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# Reactive Molecular Dynamics Simulations of Shocked PETN

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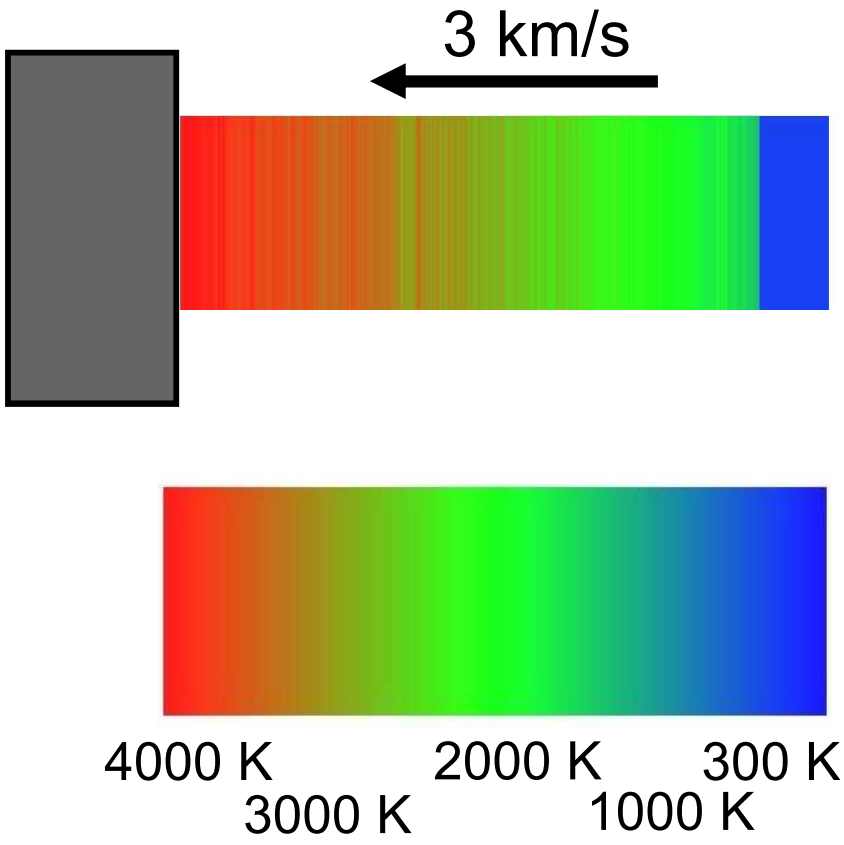



Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

# Reactive forcefields provide QM information at MD speed

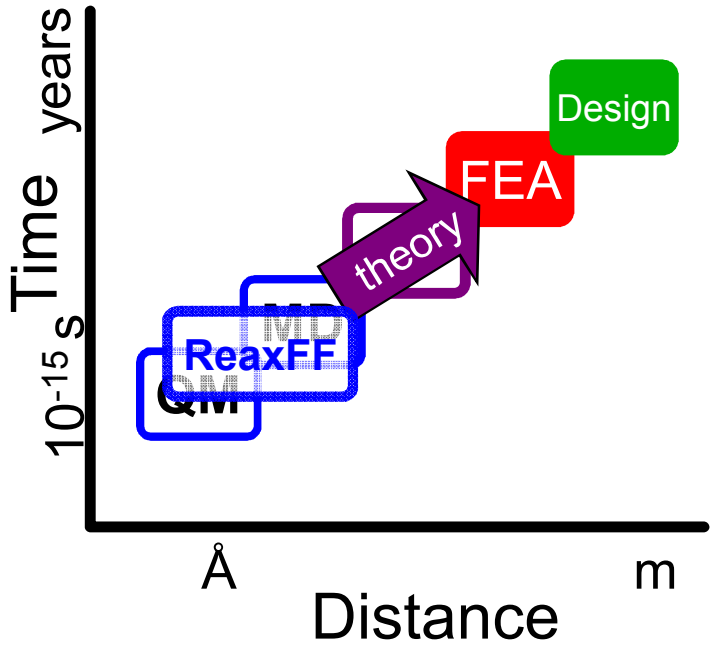
ReaxFF

GRASP

full atomic trajectories

Analysis

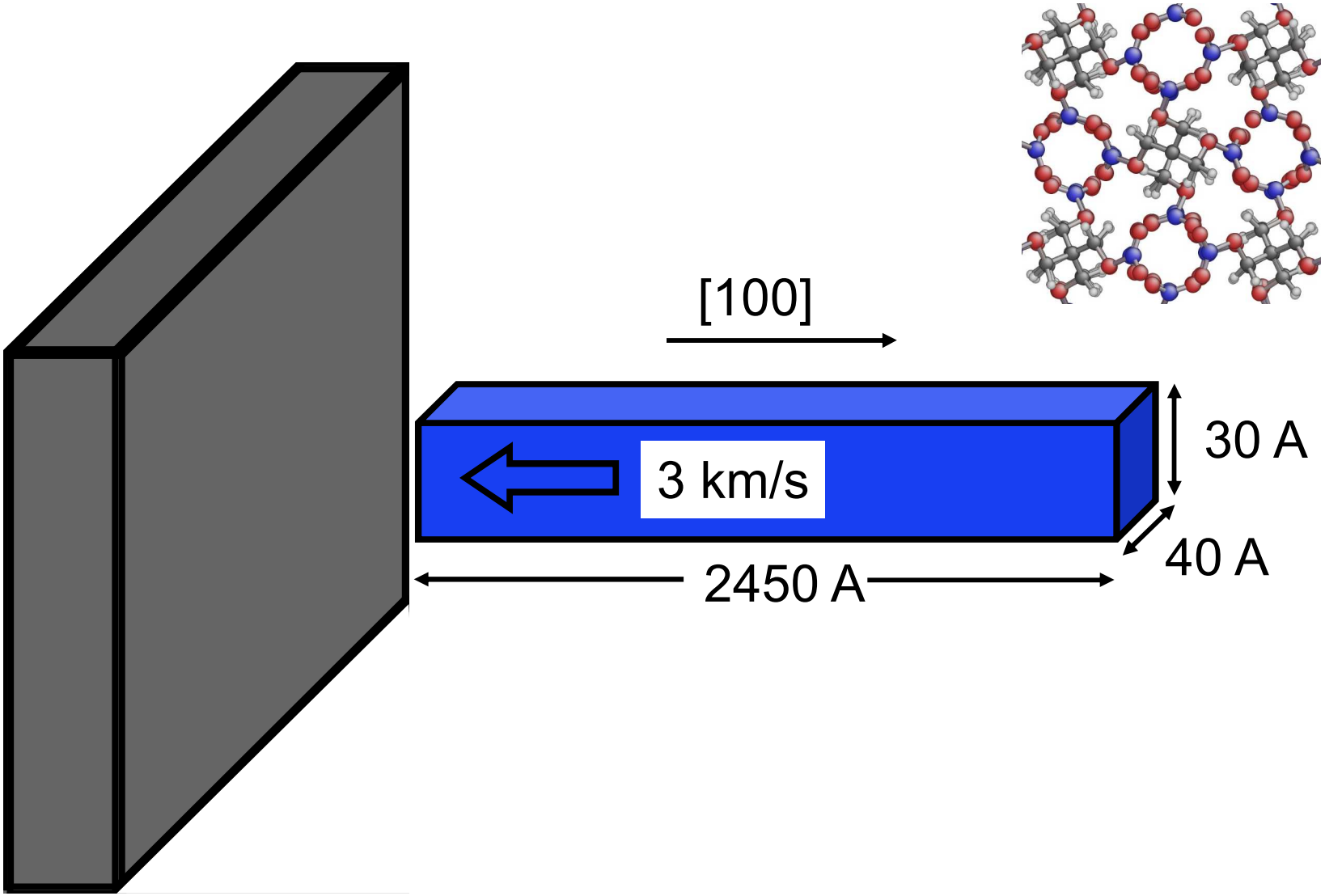
Chemical Insight




**Bonds and charges are calculated self-consistently at every step**

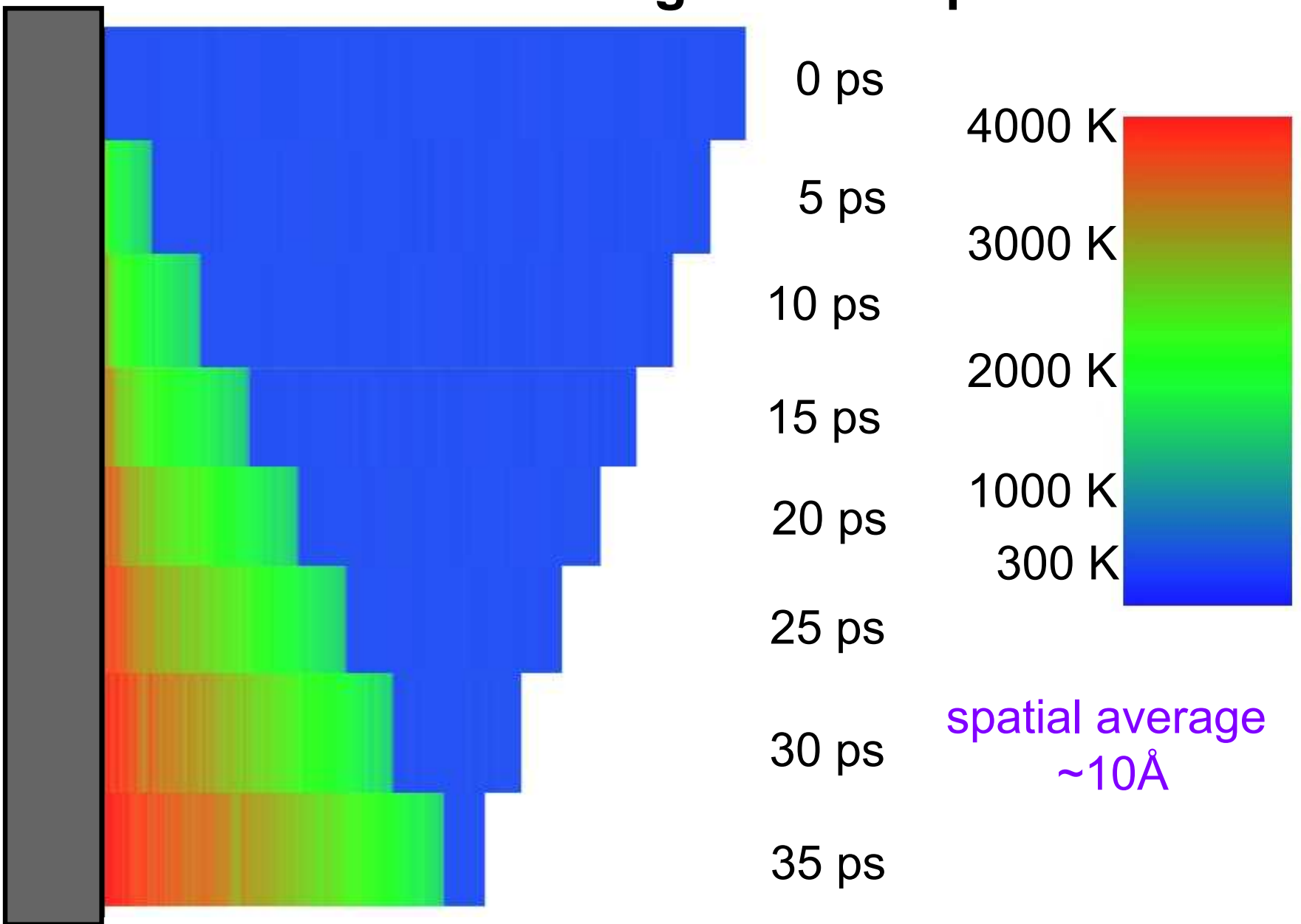
ReaxFF: van Duin, Dasgupta, Lorant, Goddard J. Phys. Chem. A 105, 9396 (2001)

