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Micron-scale Reactive Atomistic Simulation of Void Collapse and Hotspot Growth in PETN

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NNSA National Nuclear Security Administration

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Introduction

- Material defects and heterogeneities such as dislocations, grain boundaries, entrained gas, and porosity play key roles in the shock-induced initiation of detonation in energetic materials.
- Previously, we have performed a LAMMPS/ReaxFF NEMD shock simulation of a PETN crystal containing a 20 nm cylindrical void. We observed void collapse-induced hot spot formation and an exothermic reaction zone.
  - Size: 0.3 µm × 0.2 µm × 1.3 nm; 8.5 million atoms
  - Impact velocity: 1.25 km/s (U_S= 4.64 km/s, P = 2.5 GPa)

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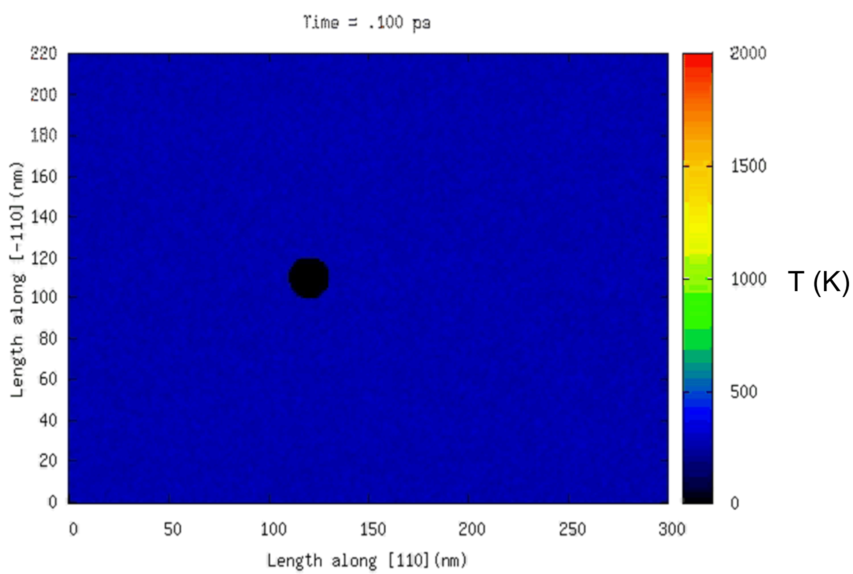
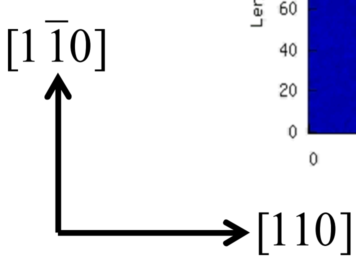
- **APS SCCM:** T.-R. Shan, A. P. Thompson, J. Phys.: Conf. Ser. 500, 172009 (2014)
- **IDS:** T.-R. Shan, A. P. Thompson, Proc. 15th International Detonation Symposium, Accepted for publication (2014)



