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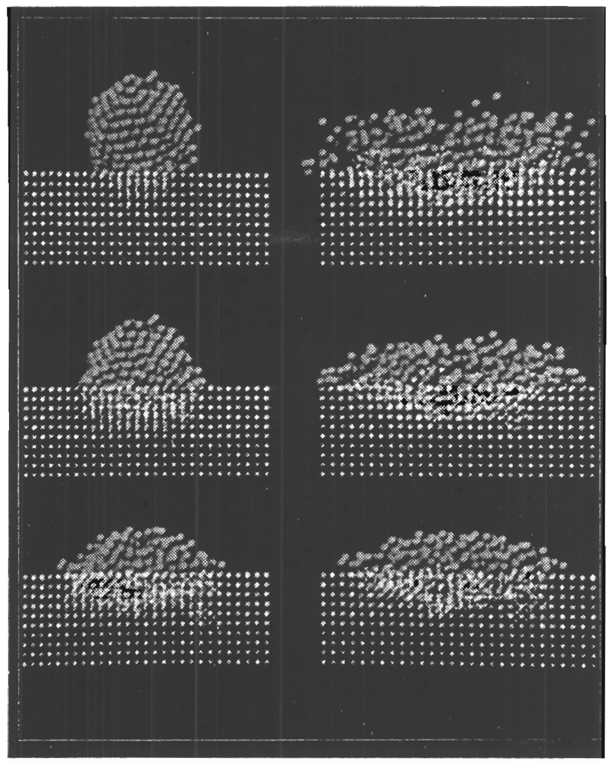
THE DYNAMICS OF MICROSCOPIC CRASHES: COLLIDING CLUSTERS CREATE "NEW CHEMISTRY" AT HIGH TEMPERATURES, PRESSURES AND DENSITIES

Chain-reaction freeway collisions create surprisingly powerful forces, particularly for hapless drivers caught in the middle of them. In the July 17 issue of Science, Georgia Institute of Technology researchers suggest that similar forces generated on a microscopic scale as clusters of atoms or molecules crash into solid surfaces may produce new chemical environments that can promote new reaction processes.

Using molecular dynamics simulations on powerful supercomputers, Dr. Uzi Landman and Dr. Charles Cleveland of Georgia Tech's School of Physics studied the dynamics of collisions between clusters of atoms and a solid surface. Those collisions -- at supersonic speeds -- generate extreme pressure, density and temperature pulses.

Their findings may open the door not only for new types of chemistry, but also for insights into new surface processing techniques, new means for depositing surface films, and an improved understanding of the molecular-scale mechanical response of materials.



Supercomputer simulations show what happens as a cluster of atoms crashes into a surface. (Color slides and B&W prints available)

"This kind of collision produces a transient medium characterized by extremely high density, pressure and temperature, and under such conditions one can expect that new chemistry will happen," said Landman. "We have very little knowledge about chemistry under these extreme conditions. Compounds that

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may not form under normal conditions may be produced under these circumstances."

Clusters moving at 2-5 kilometers per second create pressures of up to 100,000 atmospheres, and temperatures as high as 4,000 degrees Kelvin -- more than ten times room temperature -- when they hit a solid surface. Georgia Tech modeling shows that the volume of materials which are normally quite incompressible could be reduced by as much as 40 percent in such an environment.

Under such extreme conditions, which last for brief times on the order of picoseconds, atoms are moved much closer together than normal and their ability to share energy is greatly reduced.

"Most of our analytical theories and our knowledge of equilibrium thermodynamics are invalid under these conditions," Landman added. "It is like the chemistry inside a hand grenade, a very explosive sort of situation."

Chemists now use materials known as catalysts to promote reactions which do not occur at sufficient rates under normal conditions. Landman believes the collision of clusters could act to catalyze and promote reactions that are difficult or impossible to generate otherwise.

The microscopic crashes create extreme consequences because the hundreds of atoms in the cluster interact with each other much like the automobiles in the chain reaction freeway collision.

As atoms in the leading edge of the cluster contact the solid surface, their velocities drop precipitously. But the atoms immediately behind them are still moving at high speed, and that causes an atomic pile-up as they crash into the front edge of the cluster. The pile-up creates in the inertially confined medium a phenomena known as a shock wave, which for a few picoseconds compresses the cluster into a much smaller volume.

That compression unleashes tremendous energy able to break chemical bonds and alter other atomic characteristics.

"You concentrate large amounts of energy in a small volume of space over a very short period of time," Landman noted. "That's the new aspect this brings to chemistry."

Approximately three-quarters of the energy is absorbed by the substrate material hit by the cluster. That creates shock waves which can alter the surface of the material, creating tiny craters about the same width as the cluster.

"It's like a small meteorite of 500 to 1,000 atoms coming into a solid and forming a crater," he said. "It forms a very significant but localized deformation."

After the impact, shock pulses also move in a direction opposite to the shock wave traveling through the solid. That causes portions of the cluster to explode outward and laterally, ultimately spreading across the surface of the solid.

The speed at which the clusters strike the surface can be important, the researchers found. At velocities close to ten kilometers per second, the cluster may embed itself in the surface, but at less than one kilometer per second, collision forces decline significantly.

Because materials aggregates under such transient high pressure, temperature and density conditions have not been studied before, it is difficult to predict the kinds of chemical reactions that may result. Landman speculates that organic molecules may emerge: "It is not unlikely that such extreme conditions could produce molecules of biological significance if you choose the collision partners properly."

Landman hopes other scientists will study the phenomena experimentally, investigating in laboratory experiments the observations made through theoretical supercomputer-based simulations.

The Georgia Tech researchers studied the effects of crashing argon clusters into a surface of sodium chloride, but Landman said the results apply to broad classes of materials.

Since submission of the Science paper, Landman, Cleveland and Dr. H.P. Cheng -- also in the School of Physics -- have been exploring how the microscopic crashes will affect tiny salt crystals of sodium chloride and sodium fluoride. The research suggests that a new type of fragmentation or fracture may occur, opening yet another set of research possibilities.

"What we find is a selective fracture effect," Landman said. "When these nano-crystalline clusters hit a solid surface, they fracture in a very selective way. These nano-fracture events do not proceed by the same mechanisms as fracture of macroscopic bodies."

Preliminary studies show that fracture in these systems can occur without the generation of dislocations -- a phenomena that may be unique to nano-scale materials.

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