DISORDERED DESIGN

Physicist David Drabold explores the materials that will build the next generation of electronics

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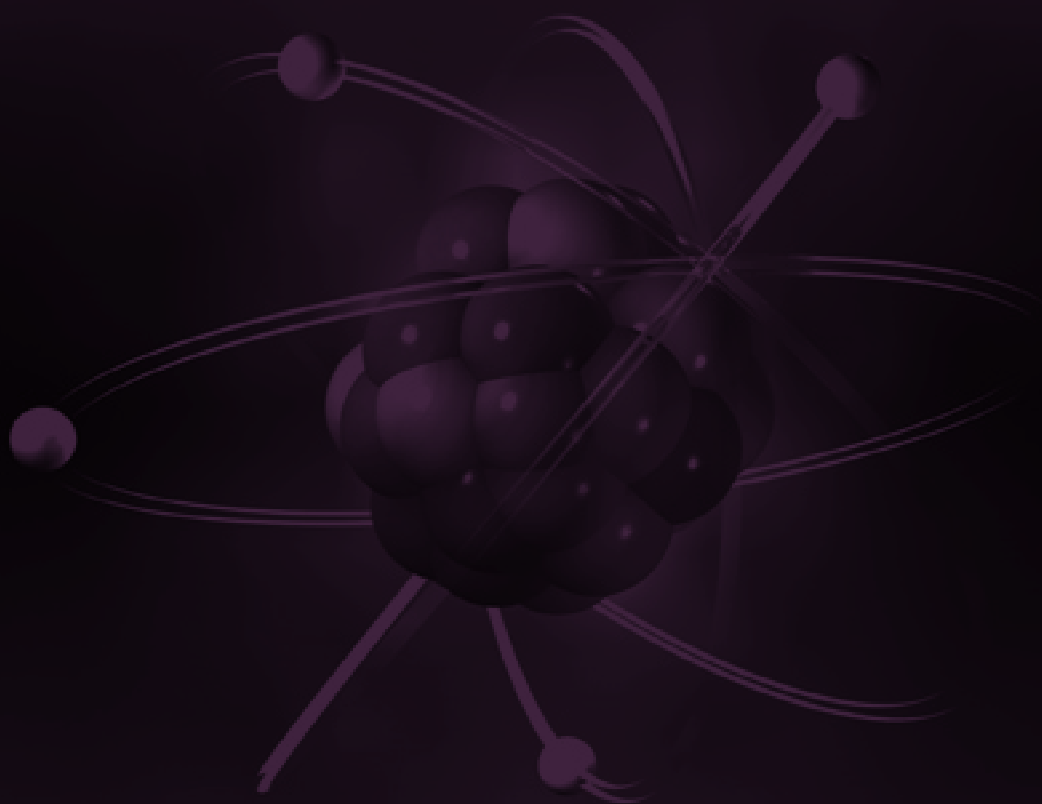
portrait by LUIZ SANTOS



"If you had asked me when I was 10 years old what I wanted to be when I grew up, I would have said a professor of history."

But when 10-year-old David Drabold wasn't devouring books on ancient Rome or medieval England, he was tinkering with radios and TVs in his basement workshop in Cuyahoga Falls, Ohio. On holidays in Detroit, he listened to his grandfather's tales of automobile technology from the 1920s, when that industry was brand new.

Then there were the clear winter nights he spent huddled over his backyard telescope, which inspired him to model the motion of the planets on his programmable calculator.

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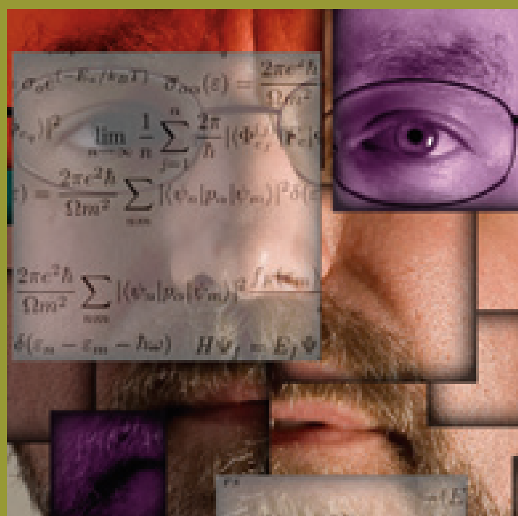

"It's the quintessential mechanics problem, right?" the Ohio University physicist remembered. "It's kind of funny — I'm a computational theorist now, and I'm not within a mile of astronomy or astrophysics, but in the sense that I was using a computer to model a physical process, I still do that today."

