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Long timescale dynamics of shocked nitromethane LAURENCE FRIED, EVAN REED, RIAD MANAA, Lawrence Livermore National Laboratory, KURT GLAESEMANN, JOHN JOANNOPOULOS, Massachusetts Institute of Technology — We present the farthest ever glimpse behind the shock front in a chemically reactive molecular dynamics simulation by applying a multi-scale shock wave simulation technique to the study of chemical reactions in shocked nitromethane (CH3NO2) represented by the DFTB tightbinding method. Shock speeds from 5.5 km/s to 8 km/s are simulated for durations up to 0.8 ns demonstrating substantial computational savings compared with the non-equilibrium molecular dynamics (NEMD)shock simulation approach. These simulations indicate that the reaction zone in detonating nitromethane is greater than 0.3 μm in length. Ionic species are found to be prevalent in the early reactions of shocked nitromethane. Results are consistent with available experimental data. As a validation of our multiscale approach, we compare spatial wave profiles computed with the multiscale technique to profiles computed using the NEMD approach.

Laurence Fried
Lawrence Livermore National Laboratory

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