# The simulation has a single crystal hitting a piston

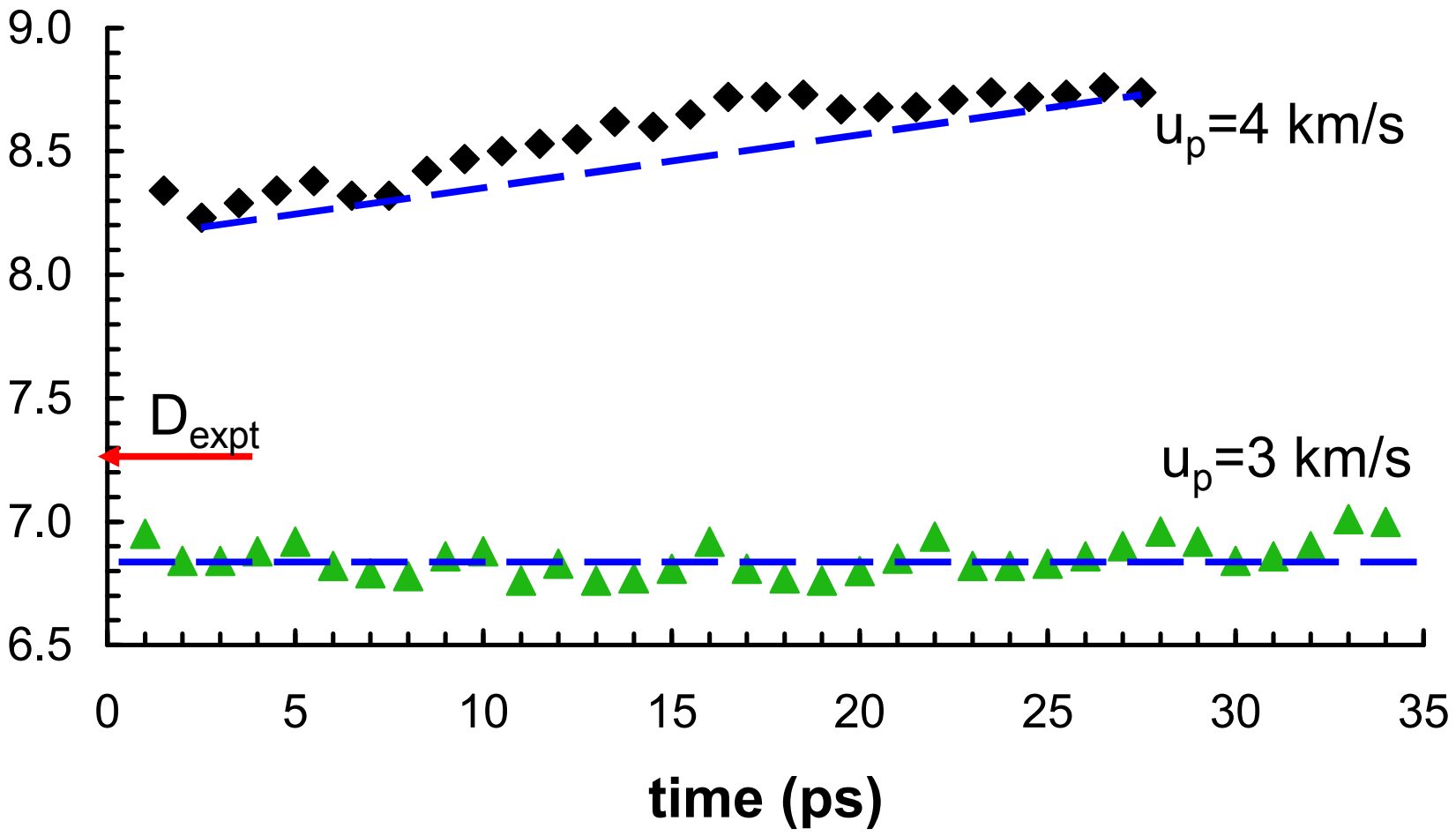



**We simulate piston velocities of 3 km/s and 4 km/s, attempting to bracket the shock to detonation transition**

# Temperature dramatically increases as the shock front moves through the