Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Toward a reaction rate model of condensed-phase RDX decomposition under high temperatures[1] IGOR SCHWEIGERT, US Naval Research Laboratory — Shock ignition of energetic molecular solids is driven by microstructural heterogeneities, at which even moderate stresses can result in sufficiently high temperatures to initiate material decomposition and the release of the chemical energy. Mesoscale modeling of these "hot spots" requires a chemical reaction rate model that describes the energy release with a sub-microsecond resolution and under a wide range of temperatures. No such model is available even for well-studied energetic materials such as RDX. In this presentation, I will describe an ongoing effort to develop a reaction rate model of condensed-phase RDX decomposition under high temperatures using first-principles molecular dynamics, transition-state theory, and reaction network analysis.

[1]This work was supported by the Naval Research Laboratory, by the Office of Naval Research, and by the DOD High Performance Computing Modernization Program Software Application Institute for Multiscale Reactive Modeling of Insensitive Munitions.

Igor Schweigert
US Naval Research Laboratory

Date submitted: 15 Nov 2013 Electronic form version 1.4