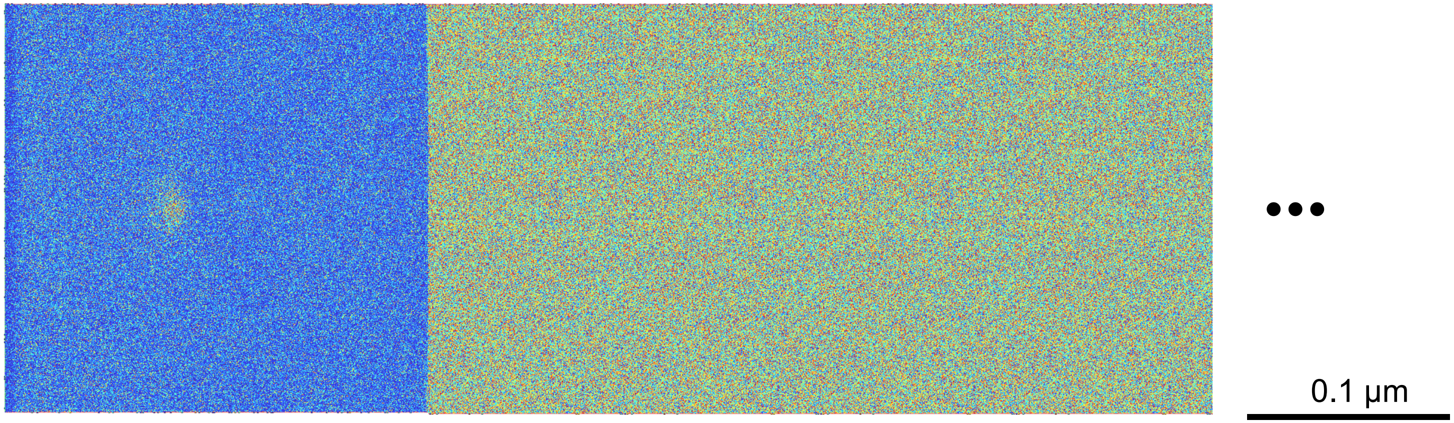
0-64 ps



Formation of hot spot observed, but
- **Is it growing?**
- **Is it leading to detonation?**

Computational setup

- Continue shock simulation after shockwave almost reached free surface
  - Conventional way is to add more uncompressed material



    - Disadvantage: adds significant amount of computational expense

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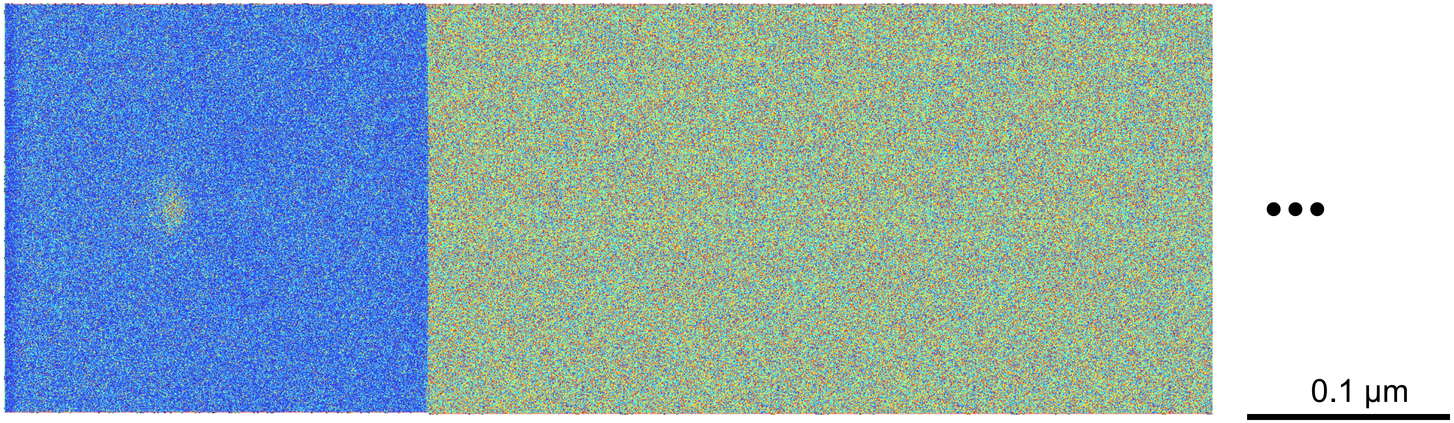
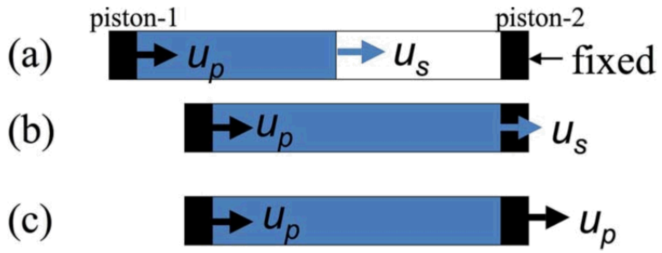


    - Disadvantage: adds significant amount of computational expense
  - We utilize the "shock-front absorbing boundary condition (ABC)"