sample

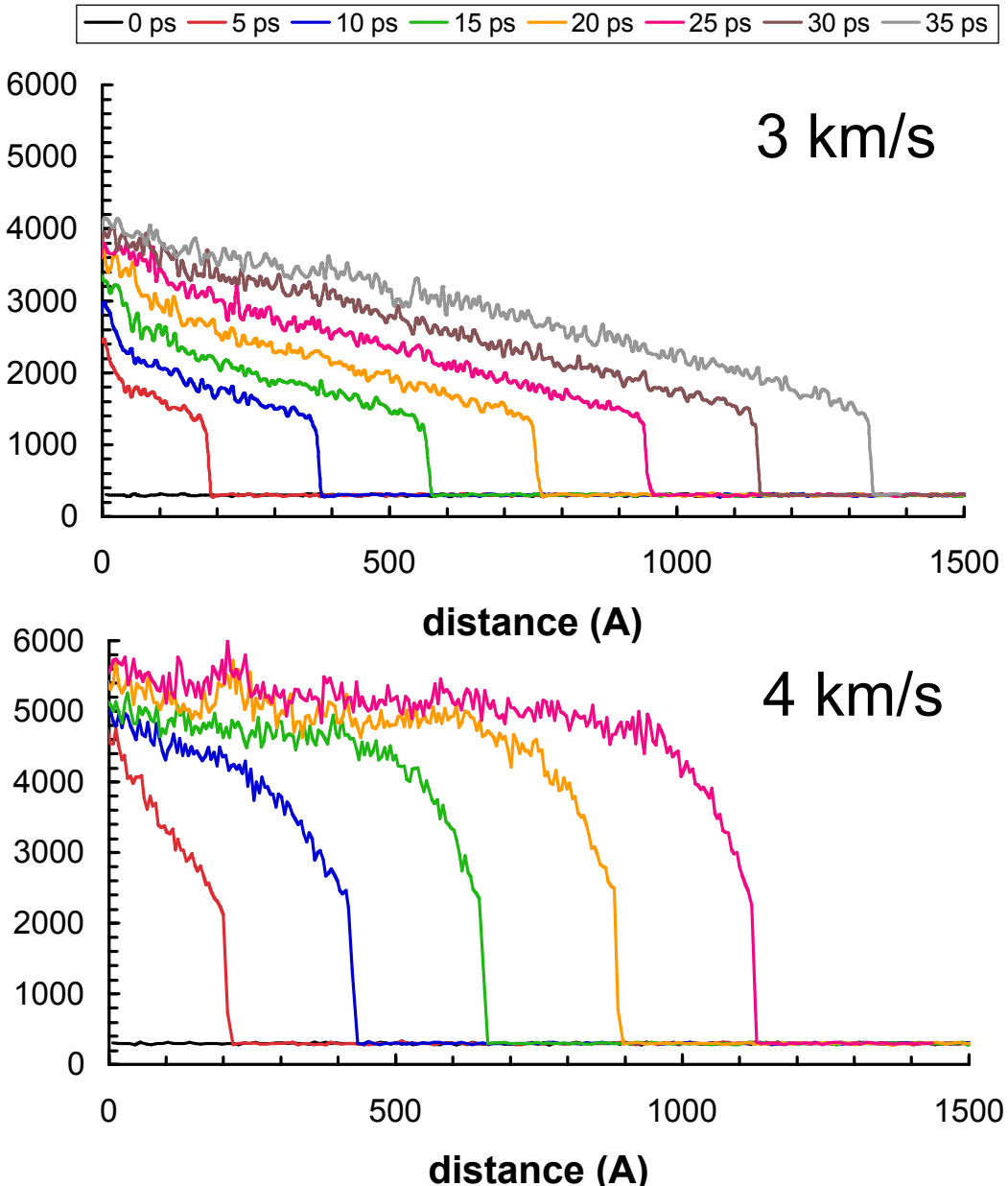


# The stronger shock leads to an accelerating shock velocity



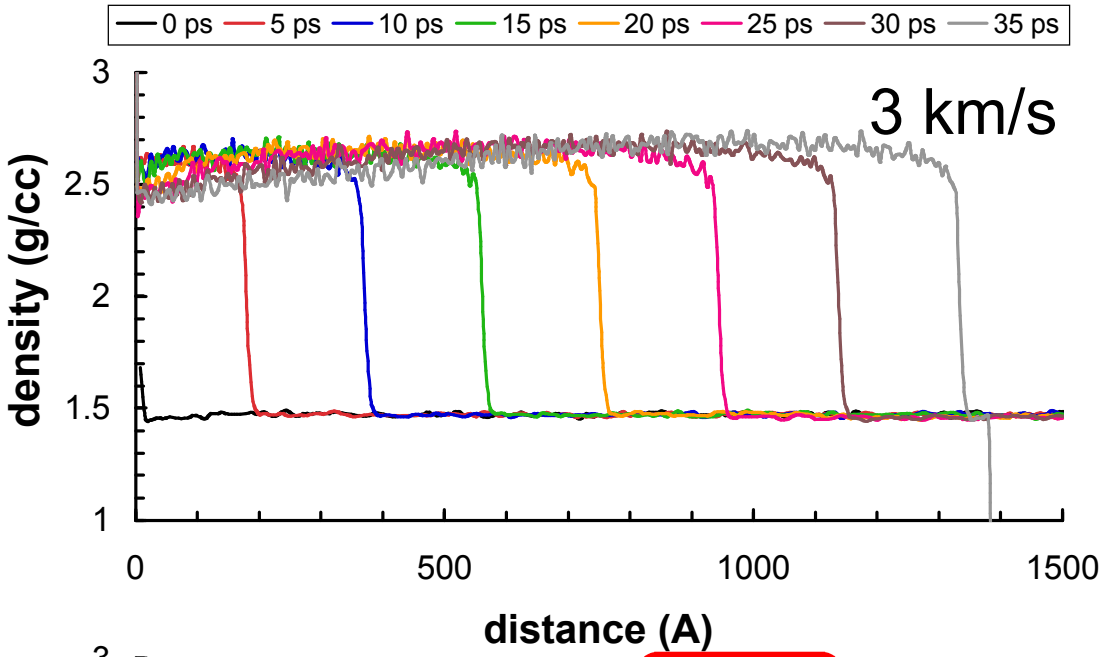

$D_{expt}$ calculated for a density of 1.47 g/cc from
Green and Lee, 13th International Detonation Symposium, Norfolk, VA (July 2006)

