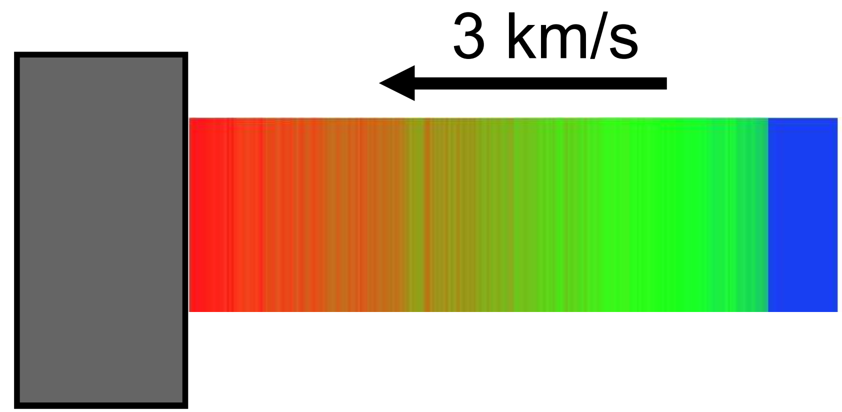
SAND2008-3458P

Explosives under Shock: Simulating PETN using Reactive Molecular Dynamics

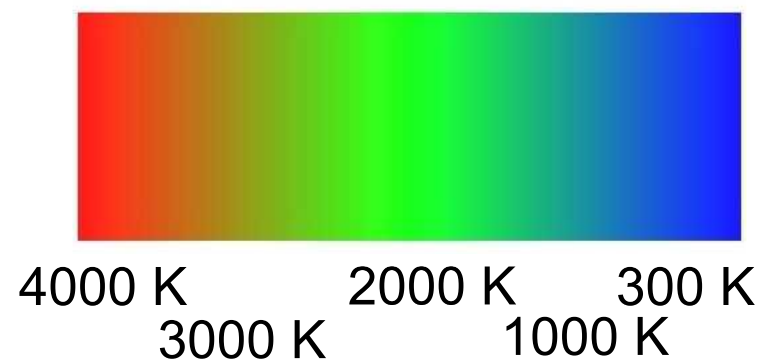
Joanne Budzien

1814, Computational Materials Science and Engineering

Sandia National Laboratories



In collaboration with:
Aidan Thompson, SNL
Sergey Zybin, Caltech

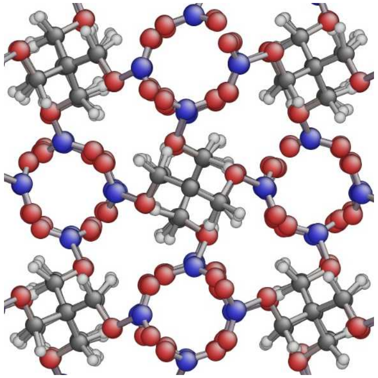


Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

This work uses molecular dynamics simulations to shock a PETN crystal

$$\vec{F} = m\vec{a}$$

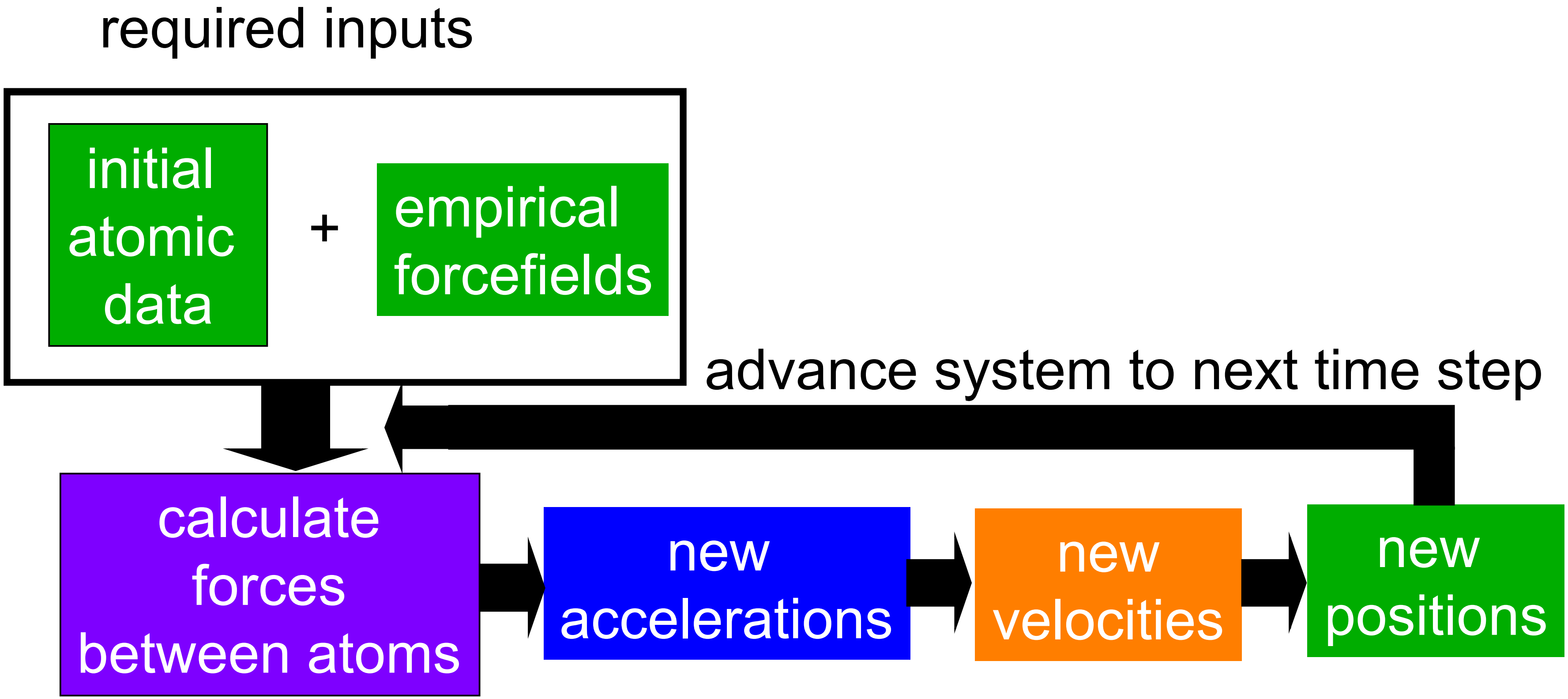
The basics of molecular dynamics



The chemistry of PETN

Comparison of two shock velocities

Molecular dynamics simulations investigate the dynamic properties of atomic systems