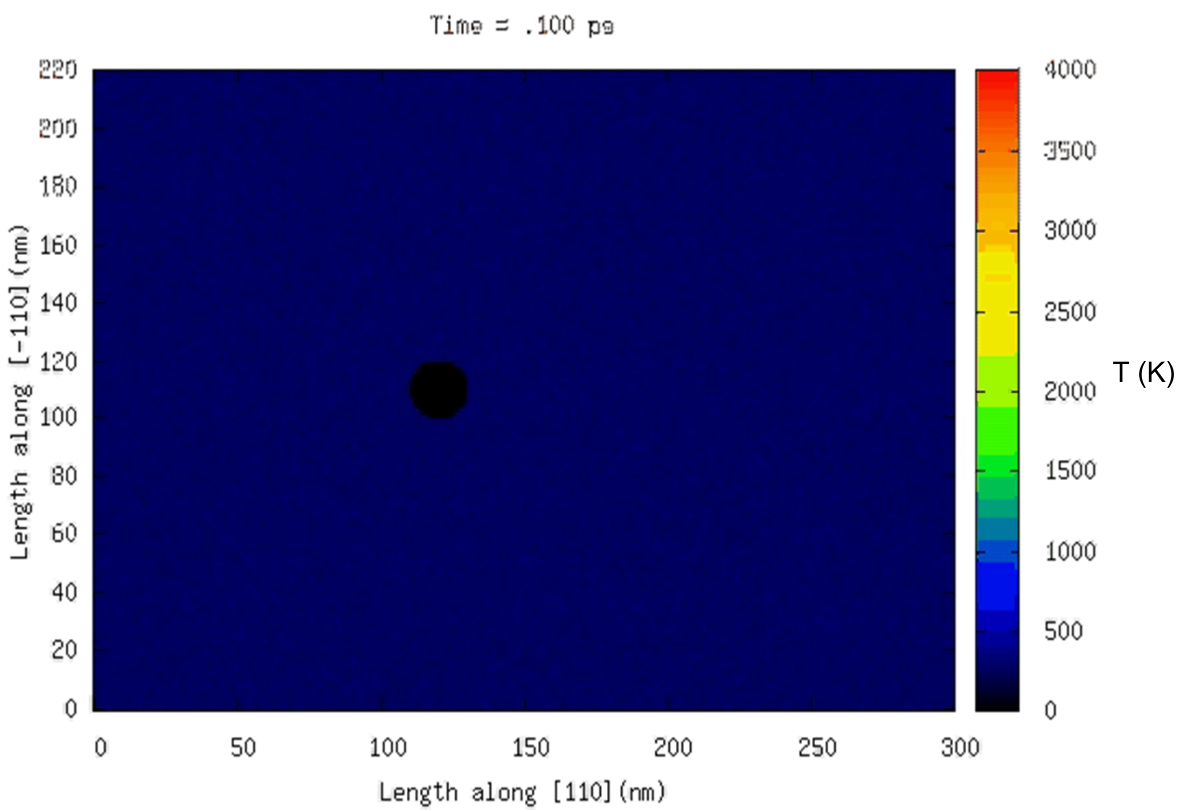


A. V. **Bolesta**, L. **Zheng**, D. L. **Thompson**, and T. D. **Sewell**, *Phys. Rev. B* 76, 224108 (2007).

Objective: To observe hotspot growth and identify growth mechanism

Results: hot spot growth

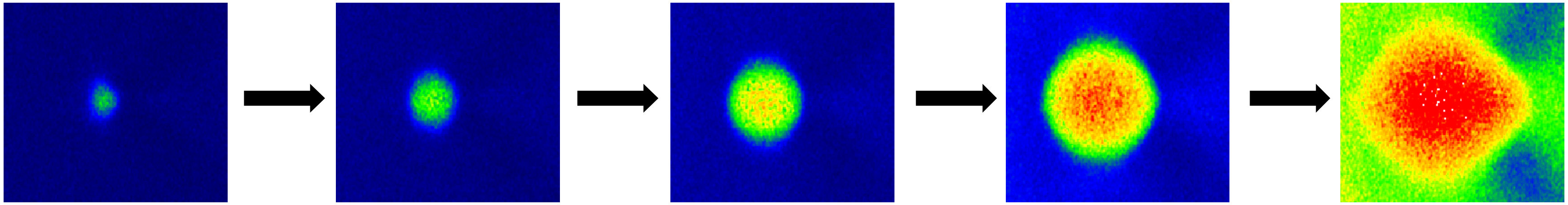
- Normal NEMD shock runs from 0 – 64 ps
  - Observed hotspot formation due to void collapse
- Shock-front ABC runs from 64 – 500 ps:
  - Observed hot spot growth due to coupling to exothermic chemical reactions