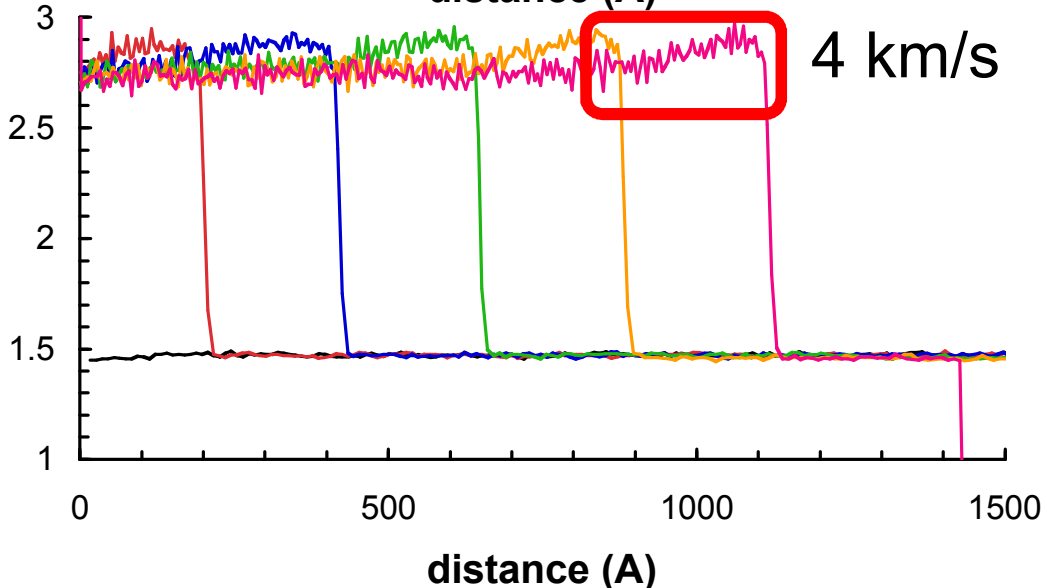
# Dramatically increased thermochemical response seen for a stronger shock