$$\vec{F} = m\vec{a}$$

At each time step,
equations of motions are integrated using the atomic information

Reactive forcefields provide QM information at MD speed

ReaxFF

↓

GRASP

↓

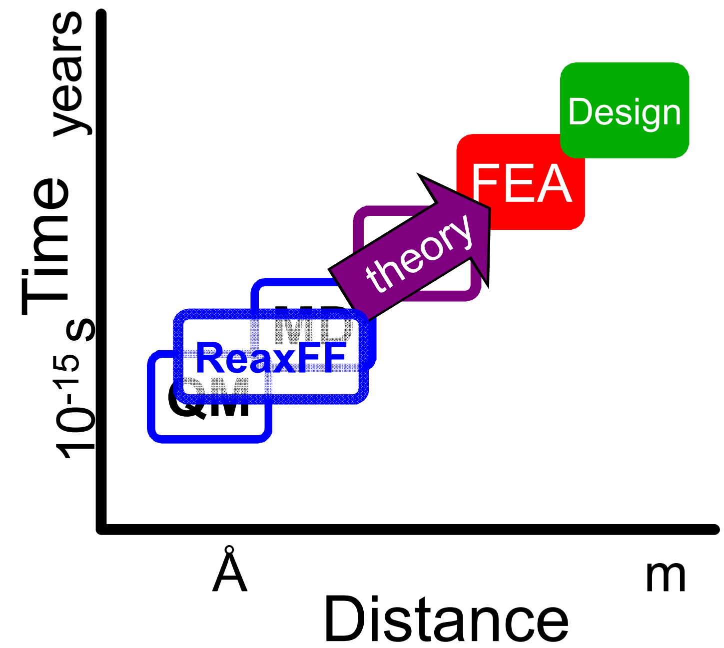
full atomic trajectories

↓

Analysis

↓

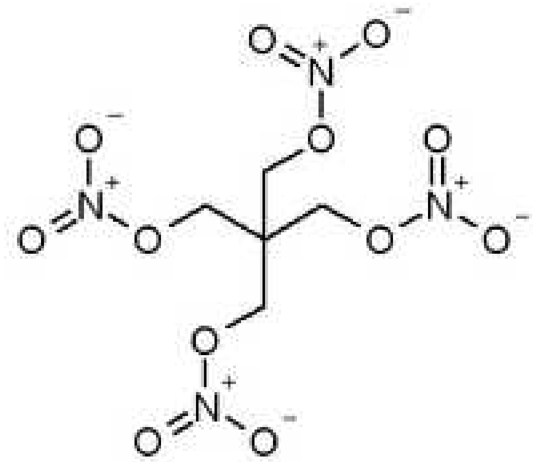
Chemical Insight



Bonds and charges are calculated self-consistently at every step

ReaxFF: van Duin, Dasgupta, Lorant, Goddard J. Phys. Chem. A 105, 9396 (2001)
GRASP: A. P. Thompson, SNL