Drabold devises equations to describe the behavior of atoms in the newest electronic materials. But while he could observe the planets' paths with relative ease from his backyard, he can't directly observe the paths of electrons flowing through these materials. He combines the data from his colleagues' experiments with what he knows about quantum mechanics and probability to work backward to the equations.

On a recent cold February day in his office in Clippinger Lab, Drabold recalled how his desire to solve complex physics problems eventually eclipsed his original career goal as a historian. Now, reading history books and collecting rare coins are what he does when he needs a break from deciphering the physics of tomorrow's electronics.

A bachelor's degree in applied mathematics and a master's in physics from the University of Akron led him to a doctorate in physics from Washington University in St. Louis. From there, he went on to two prestigious postdoctoral fellowships: one in physics at the University of Notre Dame, and another jointly in physics and materials science and engineering at the University of Illinois at Urbana-Champaign. He joined the Ohio University faculty in 1993, and except for the occasional sabbatical, hasn't left since. He's Distinguished Professor of Physics (the highest academic distinction at Ohio University), and a Fellow of the American Physical Society and the British Institute of Physics.

THE MATERIAL WORLD

Drabold studies disordered and amorphous materials, meaning that the atoms aren't arranged in neatly repeating patterns as in crystals. Some materials' structures are so predictable that their atoms resemble bricks in a wall; by comparison, Drabold's materials look more like wild frescoes designed by abstract artists. The patterns aren't easy to discern, and the math that describes them is complex. His methods for modeling these materials are being utilized by scientists across a broad range of disciplines, as they develop the next generation of electronics.

Case in point: Pure silicon, the essential element of today's electronics, has a regular crystal structure, with atoms periodically stacked one on top of the other. Scientists have understood much of how electrons move through silicon since the 1930s.

But jumble the atomic positions and add some hydrogen atoms, and you get a different material entirely: hydrogenated amorphous silicon. The atoms form a quirky latticework that looks entirely random. The material still conducts electrons, but when exposed to heat or light, its conduction changes dramatically.

Why that happens is a mystery, one that Drabold is trying to

A Distinguished Career

PUBLICATIONS
More than 140 academic journal publications, 2,700 citations by other scientists, one book published, and one forthcoming.

CURRENT RESEARCH GROUP
4 doctoral students, 1 postdoctoral, all supported by external funding.

MAJOR UNIVERSITY AWARDS
Distinguished Professor Award and Presidential Research Scholar (2002-2007). *Ohio* Magazine's "Excellence in Teaching Award."

CURRENT FUNDING
National Science Foundation, Army Research Office. Previous support: Office of Naval Research, Motorola, Inc., and Axon Technologies, Inc. Research team has more than $6 million in external funding over 5 years.

PARTNERSHIPS
University of Cambridge, University of Illinois, Penn State University, Lehigh University. West Virginia University, Arizona State University, Texas Tech University.

TEACHING
Elementary physics; graduate courses in quantum mechanics, solid state physics, and computational physics; and tutorials with the Honors Tutorial College.

[*on the web*]

www.phy.ohiou.edu/~drabold

solve. To do so, he goes literally back to the drawing board, to derive from scratch the equations that govern how silicon and hydrogen atoms in that crazy configuration interact.

Scientists already have begun incorporating hydrogenated amorphous silicon into heat-vision goggles (used to see infrared "heat" images in absolute darkness) and solar cells. But since they don't know everything there is to know about how the material works, they've hit roadblocks in cost and performance. So Drabold's theoretical work is critical to moving these technologies forward.

