Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Analysis of direct and indirect phonon-mediated bond excitation in the explosive RDX BRENT KRACZEK, PETER W. CHUNG, US Army Research Laboratory — Understanding detonation pathways is essential to controlling the sensitivity of high energy explosives. Central to these pathways is initiation, the initial chemical reactions that lead to detonation. Phonons play an active role in initiation caused by compressive wave energy, such as those caused by shock loading, by converting the wave energy to thermal energy that causes bond-breaking. In the conventional model for phonon-mediated initiation energy follows an indirect route, in which the wave energy excites low-frequency phonons which in turn excite higher-frequency vibrons that break the key initial bonds in the chemical decomposition pathways. Using lattice dynamics calculations of α-RDX (the crystalline α-phase of cyclotrimethylene trinitramine), we find that a direct route of energy transfer is more likely. We have calculated the total energy available to different phonon modes and the fractions of the mode energies that go into the bonds of the material. This enabled approximation of the maximum and minimum energy exciting the bonds due to different phonon modes throughout thermal relaxation. We find that low-frequency modes provide significantly more energy than high-frequency modes to the key bonds, implying that the direct pathway is responsible.

Brent Kraczek
US Army Research Laboratory

Date submitted: 08 Nov 2012 Electronic form version 1.4