Coarse Grain Simulations of RDX Using DPD-RX: Effects of Interfaces and Voids

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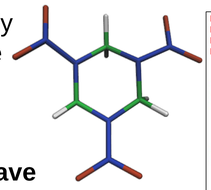
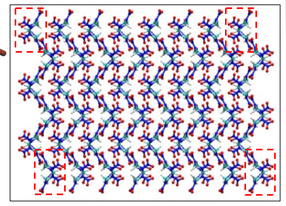
1. Introduction and Objective

RDX is a commonly used non-sensitive explosive that is a crystal at ambient conditions.

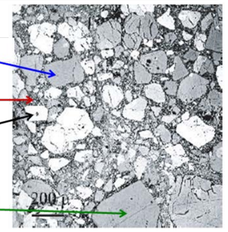




All composites have impurities and interfaces.

Several simulation systems were devised with a two-fold purpose:

- **to develop realistic RDX crystal structures**
- **test the robustness of the DPD-RX model under a variety of system conditions**

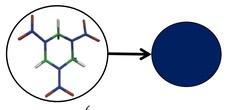


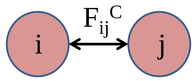
composite – microstructures – nano-scale structures

2. DPD Coarse-Grain Method

Single-site coarse-grained (**CG**) potential via *force matching* to RDX center of mass results in loss of degrees of freedom. Dissipative Particle Dynamics (**DPD**) uses additional forces (dissipative and random) to recapture lost atomistic degrees of freedom (**DoF**).

Position $\frac{dr_i}{dt} = v_i(t)$





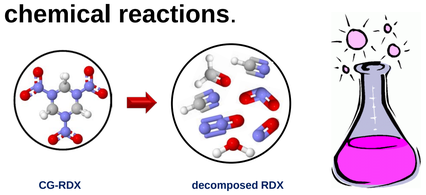
Velocity $m_i \frac{dv_i}{dt} = f_i(t) = \sum_{i \neq j} \left(F_{ij}^C + F_{ij}^D + F_{ij}^R \right)$ **Force**

CG = *more* computational efficiency *fewer* DoF

Sergei Izvekov and Joshua D. Moore

3. DPD-RX Method

The **DPD-RX** method accounts for RDX undergoing **chemical reactions**.



RDX→ 3HCN + 3/2(NO_2 + NO + H_2O)

$HCN + NO_2 \rightarrow NO + ½(N_2 + H_2) + CO$
$HCN + NO \rightarrow CO + N_2 + ½H_2$
$NO + CO \rightarrow ½N_2 + CO_2$

	Initial	Final
RDX	1.0	???
HCN	0.0	???
NO_2	0.0	???
NO	0.0	???
N_2	0.0	???
H_2	0.0	???
CO	0.0	???
CO_2	0.0	???
H_20	0.0	???

