Theoretical physicist says polymers in a vacuum may yield valuable data

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A theoretical analysis of polymer behavior suggests that large molecules should behave very differently when they are in a vacuum than when in solution. The finding suggests that with better understanding of the physics involved, analysis techniques that operate in vacuums--such as mass spectrometry and studies of organic molecules in space--could yield far more information than they do now.

"Mass spectrometry of macromolecules was a huge breakthrough. But you're only getting one number from it, the mass of the molecule, and that's that," said Joshua Deutsch, professor of physics at the University of California, Santa Cruz.

In a paper published in the November 16 issue of *Physical Review Letters*, Deutsch analyzed the behavior of large molecules in a vacuum. He said that when long, chainlike molecules are released into a vacuum, they should oscillate in characteristic ways according to their makeup. By measuring those oscillations with electromagnetic sensors, scientists might someday be able to reconstruct details of the chemical structures of the molecules.

Many important biological molecules are macromolecules, including proteins, carbohydrates, fats, and nucleic acids like DNA. In the natural world, these polymers--long chains of repeating units connected by strong chemical bonds--are always in solution in our cells. So medical researchers tend to study them in solution.

As anyone who has tried to run in a pool can attest, water restricts movement. Tiny structures such as biological macromolecules lie suspended in a cell's fluid, like spaghetti in molasses, Deutsch said. Weak chemical attractions between the solution and the molecule often enlarge the molecule, holding it in extended positions.

But in a vacuum, Deutsch realized, there is no medium to dampen movement--only the internal forces within the molecule itself. He found that this internal friction leads to very different behavior from that of a molecule in solution.

Deutsch wrote a computer simulation of the physics involved in simplified molecules containing 128, 256, or 512 subunits arranged in a single chain. When he ran the model, he was amazed to see that points on the chain would periodically get closer, then farther apart, and continue in prolonged oscillations similar to the way the sides of a bell vibrate as it rings.

"It took me completely by surprise," Deutsch said. "No one had ever looked into this before, and based on what you see in solution you wouldn't expect the system to just ring and ring like that."

After more analysis, Deutsch realized that the answer could be explained by a simple concept several centuries old. "Turns out it's just Galilean invariance," Deutsch said, referring to the principle that objects moving in a vacuum don't slow down. This means that each subunit in a macromolecule feels pushes and pulls from its neighbors, but the overall movement of the molecule is not restricted by a solvent.

"This gives rise to a far less efficient damping than you'd get in solution," Deutsch said.

The oscillations are in the radio-frequency range and are strong enough,

perhaps, to be detected in the vacuum chamber of a mass spectrometer, Deutsch said.

First developed in the early 20th century, mass spectrometers were for years confined to studying atoms and small molecules. Mass spectrometers work by accelerating molecules over a specified distance and measuring how long the journey takes. With good enough instruments, this reveals the mass of the particle.

Mass spectrometry of macromolecules at first faced a major obstacle: no one could develop a way to vaporize them intact. Then, in the early 1980s, a young Japanese electrical engineer named Koichi Tanaka discovered a method by accident after making a faulty lab preparation. He followed up on the mistake with more research, eventually developing a workable method for which he won the 2002 Nobel Prize in chemistry.

In the new paper, Deutsch suggested that a mass spectrometer outfitted with the proper instruments could measure the oscillations from a vaporized macromolecule. By comparing the measurements against known samples and theoretical predictions, researchers might learn much more about the molecule than just its mass. Characteristics such as the arrangement of bonds, placement of charges, or atomic composition could possibly be determined.

"For example, DNA, because it's a double helix, is much stiffer than a single chain," Deutsch said. "You ought to be able to measure that."

For now, Deutsch is keeping things simple. His models look at single strands composed of identical subunits, with electrical charges acting only at each end of the chain. This is a far cry from typical macromolecules, which are a tangle of chemical bonds, contain many subunits in varying sequences, and have charges dispersed along their

length. But Deutsch believes in starting simply.

"I could add that all in right now, but what would I learn?" he said. "I want to work out the basics of this system. Then the experimentalists can take it from there."

Source: University of California, Santa Cruz