

## Simulation of the solid-phase decomposition of RDX

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RDX, a cyclic nitramine, releases a large amount of energy upon bulk decomposition, making this compound an important ingredient for various propellants and explosive materials. Over the last years the decomposition pathways of this compound have been the focus of both experimental and computational studies. Both these types of study face major problems when applied to fast-reacting explosive compounds like RDX. Experimental studies are complicated due to the extremely short time-scale in which the vital initial steps of the explosion take place. These short time-scales are not problematic for computational studies, however, the quantumchemical methods that need to be used to simulate the RDX-dissociation are very time-consuming, virtually restricting their application to intramolecular reactions in single RDX-monomers, ignoring the effects of intermolecular reactions that could be important in solid-phase decomposition.

To overcome the time-restraints hindering application of computational methods from application to solid-phase RDX we have developed a bond-order dependent empirical force-field based method able to simulate the reactive behavior of CHNO-containing compounds. For systems of around 1000 atoms this reactive force field (ReaxFF) can simulate chemical reactivity at around a million times faster than quantumchemical methods, thus opening up the possibility to simulate bulk reactions, including both inter- and intramolecular rearrangements. This force field has been tested against a large set of data, including both 'non-reactive' data like heats of formation and geometries of stable CHNO-compounds as well as 'reactive' data like dissociation of single-, double- and triple bonds and the quantumchemical energies for the intramolecular dissociation pathways for RDX. To demonstrate the potential of the reactive force field method we have applied it in a series of shock simulations, in which small RDX-crystal fragments are collided with each other at increasing velocities. These simulations show a distinct impact detonation threshold for RDX, above which the explosive reactions commences. Furthermore, the simulations performed at impact velocities above the detonation threshold yield product distributions that looks very reasonable. By being able to identify such macroscopical parameters as detonation thresholds and explosive product distributions, the reactive force field method allows for a direct link between experimental and computational data, making it a very useful tool for the study of these chemically complicated systems.