Pentaerythritol tetranitrate (PETN) is a common explosive



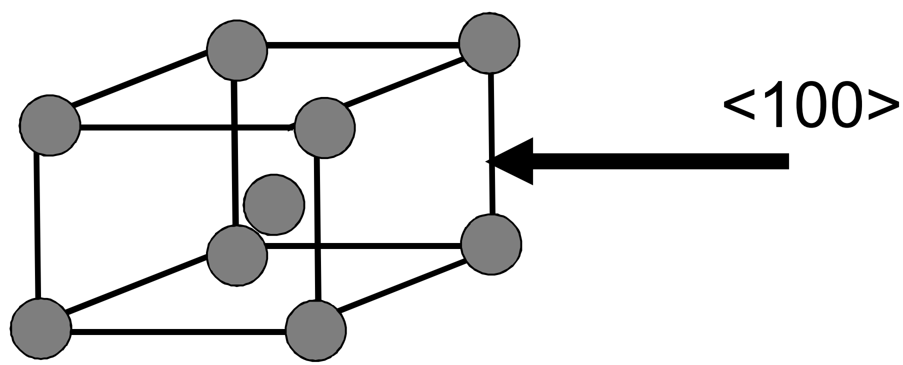
colorless crystals

T_m~141 ^{0}C

used medicinally as a vasodilator

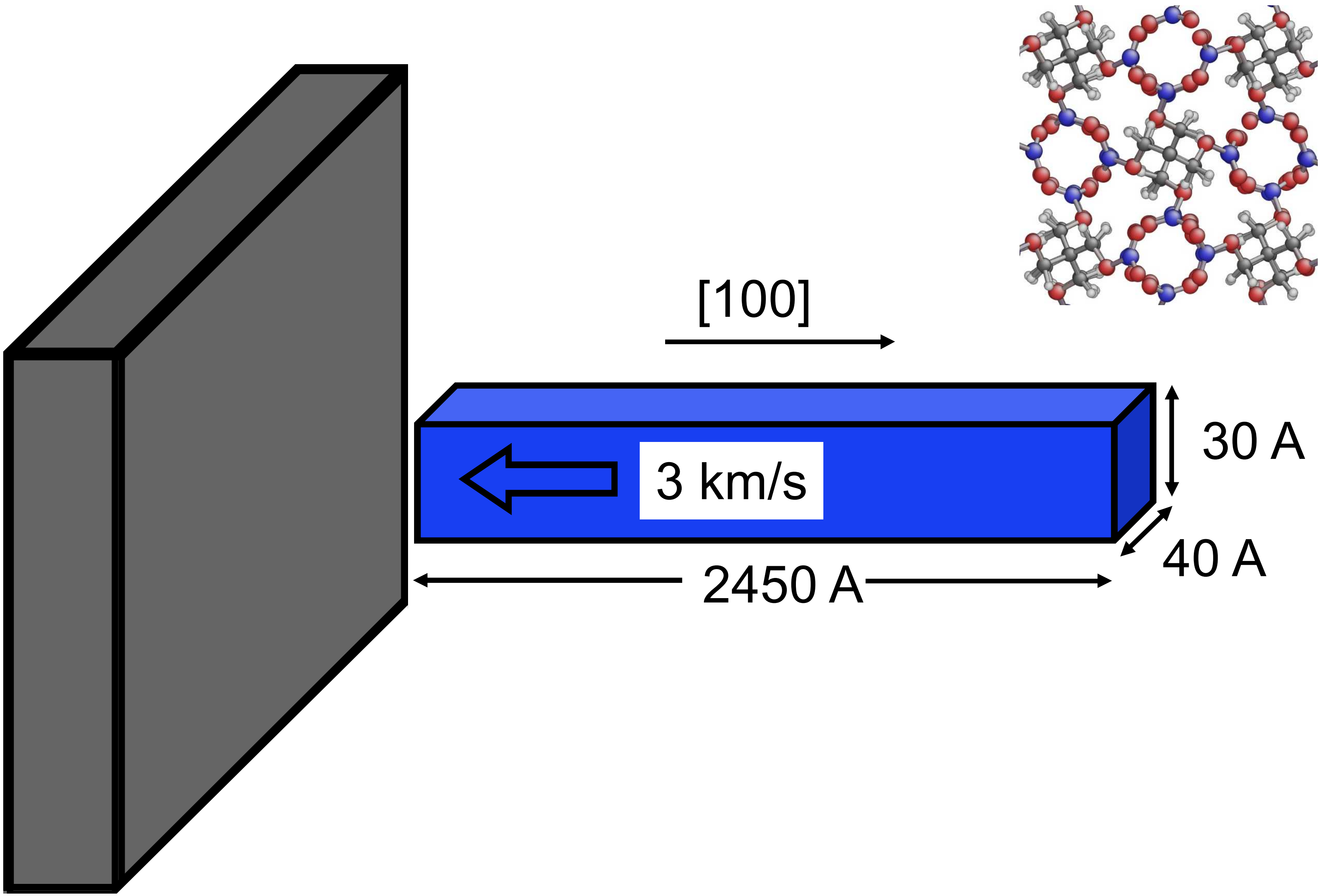
primary component of Semtex

tetragonal, $P\bar{4}2_1c$



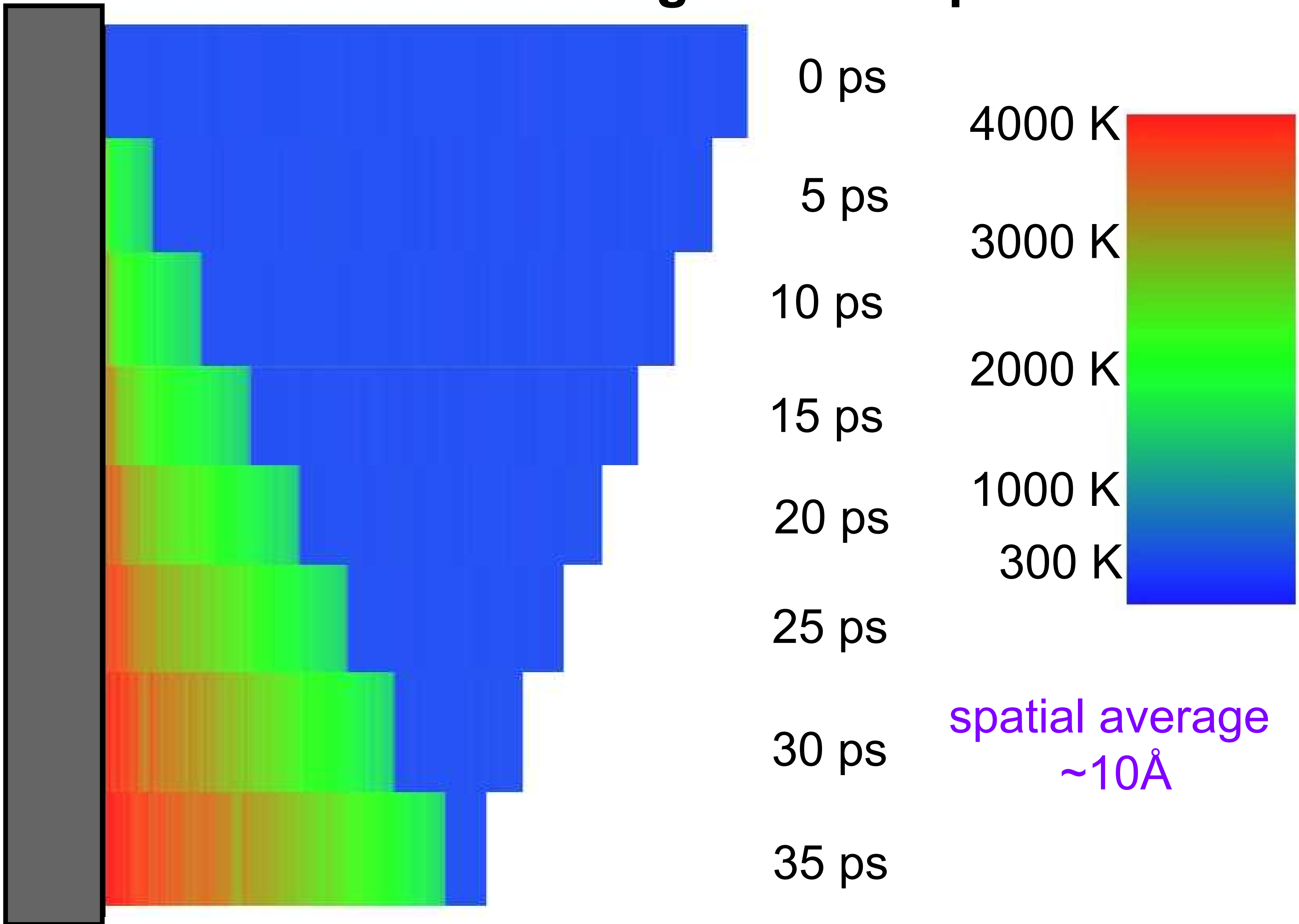
PETN doesn’t burn readily and has been found to be less shock sensitive than many common explosives.

