Smashing Chemistry in Atom Clusters

Theorists simulating experiments on a supercomputer have discovered that splattering clusters of atoms against a hard surface yields extreme conditions that can lead to a new kind of chemistry.

Because of how energy shifts the instant a cluster hits a hard surface, the cluster's core temperature can increase 10-fold, and the pressure skyrockets, possibly reaching a million times atmospheric pressure, says Uzi Landman, a physicist at the Georgia Institute of Technology in Atlanta.

During this brief instant, "there's a chance to look at reactions that are difficult to see in other ways," says A. Welford Castleman Jr., a chemist at Pennsylvania State University in University Park.

Landman and Georgia Tech physicist Charles L. Cleveland first observed these conditions when they hurled a computer-generated cluster of 561 argon atoms against a simulated salt surface at about 3 kilometers per second. The impact creates a shock wave in the cluster: Atoms in the front of the cluster abruptly stop, and atoms farther back pile onto the front ones, the researchers report in the July 17 SCIENCE.

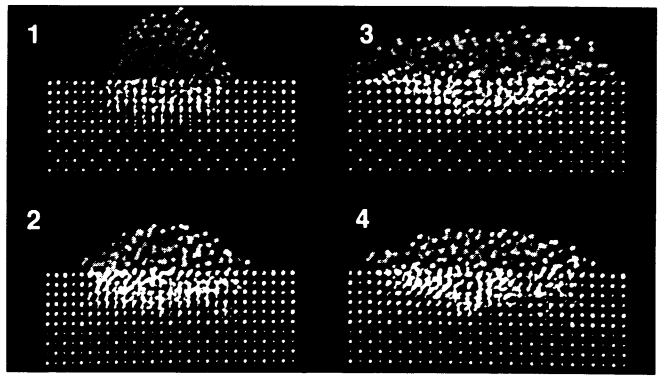
Within 3 picoseconds, this wave travels back to the trailing edge of the cluster. Then the cluster flattens and spreads out along the salt surface, with some argon atoms penetrating the salt and others evaporating. Finally, the argon atoms regroup as a patch on the salt surface.

Extreme conditions develop inside this pileup. As the cluster hits the surface, all the atoms try to scatter outward. But the outer ones don't move fast enough, so they briefly trap inner ones. The pressure inside builds to levels typically seen inside diamond anvil cells. The atoms can heat up to 4,000 kelvins, and the density of the cluster's core increases by 50 percent, Landman explains.

Should clusters contain several elements, the impact could cause them to combine in ways they would not otherwise, Landman notes. Also, the conditions appear and disappear so fast that reactions have time to create an intermediate compound but not enough time to convert that compound to more typical products. "You can get chemicals that you are not able to produce otherwise," he says.

To carry out this powerful simulation, Landman's group first developed mathematical ways to express all the interactions between salt's chlorine and sodium atoms and argon. A supercomputer takes about 10 hours to carry out a collision "experiment," he says.

"At any given time, we know where each atom is and how it influences every other atom," Landman says. But to make sense of the millions of bits of data generated, he and his co-workers had to figure out how to group data so that they could spot key details without being misled by individual fluctuations. To do this, they have the computer lump near-by atoms, averaging their information into a sphere. The whole cluster then breaks down into four spheres, whose properties the computer monitors and analyzes.



Landman/Georgia Tech

Sequence shows a simulated argon cluster crashing into salt.

"It's a pretty significant calculation," Castleman says. "I am sure it will stimulate more experiments."

Already, Robert L. Whetten at the University of California, Los Angeles, has been investigating reactions between clusters and surfaces. "I think whatever comes out [of laboratory experiments] will be interesting," Landman says.

Landman's new method of analysis also revealed that salt absorbs three-quarters of the speeding cluster's energy, much more than expected. "We learned how important it is to include the dynamics of the substrate itself," he says.

The impact creates a crater in the salt, and that could lead to defects in commercially important thin films made with deposition technologies, he notes. To avoid that damage, he suggests shooting the incoming atoms at the deposition surface at an angle or at lower velocities.

On their computer, Landman and his colleagues have also splattered gold clusters against nickel to model the molecular dynamics of gold-plating processes. Other preliminary simulations, involving clusters of nitrogen molecules, showed that those molecules tended to break apart, building Landman's expectations that new chemical reactions could occur in such clusters, he says. *— E. Pennisi*

Heart risks: This is nutty

Physicians generally counsel people with an elevated risk of heart disease to eschew high-fat foods. Nuts, which derive 70 to 90 percent of their calories from fat, should rank high on that list of dietary no-no's, right?

Not necessarily. A study of 31,200 Seventh Day Adventists suggests that people who nosh on nuts five times a week, compared with people who rarely eat them, may halve their risk of heart attacks and coronary death.

Most Seventh Day Adventists consume very little alcohol, meat, and caffeine, and health researchers suspected this might help explain why Adventists live longer than other Americans and suffer one-seventh as many heart attacks. To investigate these dietary factors, Gary E. Fraser and his colleagues at Loma Linda (Calif.) University mailed a detailed diet and lifestyle questionnaire to every Adventist over age 24 in California. His team then surveyed respondents annually, confirming heart attacks or coronary deaths through medical records.

After adjusting for potentially confounding variables such as weight, smoking, and hypertension, the researchers found that only nuts and, to a lesser extent, whole-wheat bread showed any strong link with coronary events. Both foods lowered risks, they report in the July ARCHIVES OF INTERNAL MEDICINE.

Adventists who ate nuts at least once a week lowered their heart risks by 25 percent. Munching nuts five or more times a week roughly doubled the apparent protection. A survey of randomly selected participants suggested that peanuts accounted for 32 percent of the nuts eaten, almonds for 29 percent, and walnuts for 16 percent.

"Has the magic bullet arrived? Is it the humble nut?" asks William P. Castelli, director of the Framingham (Mass.) Heart Study. In an editorial accompanying the research report, Castelli notes that "a preview of a feeding trial" by Fraser's team hints that nuts may exert their protection by altering blood lipids. *— J. Raloff*