UT chemical engineer simulates nanoscale systems to understand

From plastics that heal themselves to bulletproof vests that harden on impact, a host of new, “smart” materials based on nanotechnology are on the way. These materials respond to environmental changes in smart ways based on their design — a design that requires a precise understanding of nanoparticles and their behavior.

“From iPods to computers to the chairs that we’re sitting on, all of these everyday objects contain materials that somebody synthesized, typically based on a trial-and-error process,” said Thomas Truskett, associate professor of Chemical Engineering at The University of Texas at Austin. “The question is: can we go into the laboratory and create a more efficient process where the desired outcomes at the macroscopic scale suggest to us the forces that drive that outcome on a microscopic level?”

The incredible potential that nanoparticles (materials smaller than one ten-millionth of a meter, or a thousand times smaller than a single hair) hold for industrial applications is founded on our increasing ability to design and synthesize particles molecule by molecule. With the potential to spark new technologies that help solve our energy and climate crises, nanotechnology is already driving 21st century innovation. However, much remains unknown about the behavior of particles in the nano-regime, and this gap in understanding threatens to hinder the field’s growth.

One important question in nano-engineering is how to understand and manipulate the speed at which nano-scale particles move, or “diffuse,” in materials.

“In many cases, theory successfully predicts the most stable structure a material will adopt, but it doesn’t predict how fast these structures will form,” said Truskett. “It’s an important practical question, because when you’re trying to create a new material, you want to understand the time-scales involved in getting to the final state.”

Truskett uses the metaphor of a crowded subway car to explain the dynamics of the systems he studies. If you are trying to get from the front to the back of the car, several things might
determine your rate of transit: the number of people around you, their size, and the way you move people around — a gentle touch on the shoulder or a big, belligerent push.

These same dynamics are at work inside a solvent, where particles, interacting through electrostatic, hydrodynamic, and quantum mechanical dispersion forces, move past each other, distributing their concentrations and forming stable structures. However, the question of whether one can systematically tailor the way particles interact and move by changing their shape, size and structure, is only beginning to be quantitatively addressed by scientists.

“It turns out that if you provide a gentle force, you can break the structure around you enough to move more quickly through the crowd,” said Truskett. “We’re trying to figure out how to make nanoparticles do just that.”

Using the Lonestar supercomputer at the Texas Advanced Computing Center (TACC), Truskett simulated these complex fluid systems to explore how size and other factors impact the rate of movement of nanoparticles, and to determine whether it was possible to alter their dynamics in a predictable way.

He discovered that the smallest particles are not always the speediest. In fact, it might just be the “gentle push” that can best hurry particles into place. By virtually grafting polymer chains to the surface of the particles, Truskett was able to create a ‘fuzzy’ layer that provided the gentle force needed to let nanoparticles glide past each other.

Such changes in how easily the particles in a material move past one another can mean the difference between the creation of a viable material and a non-starter. “If a process takes a long time to get to the end, it might not be viable commercially,” Truskett said.

This line of investigation helps advance our fundamental knowledge about nanoparticle behavior and motion. For his contributions, Truskett earned a grant from the Welch Foundation; a National Science Foundation CAREER award for early research; a Sloan Research Fellowship; a David and Lucile Packard Foundation Fellowship; and the Allan P. Colburn Award for Excellence from the American Institute of Chemical Engineers.

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Thomas Truskett, professor of chemical engineering at The University of Texas at Austin

The Glassy State

The glassy state presents another promising avenue of exploration for Truskett.

“Everybody knows what common window glass is, but very few appreciate that almost any substance can form what’s called a ‘glassy state,’” said Truskett.

‘Glass’ simply refers to a material that has congealed into a disordered solid. Ice cream is a glass, as are many everyday plastics and polymers. Glasses are formed by taking a liquid that’s disordered and cooling it very rapidly, or increasing the concentration of particles in a solvent faster than they can order themselves. In either case, the atoms don’t have time to form a crystalline structure and consequently display unique properties, often at the nano-scale.

Although scientists understand part of the big picture when it comes to glass, there are still many questions regarding the glass transition. In 2005, Science Magazine dubbed the problem one of the 125 biggest scientific mysteries, and it’s one that Truskett attempts to unravel via computational simulations on Lonestar at TACC.

“Attractive glasses” are interesting because they display properties quite different from those that occur in regular atomic materials. For instance, if you increase the strength of attraction between some particles, or decrease their temperature, the particles move...
faster. When you apply shear force to some of these materials, they thicken, becoming more viscous. Truskett’s group has made strides to develop a microscopic explanation of these trends.

There is a lot of technological interest in understanding nanometer scale particles that form glasses, says Truskett. If you combine particles that have a certain property with solvents that have a different property, you can create a condensed phase, like a glass, where the combined properties are better than the two systems on their own.

One application being developed using this principle is a bulletproof armor that has the flexibibility of a liquid material, but solidifies when hit. Another example is an auto-responsive material that heals itself when it cracks.

“There are lots of examples of ‘smart materials’ where you’re leveraging nanotechnology to create materials that respond to their environment in ways that make them more sustainable,” said Truskett. “A phase change that’s triggered by an external stimuli is a powerful way to realize some of these smart material structures.”

To be successful, both applications require a more solid understanding of the glass transition, which is aided by numerical simulation.

Truskett’s simulations of simple systems help him hypothesize about the basic rules that govern real materials. Working with collaborators Shekhar Garde at Rensselaer Polytechnic Institute, Jeffrey Errington at SUNY-Buffalo, and Vincent Shen at National Institute of Standards and Technology, among others, he subjects his theories to both detailed atomistic simulations and laboratory experiments to test their validity.

By learning how to tune nanomaterials so they behave in a specific and useful way, Truskett is advancing the development of new “smart materials” and applications, and helping to bring forth the era of nano-invention.

“In industry, there’s still a lot of trial and error,” said Truskett. “But with a clearer understanding of how to make new materials, the limits would be our imagination, and not the process itself.”

To learn more about Truskett's projects, visit his research group's website.

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