The simulation has a single crystal hitting a piston

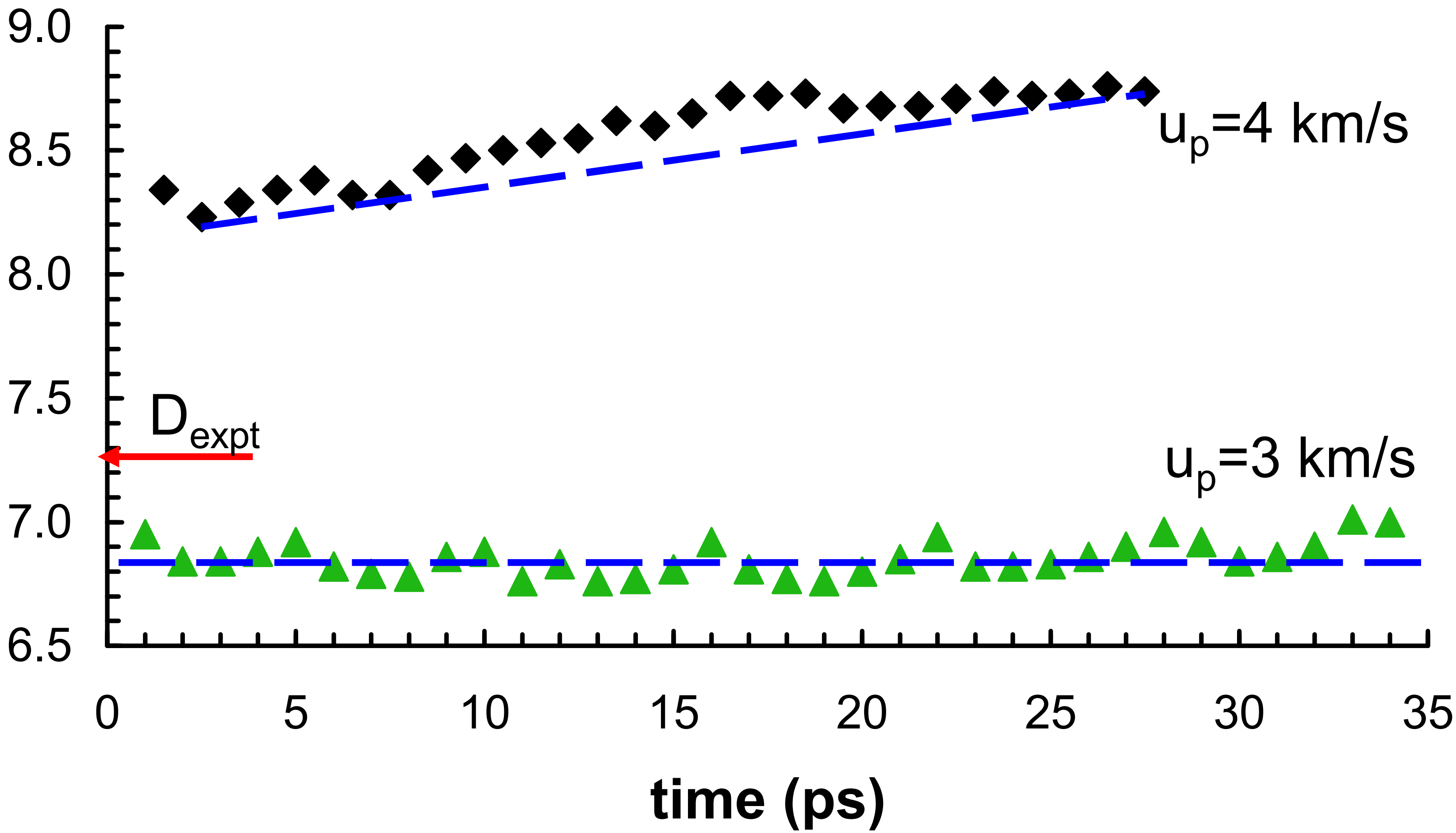


We simulate piston velocities of 3 km/s and 4 km/s, attempting to bracket the shock to detonation transition

