atomic-scale control of step-flow growth that is essential to the production of incredibly pure electronic materials, such as the semiconductors used in virtually every modern device. "As early as the 1950s," Williams says, "researchers realized that the energies required to develop [these materials] weren't consistent with the properties of a flat surface."

On the nanometer level, steps create fluidity on a material's surface. "Atoms can come off the edge of one step, becoming a source of free atoms, and fuse onto other terraces or plateaus," Williams says. "When we're looking at an electronic device that might be made up of a total of 100,000 atoms, you need to be able to predict 'every wart on the face of a crystal.'"

Through the 1990s, her research group explored these dynamic processes, developing and applying experimental methods to measure the underlying statistical mechanics of one-dimensional steps (10).

In 2000, Williams was named as a distinguished university professor, a prestigious title at the university that includes Nobel Prize winners William D. Phillips, a fellow physicist, and economist Thomas Schelling.

Flexible Devices

Williams' recent work has moved away from silicon-based materials. She now investigates the thermodynamic properties of next-generation electronic materials such as organic semiconductors and graphene, a one-atom-thick layer of well-ordered carbon graphite. This polycyclic hydrocarbon has one of the lowest electrical resistances of any material at room temperature.

Williams says that graphene "has the potential to be a very fast semiconductor, better than gallium arsenide or silicon materials. Everybody's excited to see something new, but there are many questions that have to be answered about how well it can be controlled."

One of the first challenges to controlling the carbon material's properties was determining why it wasn't conducting electrons as freely as condensed matter physicists predicted. Along with UMCP's Michael S. Fuhrer, Williams investigated the material's apparent "roughness." They demonstrated that this undesired property was not inherent and that, instead, it came from the silicon material on which scientists traditionally had mounted graphene (11).

"That result is cool," Williams says, "because we can try to put it on a smoother surface and see if we can remove this limitation."

Nanoelectronic materials offer many exciting possibilities, such as the development of flexible electronics. Williams' group fabricated an electronic circuit on graphene, opening the door for the production of devices that can twist and bend without breaking (12).

"All of our present solid electronic devices could be put onto thin layers of plastics using printed graphene circuits," she says. Williams thinks that applications using this high-speed material will be developed in the next 5–10 years.

Her Inaugural Article moves further away from standard silicon-based materials. With assistance from fellow professors John D. Weeks and Janice Reutt-Robey, Williams examined the thermal motion of the organic thin film acridine-9-carboxylic acid. Electron motion in ACA and similar materials is slower than silicon-based semiconductors, but the films act like silicon and turn on and off with a "gating" voltage. Thermal fluctuations in the films may help scientists design self-assembling systems for use in nanoelectronics or photovoltaic cells, which convert sunlight into electricity.

This research paves the way for cheap devices that would not rely on the relatively expensive processes required to manufacture silicon semiconductors. Organic thin films could also be used for biologically based electronics, from drug delivery nanomachines and biosensors that detect carcinogenesis, to biocomputers that effectively mimic neural networks.

"Entropy, randomness, and disorder are a part of life," Williams says. "In nanotechnology, the defects themselves may become intrinsic properties. We see this in the biological world, where error correction is built into systems like DNA replication."

Williams signing the membership book at her NAS inauguration.

Beyond the Surfaces

As she continues to leave her mark on the world of surface physics, Williams realizes that her appointment to the National Academy of Sciences comes with significant responsibilities. To help promote science to the younger generations, she directs outreach activities that bring physics and physicists into middle and high schools in Maryland. In addition, over the past decade, she has provided counsel to government projects and says that she could foresee a future in which she spends more time in the policy world.

In her current appointment to the Congressional Commission on the Strategic Posture of the United States, she will help review the country's arsenal of non- and counterproliferation programs and defense systems. Expanding these activities while her lab continues to investigate materials for next-generation technologies "would be a new challenge," Williams admits.

But the field in which she has spent the better part of the past 3 decades is rapidly changing. "It's going to be exciting to explore these new electronic materials pushing, perhaps, new quantum phenomena that are intrinsically different from the transport behavior we have previously seen. There's also a world moving toward biological analogies in developing electronic systems, like error correction."

Williams believes that electronics eventually will be ubiquitous. But, she says, "we must continue to create technology that lowers our ecological and environmental footprint. We'll have a better life, but not if we trash the Earth while we're doing it. Dealing with these issues is absolutely the direction science has to take."

Farooq Ahmed, *Freelance Science Writer*

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