**Both systems started at 300K**

# Peak density is higher and sharper for stronger shock

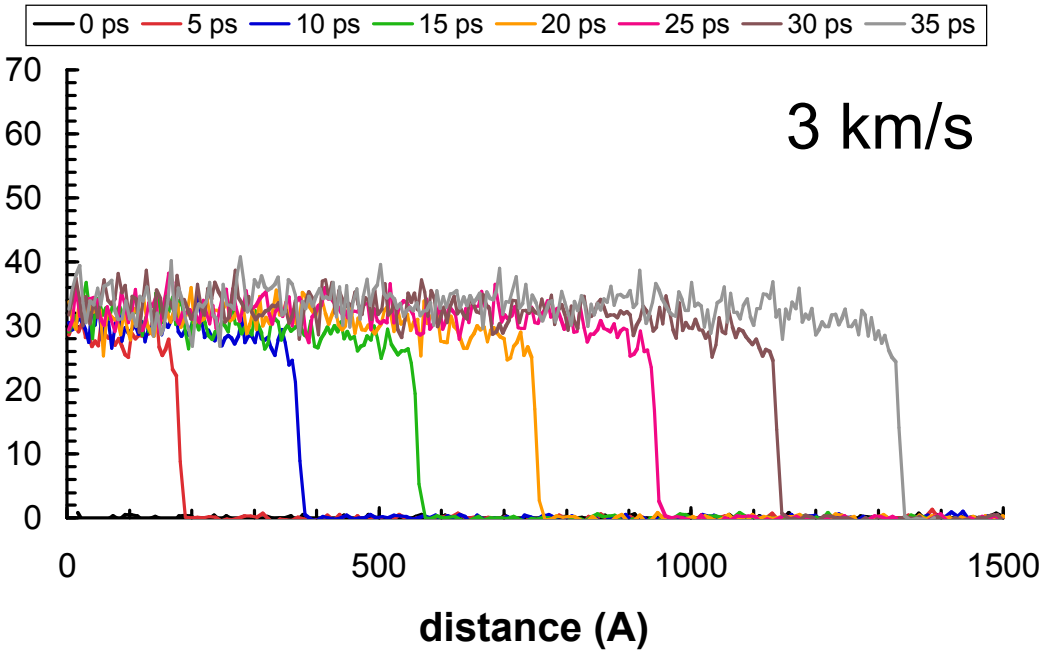


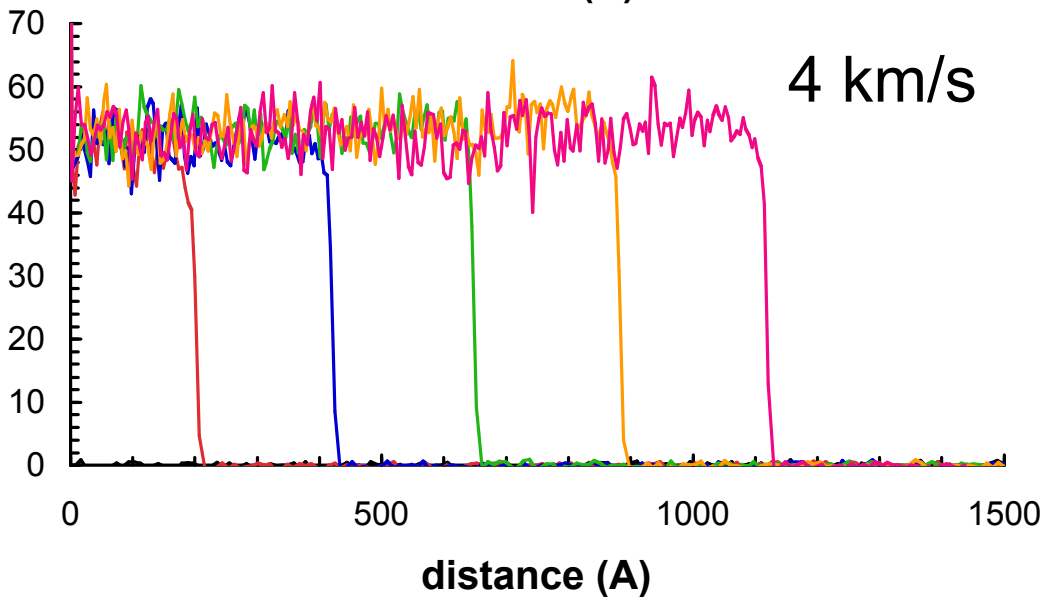




**Both systems start at $\rho$=1.47 g/cc**

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

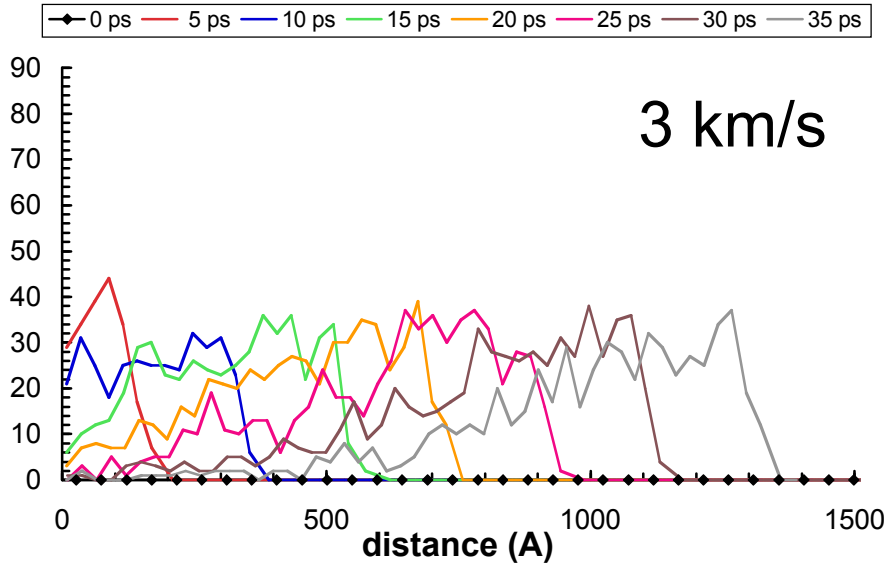
# Pressure is significantly higher for the stronger shock

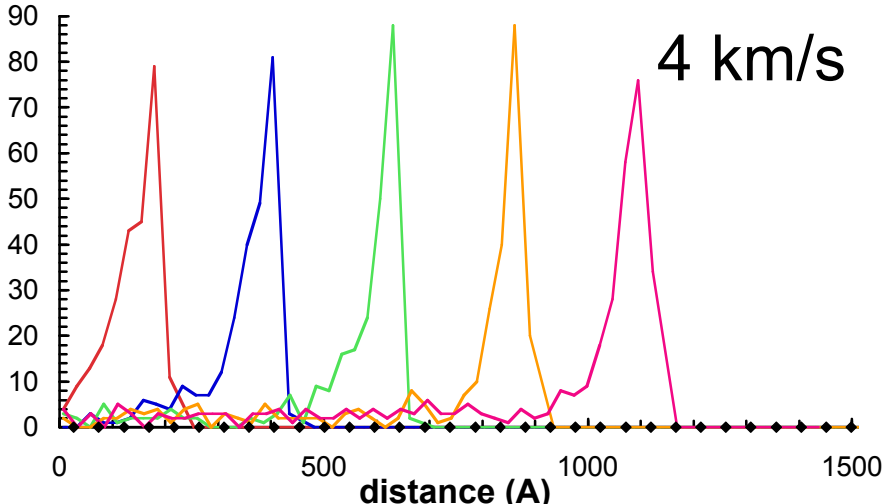


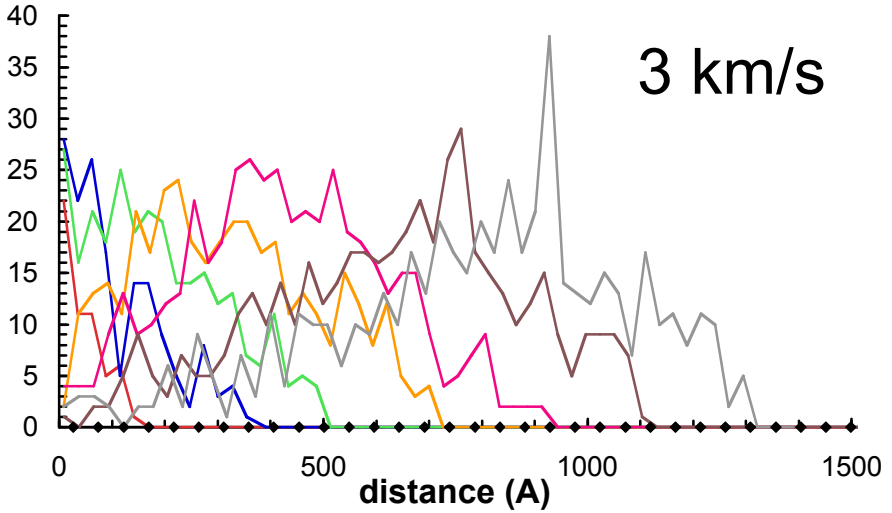
# The stronger shock has the primary products quickly react to become secondary products

