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Birck Nanotechnology Center, Room 2001

High Explosives: Chemistry at Supersonic Speeds

Safely controlling the behavior of high explosives is an extremely challenging scientific problem at the interface of hydrodynamics and chemistry. The same energetic materials can be used as propellants, with burn rates ~mm/sec, or in detonations, with propagation velocities of km/sec, depending upon the ignition and confinement conditions. Understanding how the reaction chemistry couples to these local conditions is then critical for improving the safety margins in the use and design of energetic formulations. This can be addressed using reactive molecular dynamics simulations, though fairly large-scale simulations are required in order to describe the features of interest. Reducing the results of those simulations to simple models that can be used in hydrodynamics simulations then becomes the challenge. A new method for analyzing the complex chemistry found in these large simulations will be presented and discussed.

Ed Kober received his BS in chemistry (with honors) from Caltech in 1977 and his PhD in inorganic chemistry from the University of North Carolina at Chapel Hill in 1982. He started working at Los Alamos National Laboratory in 1985 in the area of molecular simulations applied to spectroscopy and reaction analysis. He has subsequently also performed research in the areas of mesoscale and continuum hydrocode simulations, primarily related to high explosives and shock physics. He has served as both a group leader and project leader in the area of high explosives simulations. His current research interests are methods for analyzing molecular dynamics simulations and general techniques for the integration of multiscale simulations.