Temperature dramatically increases as the shock front moves through the sample

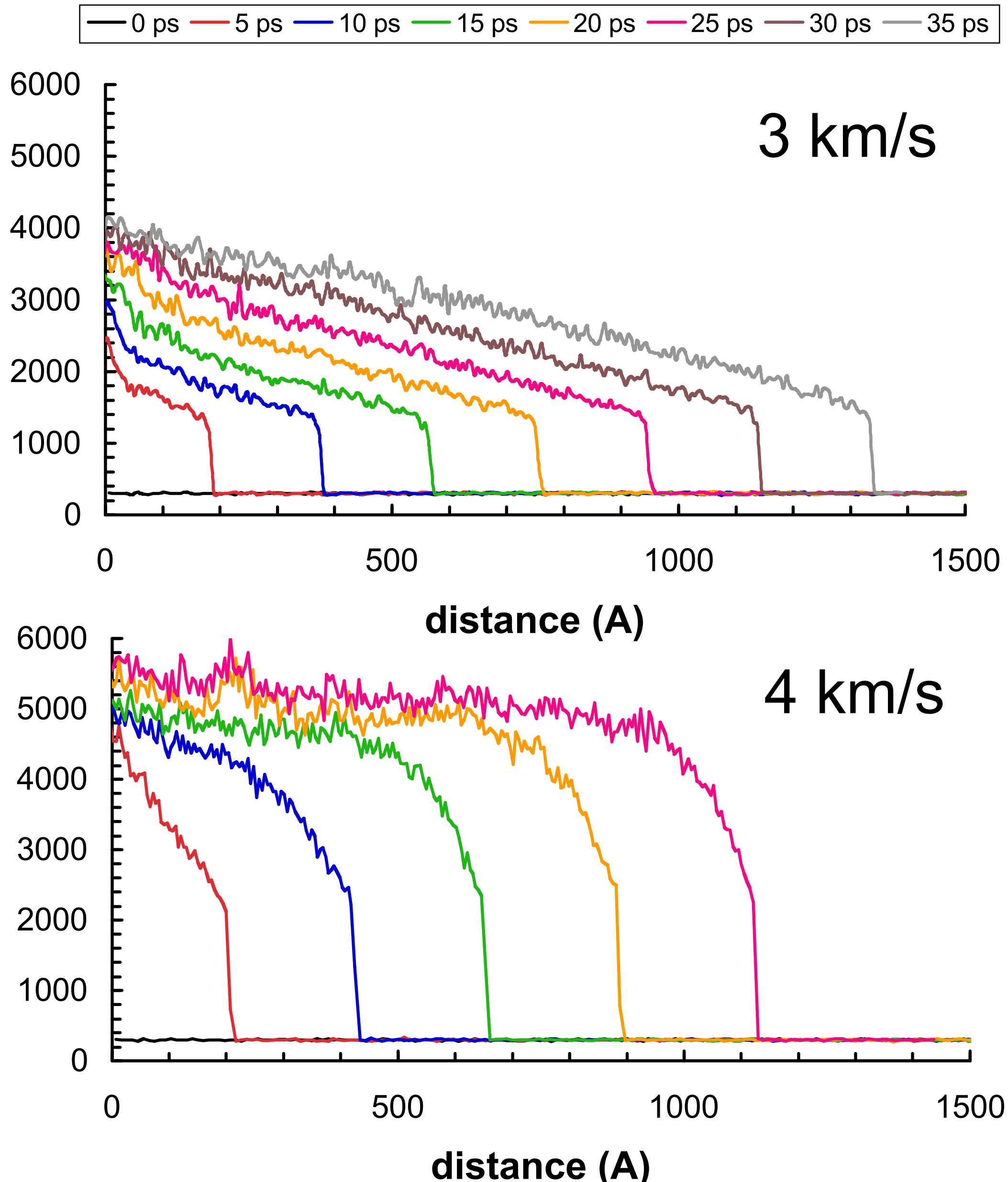


The stronger shock leads to an accelerating shock velocity



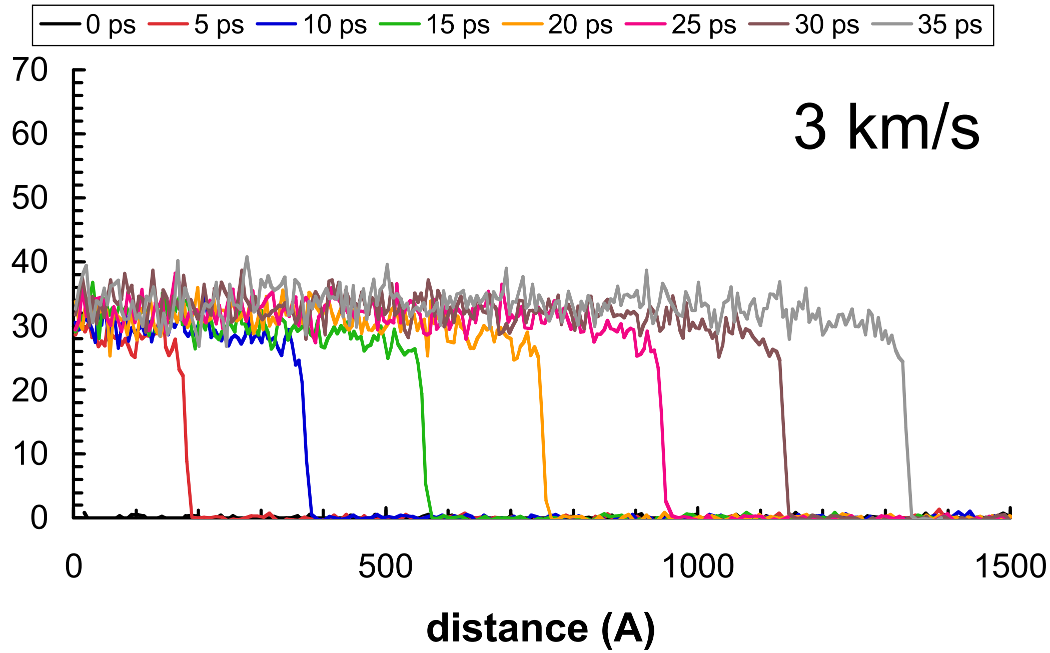
D_{expt} calculated for a density of 1.47 g/cc from
Green and Lee, 13th International Detonation Symposium, Norfolk, VA (July 2006)

