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Simulations of the chemistry of shocked energetic materials on the nanosecond timescale¹

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The initiation of chemistry by a shock wave occurs through complex interactions between chemical and mechanical mechanisms. The first few nanoseconds after shock arrival is a crucial time period, where the initiation of exothermic chemical reactions leads to the growth of local hot spots. We are simulating these mechanisms in two ways. First, we are performing atomistic simulations of shocked TATB using a modified version of the ReaxFF force field. We have found that modification of ReaxFF is necessary in order to accurately model charge transfer and ionization under sustained high density conditions. We have simulated overdriven detonation waves in TATB using the multi-scale shock technique (MSST). In our simulations of overdriven shocked TATB, we find that large-scale graphitic structures encompassing thousands of atoms form after 1 ns. A second simulation technique uses continuum mechanics with an anisotropic crystal-level plasticity model for shocked HMX. We use a thermochemical approach to model the equation of state and chemistry of the shocked energetic material. In the simulations a pore is compressed by a shock wave, resulting in material deformation and chemistry. We find that simulations with crystal-level plasticity predict chemistry that is localized in fluid regions. The results of the crystal plasticity model will be compared with a more traditional treatment of plasticity in HMX via shock viscosity.

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