

Exercise for Empirical Reactive Force Fields

Shock compression of RDX

ReaxFF is an empirical force field that can treat bond breaking and bond formation. The code was developed at CalTech by Adri van Duin and Bill Goddard. If you are interested in using the code, contact Bill Goddard: wag@wag.caltech.edu.

This exercise will introduce you to atomistic simulation of shocked explosives. It will demonstrate the usefulness of the Reax force field for prediction of shock-induced chemistry. For more information, see Strachan, et al, *Phys Rev. Lett.*, 91(9), 098301 (2003).

The material is RDX, cyclic-[CH₂N(NO₂)₃], and the simulation will involve the collision of 2 unit cells of the material at 10 km/s (10 nm/ps). (One unit cell contains 8 molecules – 168 atoms.) This is a strong shock, allowing you to see results with a reasonable amount of computer time.

The simulation has been run for 100 fs, to make your run-time shorter. The initial geometry is located in 'initial.xyz'. Your starting configuration and velocities are in 'vels'. The sample was equilibrated at 300 K, then the velocity for each atom was increased or decreased by half the impact velocity (in this case, $v_{inp} = 10$ nm/ps).

Input files: ffield – the force field
 control – simulation parameters
 exe – execution script
 geo – input configuration (superceded by 'vels' if 'vels' is present)
 vels – input configuration, velocities

Start the simulation by typing 'exe>&exe.log&'.

Output files: fort.71 – energy and temperature data
 xmolout – trajectory in xyx format
 molfra.out – molecular composition at select timesteps

The trajectory can be viewed with Molden by typing 'molden xmolout' then clicking on Movie (top right of Molden Control window). The temperature and energies can be plotted using gnuplot.

Example:

in gnuplot, typing: plot 'fort.71' u 18:7 will show the temperature as a function of time

As the two RDX clusters collide, chemistry is induced. The reaction (as a whole) is highly exothermic, and small molecules are produced. This decomposition can be monitored using the 'molfra.out' file.