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Applying Math to Materials

Materials Scientist and Engineer David Srolovitz Joins Penn Faculty

By Janelle Weaver

The frothy foam that rises on top of beer as you pour it into a glass, the bubbles that build up in the sink after you dump dish soap into it, the smooth texture of shaving cream smeared on your face—these physical phenomena are entrancing enough on the macroscopic scale, but David Srolovitz has an entirely different perspective. Srolovitz, the inaugural Joseph Bordogna Professor of Engineering and Applied Science in the departments of Mechanical Engineering and Applied Mechanics (MEAM) and Materials Science and Engineering (MSE), is fascinated by the microscopic properties of these materials. For years, he has used computer simulations to understand mechanical deformations affecting the microstructure of a variety of materials, from crystals to foams. Using mathematical principles, he has developed intricate theories that describe how crystal grains and other structures grow in three dimensions, laying a strong foundation for the entire field of materials science.

"We are very excited that Srolovitz has joined the Penn faculty, because he is one of the world's most preeminent computational materials engineers and influential materials scientists and mechanicians of his generation," says Eduardo D. Glandt, Nemirovsky Family Dean of the School of Engineering and Applied Science. Penn has also recruited Vivek Shenoy, Professor of Materials Science and Engineering, another leading expert in computational science who focuses on modeling the fabrication, performance and physical properties of nanoscale devices and structures.

Small-scale Simulations

By studying mechanical properties at the nanoscale, Srolovitz gains unique insights into how materials behave when they're deformed. A wire, for instance, behaves very differently at the macroscopic scale than it does on the nanoscale when it is stretched. Using

David J. Srolovitz

molecular dynamics simulations, Srolovitz tracks the position of individual atoms at every moment in time to gain a more complete quantitative picture of their behavior than is possible with experiments. "The central goal of materials science is to control the microstructure of materials, and our work provides really precise descriptions of how microstructures evolve," he says.

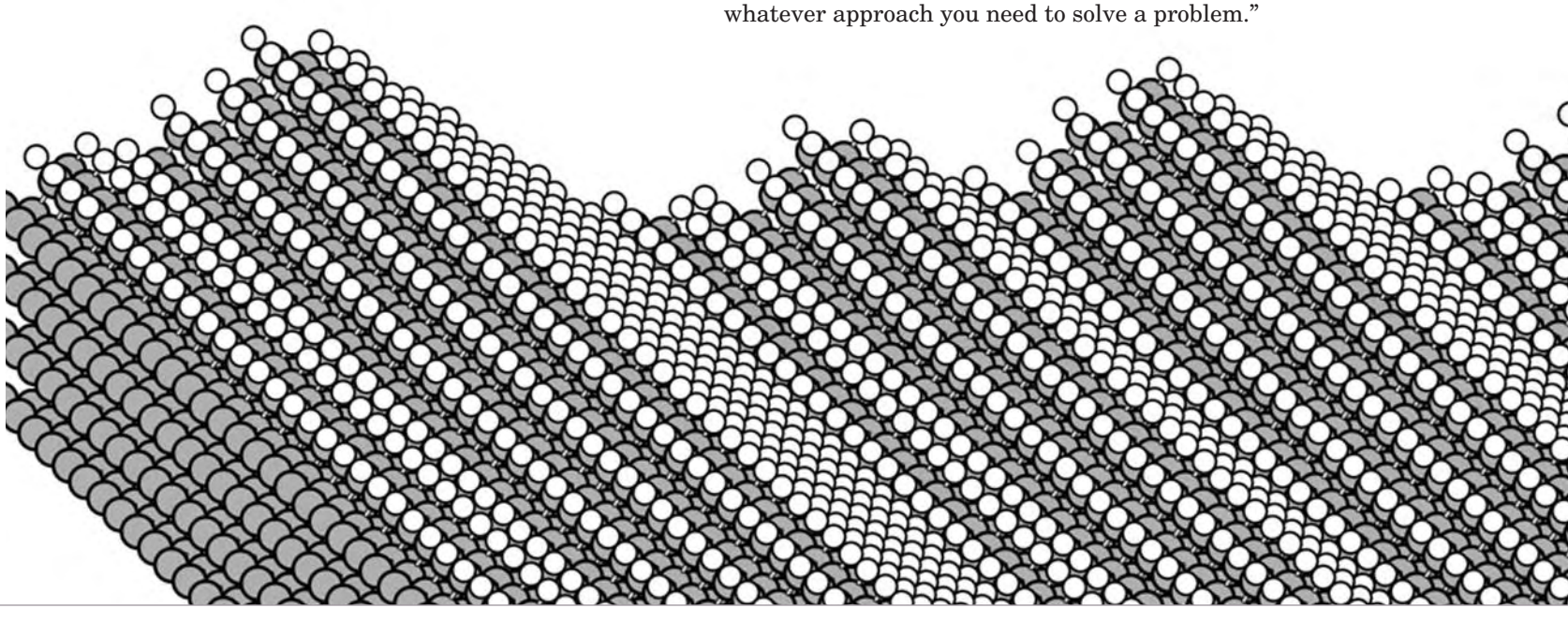
These simulations provide a glimpse of how materials behave, making it easier to develop theories. "Without simulations, you can make macroscopic observations from experiments, but then it's a big leap to try to understand what's going on at the microscopic level and to develop theories," Srolovitz says.

