# New methods are changing old materials

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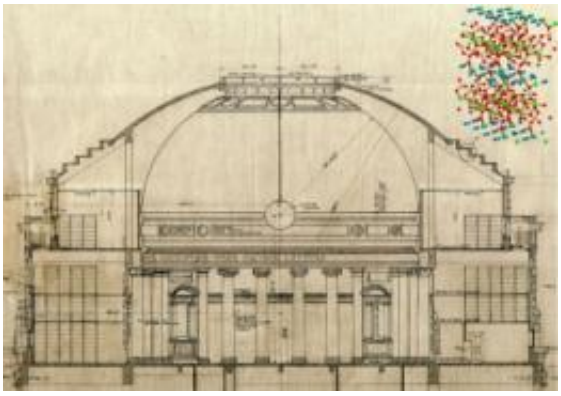

The Great Dome at MIT, shown here in an architectural draft, includes a cement liner that seals and secures the sandstone overlay. In research published earlier this year in the Proceedings of the National Academy of Sciences, a group of MIT researchers used computational materials science techniques to decode for the first time the three-dimensional structure of the basic unit of calcium-silicate-hydrate (CSH) — the paste that forms and quickly hardens when cement powder is mixed with water. An atomistic rendering of C-S-H is shown in the upper right corner of the image. Graphic created by KJ Van Vliet; architectural drawing supplied by M. Parkin; atomistic rendering of CSH generated by R. Shahsavari

(PhysOrg.com) -- A company that makes steel for bearings used in heavy trucks had a big problem. The trucks travel through harsh, perilous environments such as Siberia, and an unexpected bearing failure on a remote stretch could literally put the driver's life in danger. Knowing how long the steel would hold up under those conditions was beyond their ability to predict experimentally, so they turned to specialists at MIT.

Under applied weight, steel deforms over time at an ever-increasing rate. The exponent in the equations governing that process should be three, according to scientific theory, while experiments conducted over many decades always found it was really four or five, says MIT materials scientist Krystyn Van Vliet. Nobody could demonstrate the reason for this discrepancy — until now, using new computational techniques.

Computers were able to solve the mystery by controlling all the variables and exploring every possible variation, Van Vliet says. The analysis had to be done at the level of the individual atoms in the material — exactly how carbon atoms are spaced among iron atoms in the material, and how hydrogen atoms penetrate into that structure as the material degrades — in order to understand the behavior of the bulk material. "In laboratory experiments, it would have been impossible to do in anyone's lifetime," she says. Now, using the analytical tools developed at MIT, the company has embarked on a major program to analyze the material's degradation and find ways to improve it.

That's just one example of how the field of materials science has profoundly changed in recent years. From largely trial-and-error laboratory experiments, the field has graduated to computational methods that use first principles of physics and chemistry to evaluate thousands of different variations in material composition.

The new approach, called computational materials science, is a powerful way of discovering new materials with desired properties — such as improved charge and discharge speeds for battery materials — and of understanding and fine-tuning the properties of well-known, long-used materials such as steel alloys, ceramics, and cement composites, whose fundamental properties are still surprisingly little understood.

Although the approach has evolved over many years, its potential has been recognized only relatively recently, says Sidney Yip, MIT professor

emeritus of nuclear science and engineering and materials science and engineering, who retired from teaching duties this summer after 44 years. "By and large, the role of computers in materials science is still in the process of gaining acceptance," he says. "It's a change of paradigm that seems to be occurring at an accelerating rate."

Duane Johnson, a professor of materials science and engineering at the University of Illinois and a leading researcher in the field, agrees that this is a major change. "Today, as is reflected in many journal publications, computational materials science is a key, and often equal, partner in characterization of materials, often more than just to support experimental observation," he says. "In fact, computationally complex methods provide predictions that are becoming more and more reliable, helping direct experiments and improve materials technologies design."

That change is so profound that one of the field's leading researchers, MIT's Gerbrand Ceder, has called for a massive project somewhat analogous to the Human Genome Project, to create an exhaustive database of all possible inorganic compounds (those that don't include carbon) and their properties. He calls it the Materials Genome Project.

Computational materials science "emerged a while ago, and is in full bloom now," says Ceder, the R. P. Simmons Professor of Materials Science and Engineering. Now, his department has five or six people doing computer modeling full time, he says, and three people who do modeling based on first principles of physics. "I don't think people would have anticipated that" even a few years ago, he says.

## Working in a virtual world

Using the new computational methods, "we can use modeling almost as a microscope into the nature of materials," Ceder says. "If you can realistically simulate the materials, it's a virtual world: you can do

controlled experiments, which are difficult to do in the real world. It rapidly allows you to understand things."