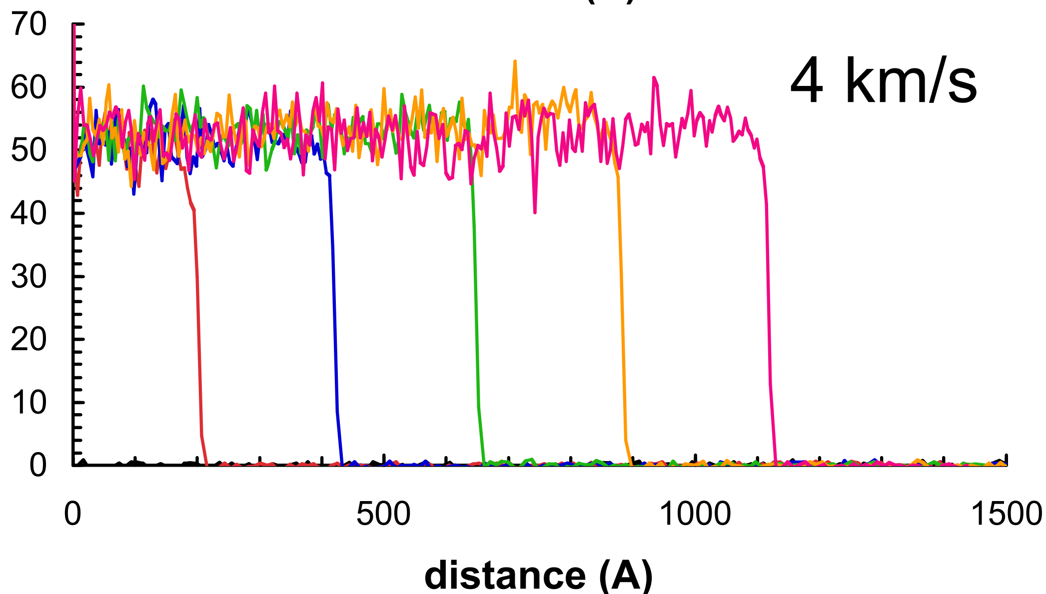
Dramatically increased thermochemical response seen for a stronger shock



