Explosives at the microscopic scale produce shocking results

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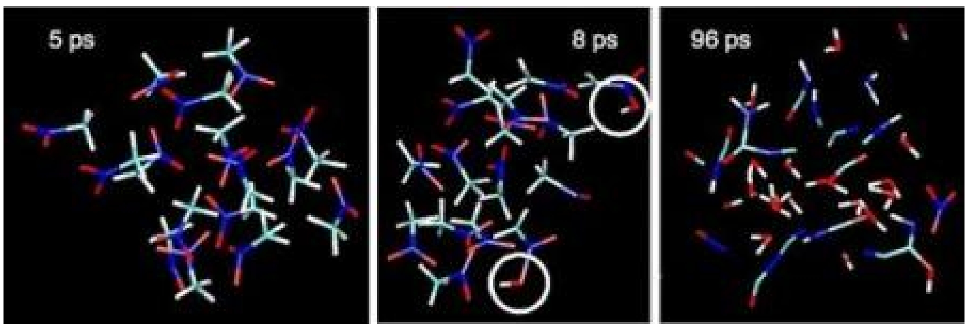

Snapshots during a simulation of detonating nitromethane at three different times. At 5 picoseconds behind the detonation shock front (1 picosecond = one millionth of a millionth of one second), the shock has compressed the nitromethane molecules into a hot, dense liquid-like state. The first reactions occur around 8 picoseconds: hydrogen atoms are transferred to the oxygen atoms on the same molecule (white circles). Near the end of the simulation at 96 picoseconds, a mixture of transient and stable molecules exist including H2O, CO2, and HNC, HNCO. (Carbon=green, Hydrogen=white, Nitrogen=blue, Oxygen=red.)

U.S. troops blew up enemy bridges with explosives in World War II to slow the advance of supplies or enemy forces.

In modern times, patrollers use explosives at ski resorts to purposely create avalanches so the runs are safer when skiers arrive.

Other than creating the desired effect (a destroyed bridge or avalanche), the users didn't exactly know the microscopic details and extreme states of matter found within a detonating high explosive.

In fact, most scientists don't know what happens either.

But researchers from Lawrence Livermore National Laboratory and the Massachusetts Institute of Technology have created the first quantum molecular dynamics simulation of a shocked explosive near detonation conditions, to reveal what happens at the microscopic scale.

What they found is quite riveting: The explosive, nitromethane, undergoes a chemical decomposition and a transformation into a semi-metallic state for a limited distance behind the detonation front.

Nitromethane is a more energetic high explosive than TNT, although TNT has a higher velocity of detonation and shattering power against hard targets. Nitromethane is oxygen poor, but when mixed with ammonium nitrate can be extremely lethal, such as in the bombing of the Alfred P. Murrah Federal Building in Oklahoma City.

"Despite the extensive production and use of explosives for more than a century, their basic microscopic properties during detonation haven't been unraveled," said Evan Reed, the lead author of a paper appearing in the Dec. 9 online edition of the journal, *Nature Physics*. "We've gotten the first glimpse of the properties by performing the first quantum molecular dynamics simulation."

In 2005 alone, 3.2 billion kilograms of explosives were sold in the United States for a wide range of applications, including mining, demolition and military applications.

Nitromethane is burned as a fuel in drag racing autos, but also can be made to detonate, a special kind of burning in which the material undergoes a much faster and far more violent type of chemical transformation. With its single nitrogen dioxide (NO2) group, it is a simple representative version of explosives with more NO2 groups.

Though it is an optically transparent, electrically insulating material, it undergoes a shocking transformation: It turns into an optically reflecting, nearly metallic state for a short time behind the detonation shock wave front.

But further behind the wave front, the material returns to being optically transparent and electrically insulating.

"This is the first observation of this behavior in a molecular dynamics simulation of a shocked material," Reed said. "Ultimately, we may be able to create computer simulations of detonation properties of new, yet-to-be synthesized designer explosives."

Source: Lawrence Livermore National Laboratory

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