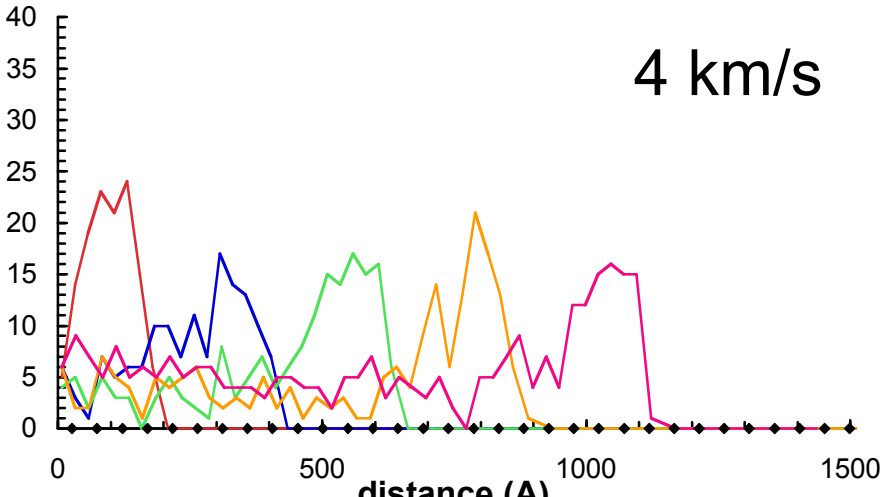
## $NO_2$



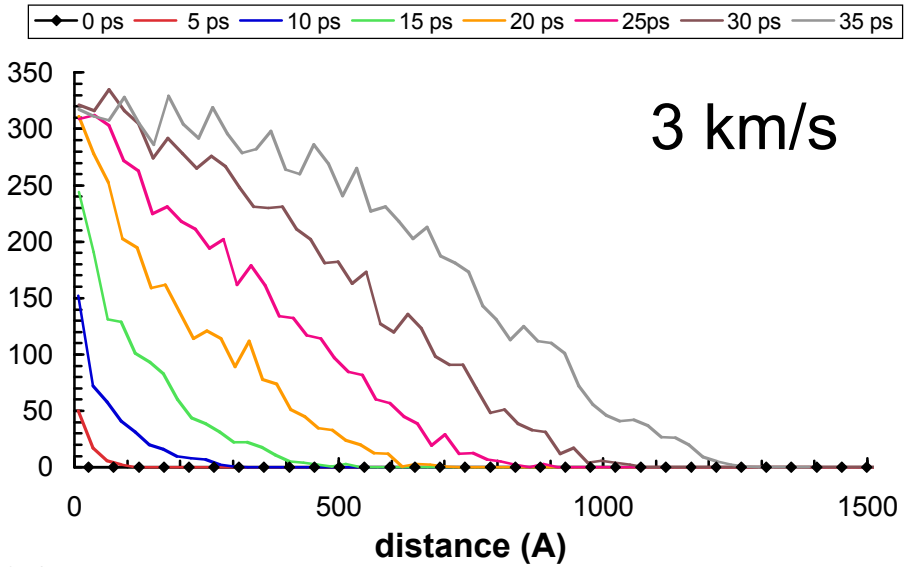

## HONO

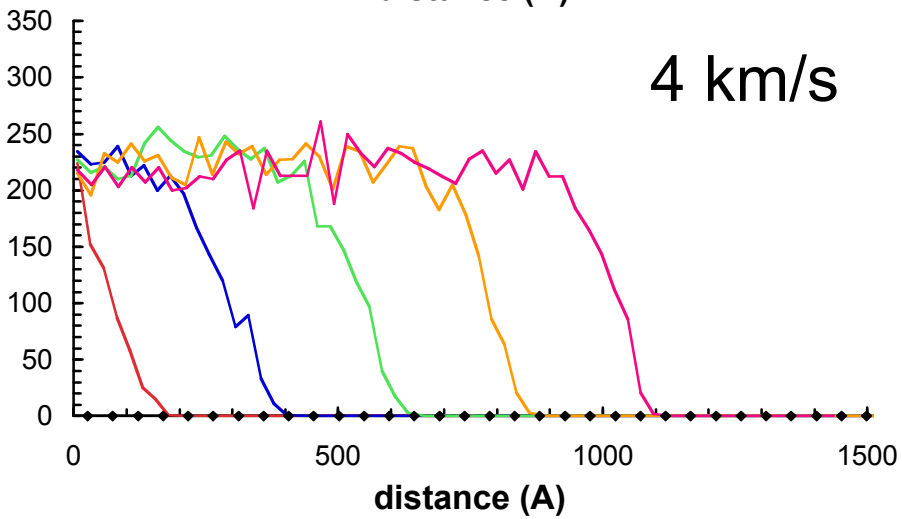


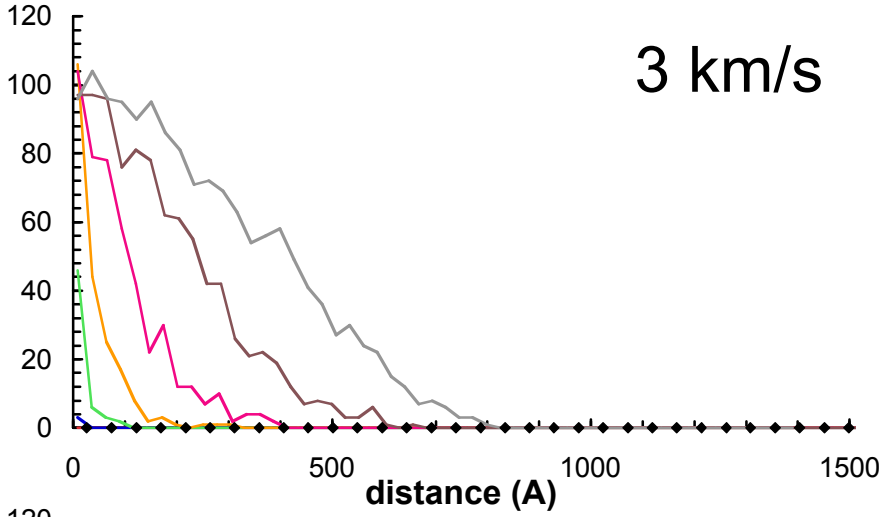
# Secondary products form more quickly under stronger shock

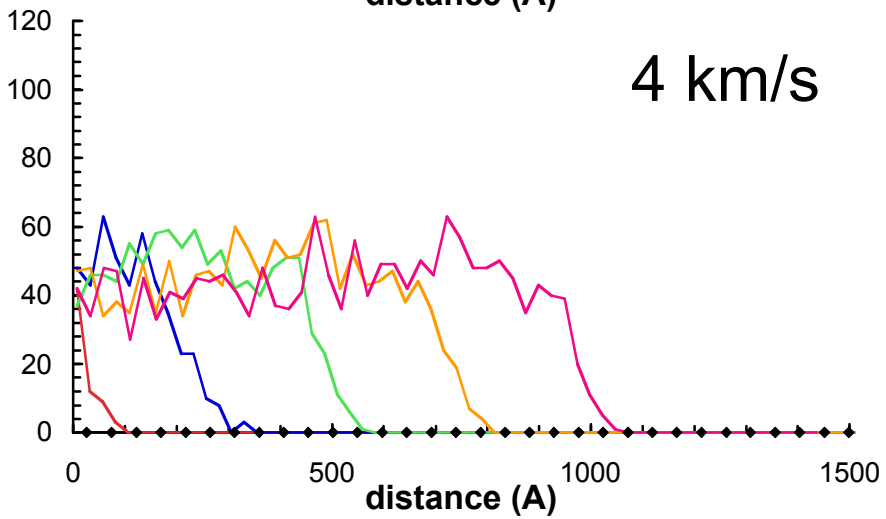