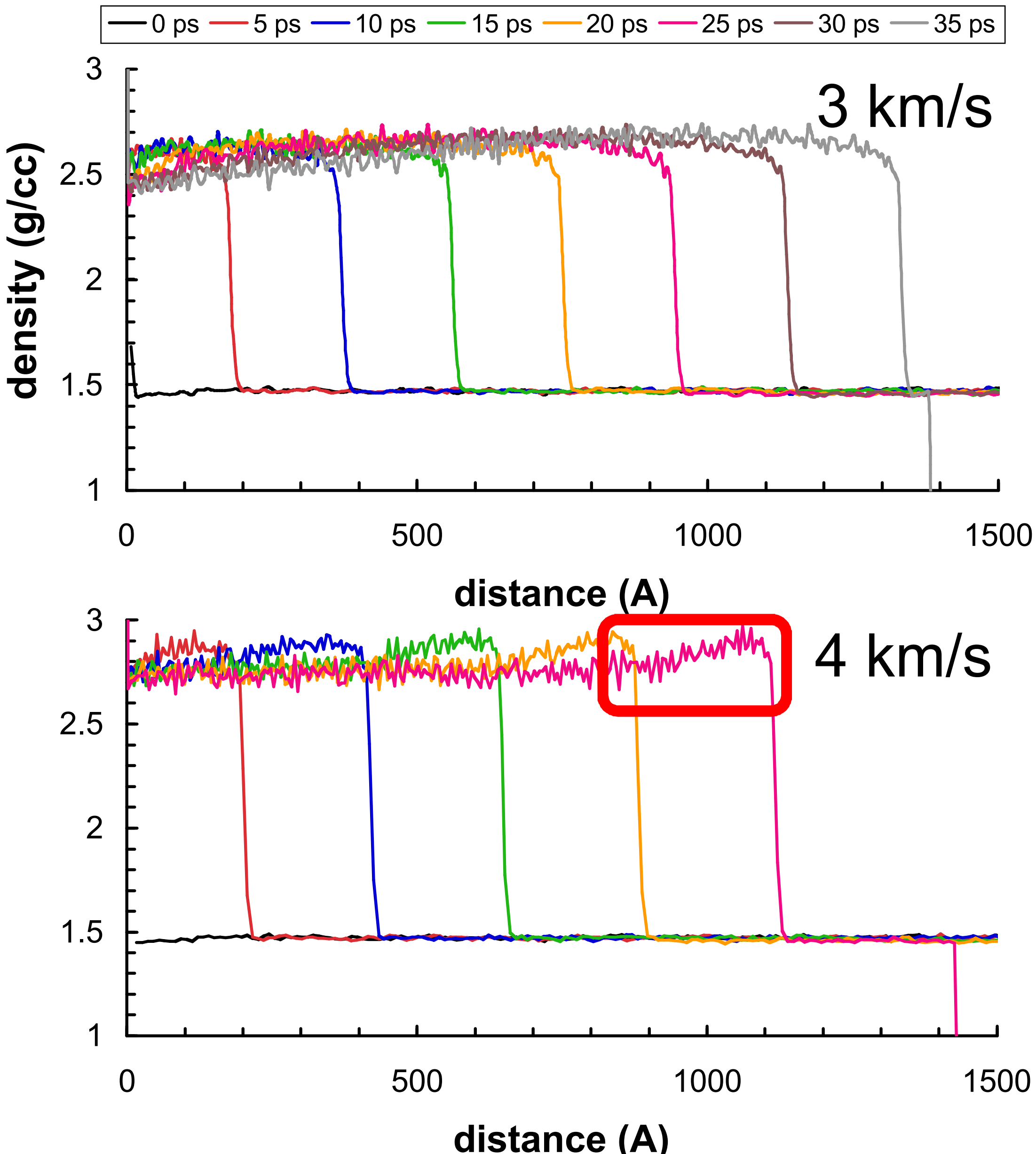
Both systems started at 300K

Pressure is significantly higher for the stronger shock





Peak density is higher and sharper for stronger shock

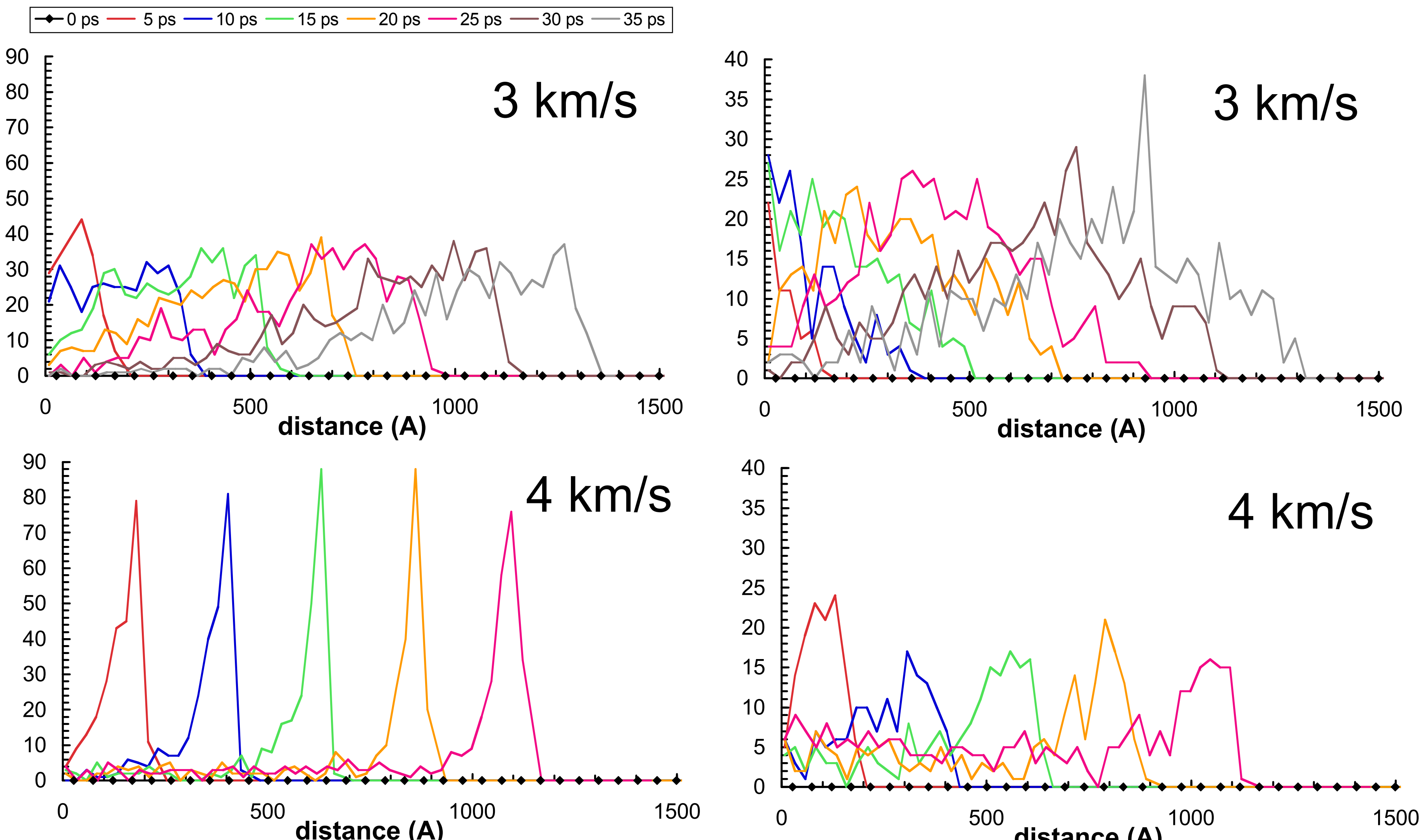


Both systems start at ρ=1.47 g/cc

4 km/s shows a noticeable peak at the shock front

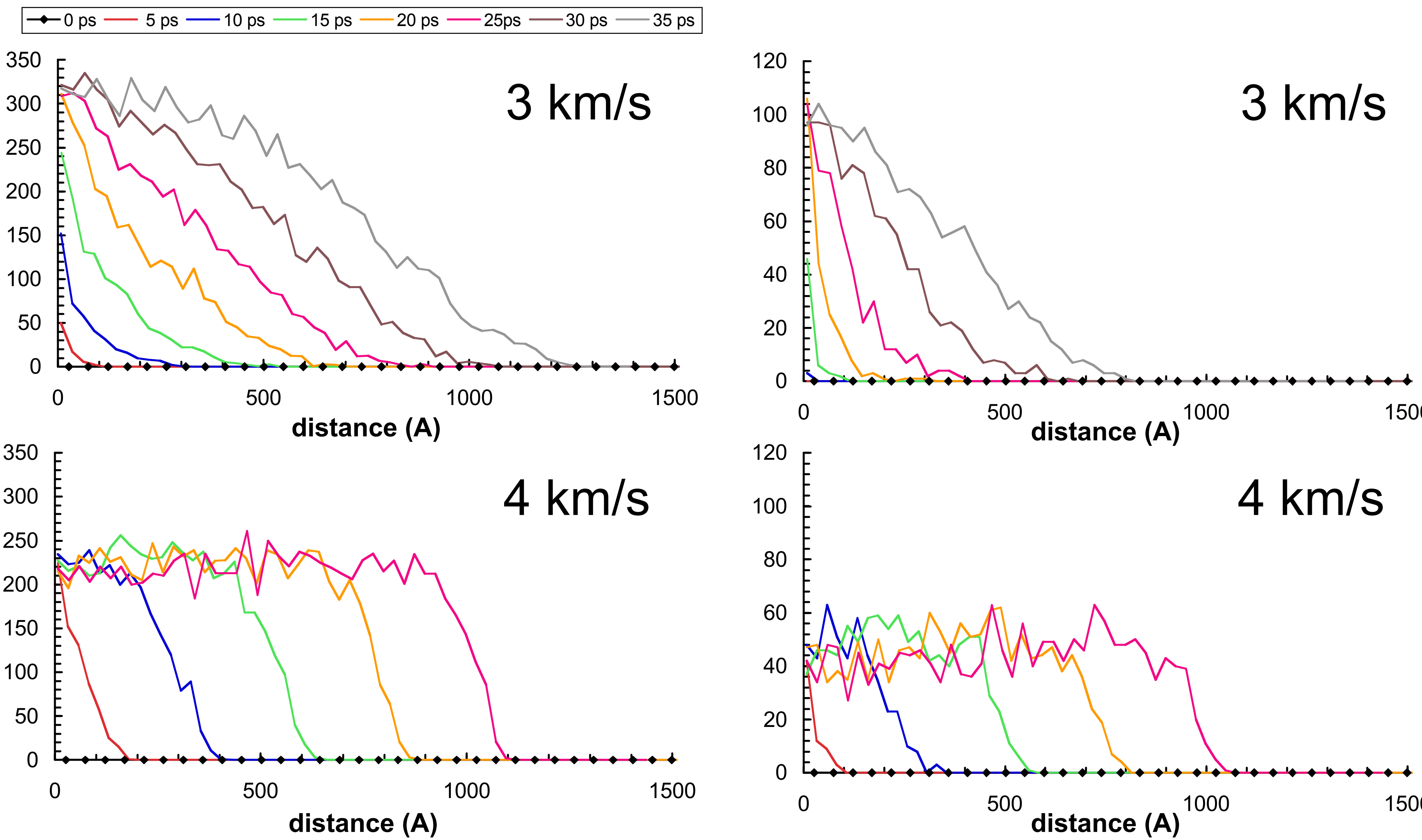