Though it's been building for many years, however, the new approach has not yet yielded many dramatic results, Yip says. "I think the word is potential. There are not that many obvious successes so far."

But there are major efforts under way to bring about those successes. MIT recently announced a new interdisciplinary project, the Concrete Sustainability Hub (CSH), to study the fundamental properties of concrete and find ways of improving them and of reducing concrete's massive carbon footprint. Amazingly, though the material has been in widespread use since the Roman Empire, the basic structure of concrete is still not well understood. "Nobody knows what its fundamental structure is at the molecular level," Yip says, though recent work at MIT has provided significant new insights into that structure.

The aim of the CSH is to produce new versions of the material, either with improved properties such as faster setting or greater durability or with a significant reduction in the carbon dioxide emitted by cement manufacturing. The five-year project, partly funded by the Portland Cement Association, the industry's trade group, is being led by Franz-Josef Ulm, the Macomber Professor in the Department of Civil and Environmental Engineering. The team working on cement science includes several computational materials modelers including Roland Pellenq, Markus Buehler, Nicola Marzari, Jeff Grossman, and Bilge Yildiz, as well as Van Vliet and Yip.

Understanding the detailed properties of materials still requires laboratory experiments — no computer models are perfect, and they may never be. But the guidance provided by the modeling allows the laboratory work to be done much more efficiently, Ceder explains. "Now, when you go into the lab, you know what you should be doing,"

he says. "It's not a random experiment anymore."

Inorganic oxides and concrete are not the only traditional materials coming under new scrutiny. Steel alloys, crucial to so much of modern life, are also not well understood. Yip explains that new, more radiation-resistant steel alloys will be essential for the proposed new generation of nuclear power plants seen by many as an important low-carbon energy source to replace plants that consume fossil fuels.

## Predicting steel's behavior

"It's a great challenge," Yip says. "If we want to extend plant lifetimes from 30 years up to 60 or 80 years, we have to make sure the material can withstand the radiation damage. Many people are working on that." For example, early computational results by Assistant Professor of Materials Science and Engineering Michael Demkowicz are pointing to several possible approaches to damage-resistant microstructures.

Already, this approach has led to some significant progress in steel formulations, says Van Vliet, the Thomas Lord Associate Professor of Materials Science and Engineering. For example, one company was finding that steel was failing prematurely, and "they knew they couldn't make it better just by processing. They knew it was failing in certain ways," and that it could fail sooner via absorption of hydrogen from water and oil. "Hydrogen embrittlement is an issue for many infrastructure applications, from bridges to nuclear power plants," Van Vliet says, and the simulations allowed the company to better understand that process. "It's very predictive," she says, allowing solutions to be developed for specific situations.

Other materials that are slowly yielding their secrets to the new computational techniques include the coatings applied to many common mechanical devices. For example, Carter says, turbine blades used in jet

engines may have coatings to protect them from high temperatures. "A bad thing would be for these blades to lose that coating," he says. "We have used computer simulations to analyze the boundary between the coating and the material" in order to understand better how the two might become separated.

Computational methods are also proving useful in explaining how materials change over time — by, say, undergoing gradual corrosion. And, in the ever-more-important field of battery research, these simulations can show how the components of a lithium-ion battery, for example, are altered by repeated cycles of charging and discharging. "It gives us new insight into the behavior of these batteries," Carter says. "We can relate the microstructure to the overall behavior" of the battery.

The whole field is evolving, and that is changing the way research is carried out and therefore the way the field is taught, says Professor of Materials Science and Engineering W. Craig Carter. "Over the next decade, how you decide to teach materials science will depend on the evolution of the computer model," he says.

MIT has played a significant role in the growth of this new approach, says the University of Illinois' Johnson. "Certainly, MIT has been a leader in promoting the area of computational materials from the beginning. They have maintained a strong group of quality researchers in computational materials science and materials physics," he says. "The MIT computational materials science faculty continue to be successful in using new and fundamental techniques."

And the science itself will continue to evolve dramatically, Ceder believes, as the computational techniques become ever more capable of automating the process of discovery and analysis. "Once you automate things, the world changes," he says.

But some things won't change. Even as the well-controlled thought experiments offered by computational materials science will drive both the education and the experiments of the next generation of engineers, the field of materials science will continue to rely on good old-fashioned, trial-and-error lab work, researchers say.

"Many materials in widespread use, like concrete, steel, and polymers, are very complex organizations of many atoms which cannot possibly be simulated by computer," says Carter. Computational materials science appears to be "generating successes in directing the nature of the experiments that should be done," he says. "But then you still have to do the experiments to find out the real properties of the material being studied. There are some properties that are almost impossible to model."

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