

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Ultrafast semi-metallic layer formation in detonating nitromethane¹ EVAN REED, M. RIAD MANAA, LAURENCE FRIED, KURT GLAESEMANN, Lawrence Livermore National Laboratory, JOHN JOANNOPOULOS, Massachusetts Institute of Technology — We present the first quantum molecular dynamics simulations behind a detonation front (up to 0.2 ns) of the explosive nitromethane (CH_3NO_2) represented by the density-functional-based tight-binding method (DFTB). This simulation is enabled by our recently developed multi-scale shock wave molecular dynamics technique (MSST) that opens the door to longer duration simulations by several orders of magnitude. The electronic density of states around the Fermi energy initially increases as metastable material states are produced but then later decreases, perhaps unexpectedly. These changes indicate that the shock front is characterized by an increase in optical thickness and conductivity followed by a reduction around 100 picoseconds behind the front. We find that a significant population of intermediate metastable molecules are charged and charged species play an important role in the density of states evolution. The transient transformation to a semi-metallic state can be understood within the Anderson picture of metallization.

¹This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Evan Reed
Lawrence Livermore National Laboratory

Date submitted: 26 Nov 2007

Electronic form version 1.4