He's made progress. In 2005, he and his colleagues discovered one reason that defects form in solar cells made from the material. And he thinks they've just figured out why it's so sensitive to changes in temperature — the feature that makes it ideal for heat-vision goggles: Electrons are confined inside pockets in the material, and those electrons are very sensitive to movement in the surrounding atoms. So incoming heat energy may jostle those atoms only a little, but to great effect to the electrons and therefore the conductivity.

Colleague Alex Kolobov, a senior scientist at the National Institute of Advanced Industrial Science and Technology in Tsukuba, Japan, is looking for Drabold to help solve another mystery: why re-writable DVDs work the way they do. Laser light alters the data on these disks by changing the structure from a crystalline to an amorphous state. Even though the technology has been commercially available since 1999, scientists don't understand exactly why the change takes place. Kolobov called simulating this transition a "major challenge," and added that Drabold "is one of the very few people who can, perhaps, do this."

Looking to the future of electronics, power generation, and computer memory, Drabold sees strong potential for disordered materials — from materials like hydrogenated amorphous silicon, to glasses and polymers. All require innovative methods to predict their properties. The ultimate goal is designing electronic materials to order.

"Ideally, you'd like to be able to say, 'I want a material with this particular property — give me the recipe.' We've taken a first step in that direction," he said.

Just determining a material's structure can be a difficult task. "If you give me the data from one experiment, one curve on a graph that characterizes the material in some way, there's literally infinity of possible structures that would be consistent with that," he said. "How do I find an optimal model expressing all we know about the material (from experiments) and from theory work at the same time?"

MAKING PREDICTIONS

For that, he often turns to Bayes' theorem, a centuries-old statistical method that was once very controversial but is now gaining a foothold in the scientific community. The method involves taking an educated guess about the likelihood of something happening, and gradually making that prediction better by factoring in results from scientific experiments.

To Drabold, calculating the likelihood that one of his computer models accurately describes a material is a "disarmingly simple" use of the theorem: "It's just two lines [of equations].... What you're doing algebraically is utterly trivial, but somehow the results are profound."

Richard Martin, professor of physics at the University of Illinois at Urbana-Champaign, recalled that Drabold was already employing innovative methods such as Bayesian statistics when he was a postdoctoral researcher in Martin's lab in the early 1990s. "David was already very mature and independent at that time, and he became the leader for much of our work," Martin said. He was especially impressed with the way Drabold was able to unite the theory from so many different fields — including statistics, mathematical analysis, and advanced numerical methods for creating algorithms — with experimental problems.

Drabold traces his use of Bayes' theorem to his graduate study, where he met one of his most important mentors, E. T. Jaynes. Though Jaynes was a physicist, he was best known for advancing the use of statistics in science. Bayesian techniques are still somewhat controversial, but they were much more so in the 1980s, when Jaynes was a strong proponent. "No matter what course [Jaynes] taught, somehow it always had a lot of Bayesian probability theory in it," Drabold said. "Somehow, coming from him, it worked."

While Drabold was still a graduate student, Jaynes paid for him to travel to a science meeting at the University of Cambridge. It was his first trip to England, and so his interest in statistical mechanics collided joyously with his interest in medieval history.

Ever since, science has brought Drabold experiences that any history buff would envy. When he returned to Cambridge for a sabbatical in 2001, the chemist with whom he was collaborating arranged for him to visit the Parker Library, at Corpus Christi College known as one of the finest libraries specializing in early medieval works in Europe. There, he read the oldest known copy of the Anglo-Saxon Chronicle, including the entry for the year 1066, when William of Normandy conquered England. (He added, with relish, that the librarian permitted him to turn the pages with his bare hands.)

Meanwhile, he said, his love of old coins lives on. From a cabinet in his office, he pulled a small but heavy box, packed with specimens that date all the way back to ancient Rome. As he showed off a few of his favorites, he mentioned a friend at the University of Michigan who is using the latest technology to study ancient coins' composition, to infer where and when they were made.

"At some point in my career, when I'm not so busy with other things, I may try to do something like that myself," he mused with a smile. "It would be great fun."