## $H_2O$



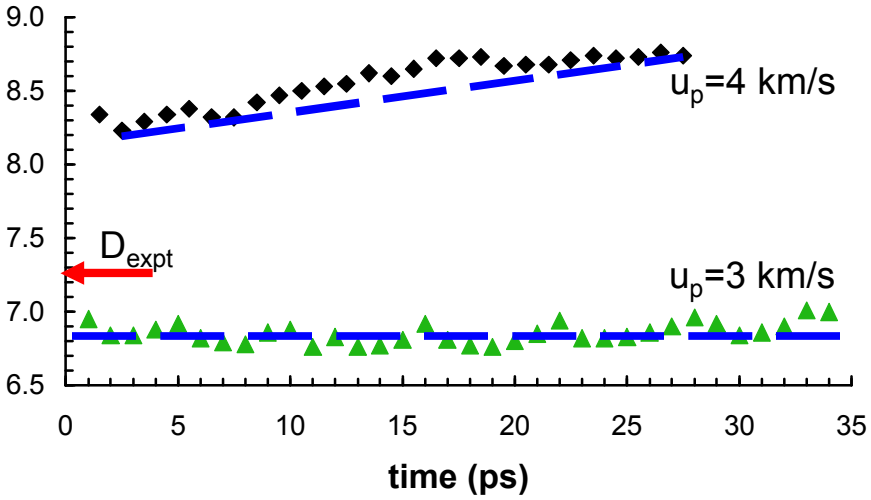

## $N_2$



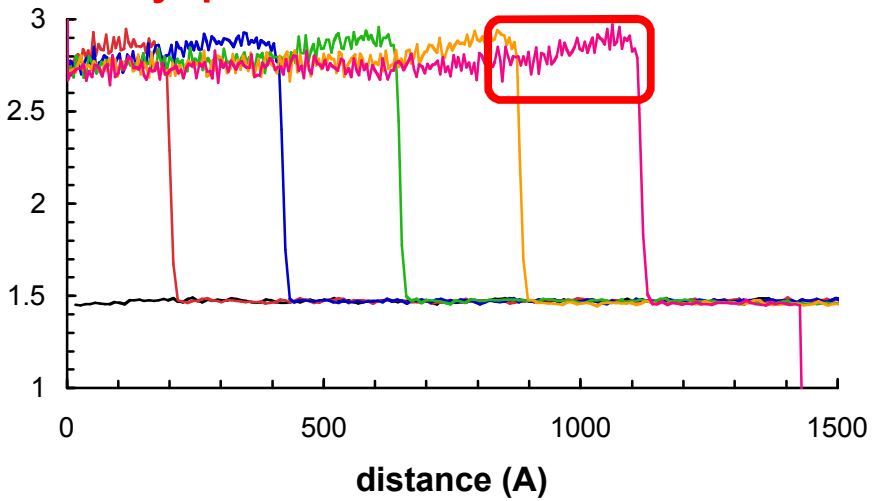



# Summary of Strong Shock Results

## accelerating shock velocity




## density peak behind shock front




## high initial temperature rise hastens chemical reactions