Understanding how the structure of materials deforms under different conditions is crucial for a range of applications, from building jet engines that are less likely to fracture when stressed to precisely controlling the properties of hair mousse. "We walk on the edge between things that are technologically interesting and good scientific questions that can be applied broadly," Srolovitz notes.

For the past several years, Srolovitz was the Executive Director of the Institute of High Performance Computing at Singapore's Agency for Science, Technology and Research (A*STAR), and prior to that position, he was on the faculties at Yeshiva University, Princeton University and the University of Michigan. The decision to join the Penn faculty was easy for him because it meant returning to the place where he got his start. Srolovitz earned master's and doctoral degrees from Penn's Department of Materials Science and Engineering. Since then, he has maintained his ties with MSE, returning to give seminars every few years. "I've spent a lot of time in this part of the country, and it feels like coming home," he says.

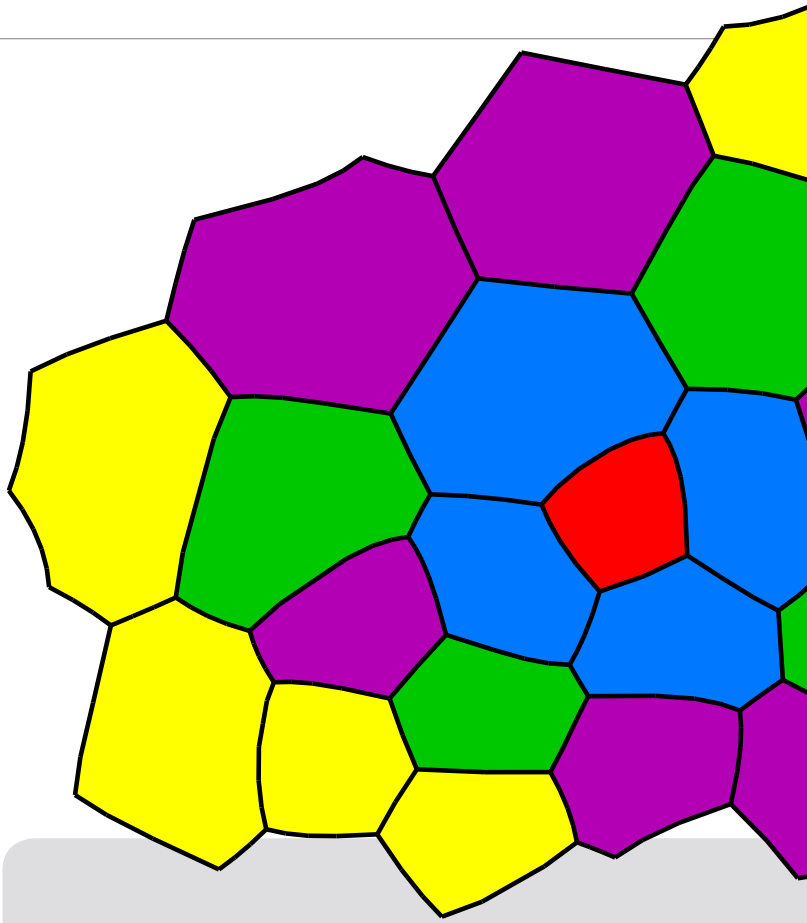
Collaboration Is Key

As a member of the Penn faculty, Srolovitz will bridge macroscopic observations with theoretical predictions by collaborating with experimentalists in the Departments of Physics and Chemistry, among others. "I enjoy working with people from a lot of different disciplines because each discipline brings its own perspective, and it's important to bring to bear whatever approach you need to solve a problem."



Penn's relatively small size makes it easy to forge collaborations, but at the same time it's large enough to achieve a critical mass of experts in various specialties, Srolovitz notes. "Penn strikes the right balance in terms of size, and because it's a world-class institution, it will allow me to collaborate with high-quality researchers on both the engineering side of the discipline as well as the basic science side."

One Penn scientist Srolovitz plans to collaborate with is Randall Kamien, professor of Physics and Astronomy, who develops precise mathematical theories to describe at the molecular level how materials fold. "Srolovitz has the intellectual range and expertise to take an abstract mathematical idea and know how to make a real material out of it," Kamien says. "Because of his remarkable breadth and eagerness to collaborate, he epitomizes what our campus is about."



Penn PICS Up the Pace

The Penn Institute for Computational Science (PICS) is a new center that will act as a central hub for computational modeling research. The premier institute will bring together faculty across Penn who are working on a diverse set of projects involving high-speed computing. Unlike many other institutes for computational science, PICS will have a broad focus, welcoming scientists from a variety of research areas, including engineering, chemistry, biology, applied mathematics, computer science and physics. PICS will also host a regular seminar series and provide technical training to students and postdoctoral fellows to allow them to take advantage of rapidly evolving computing technology. "With the launch of PICS, we are trying to make sure that Penn plays a leadership role in computational science and engineering at the national level," says Director David Srolovitz.