The stronger shock has the primary products quickly react to become secondary products

NO_2	HONO



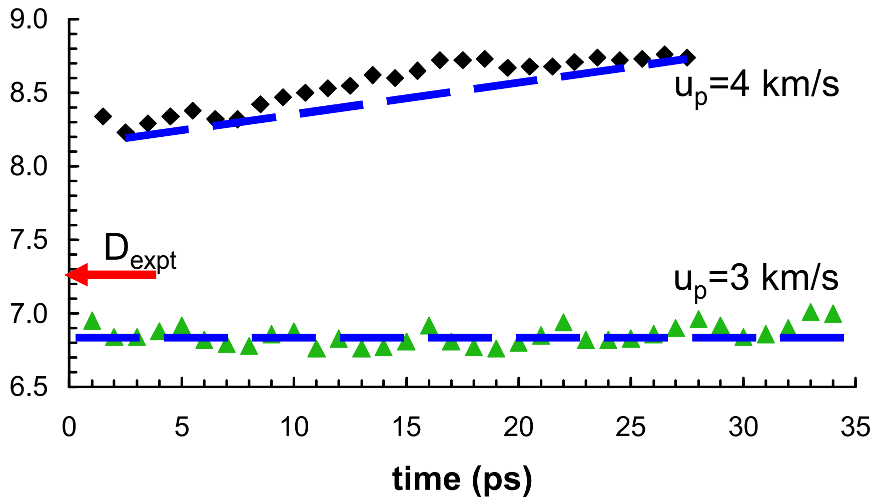
Secondary products form more quickly under stronger shock

H_2O | N_2

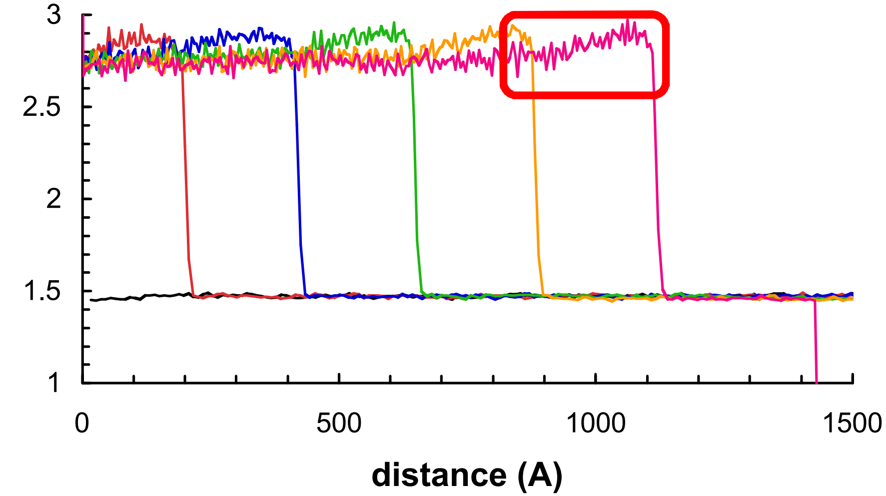


Summary of Strong Shock Results

accelerating shock velocity



density peak behind shock front



high initial temperature rise hastens chemical reactions