John K. Brennan, Joshua D. Moore, James P. Larentzos, and Martin Lísal

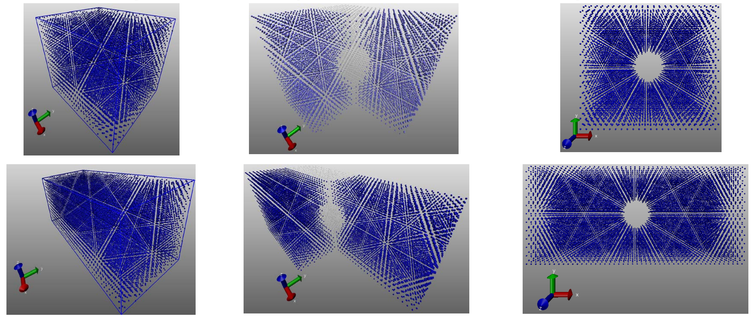
4. RDX Microstructure Simulations

DPD Simulations

Perfect Crystal | Spherical Void | Cylindrical Void

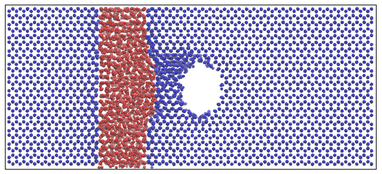
Cube

Rectangular Block

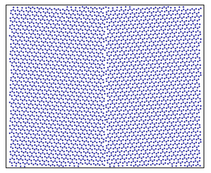


Void and Grain Boundary Simulations

time = 2ps

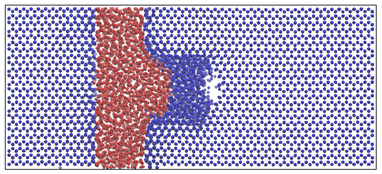


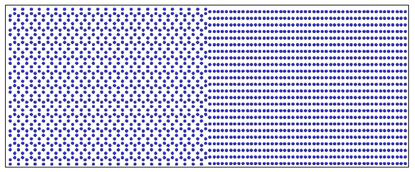
RDX reaction collapsing cylindrical void



Top: tilted grain boundary
Bottom: rotated grain boundary

time = 3ps





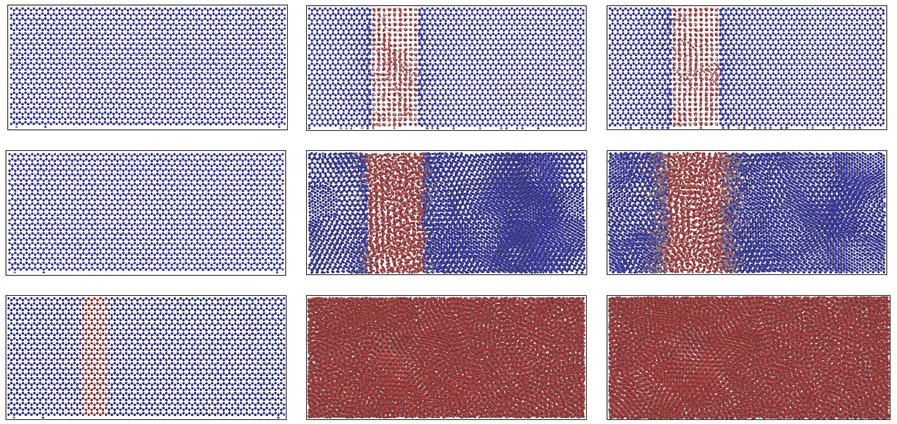
Temperature Variant DPD-RX Simulations

Simulation Time: 0ps | 30ps | 60ps

1800K

2400K

3500K



Low Temperatures:
- reaction does not propagate in timeframe
- products form Exp-6 FCC structure
- bulk crystal grain orientation tilts

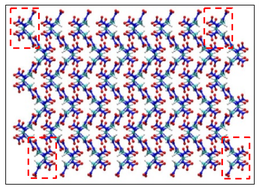
High Temperatures
- reaction propagates unrealistically fast
- lattice becomes disoriented by high pressure

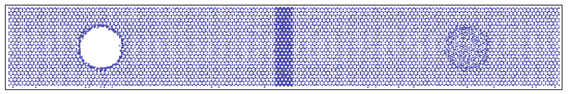
5. Results and Ongoing Work

1) Microstructures

Successfully equilibrated crystal lattice and confirmed with previous work. Created various void and grain boundaries. Ongoing simulations to:

- Create new microstructures
- Increase system sizes



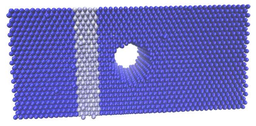


Ignition slab between cylindrical and spherical voids

2) Ignition and Ensemble Methods

Reasonable results from DPD ensembles and DPD-E in simulations thus far. Current plans to:

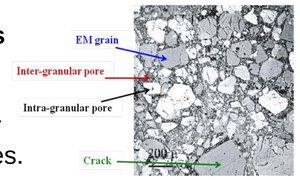
- Analyze reaction propagation through different microstructures
- Compare ignition method from high temperature to pressure shockwave
- Use DPD-H instead of DPD-E for more realistic heat conduction



3) Realistic Composite Results

Future work planned to:

- Analyze periodic boundary conditions for realistic behavior
- Implement more microstructures.



microstructures – meso-scale bridging – composite

6. Acknowledgements

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Back: Michael Sellers, Sergei Izvekov, James Larentzos
Front: John Brennan, Isaac Indgjer

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