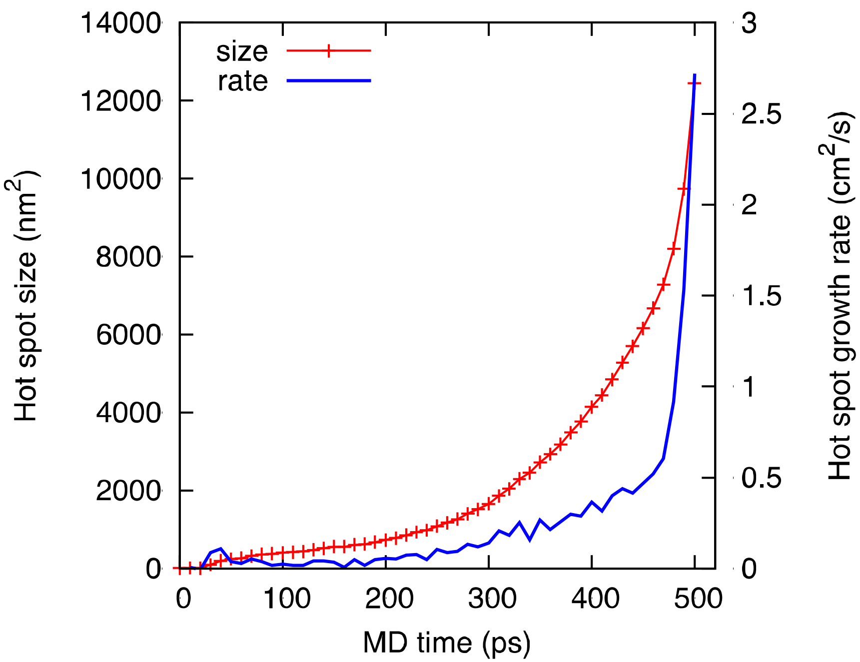
H_2O

N_2

Results: hot spot growth



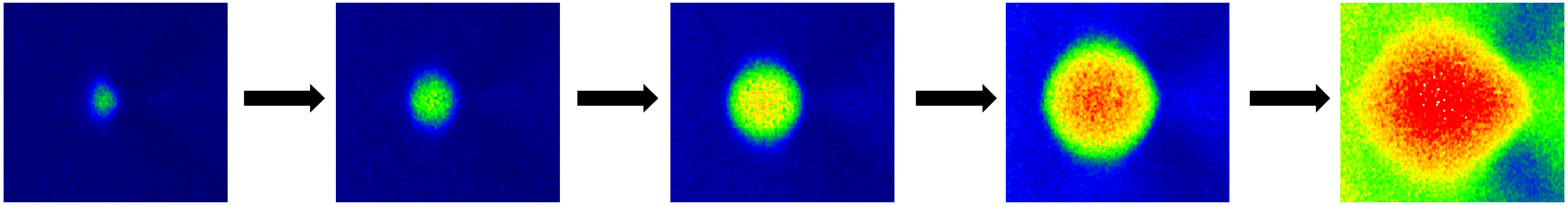
100 ps 200 ps 300 ps 400 ps 500 ps



Strong coupling

Hot spot growth ⟷ Exothermic chemical reactions

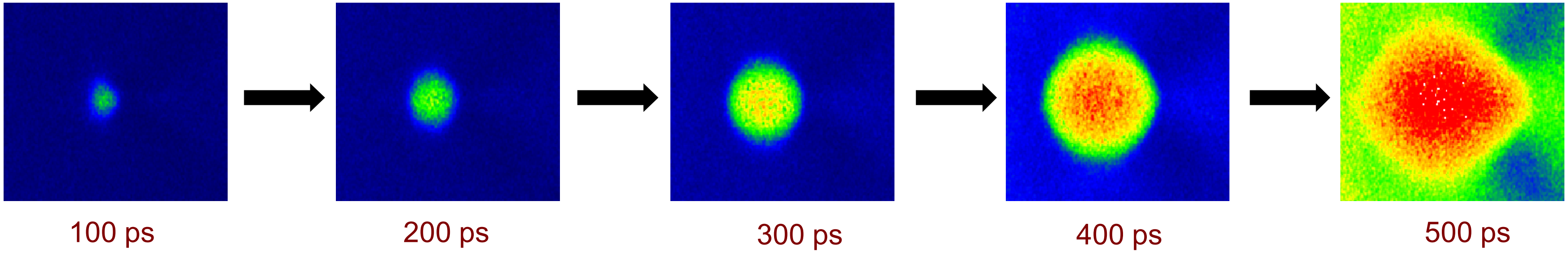
Results: hot spot morphology



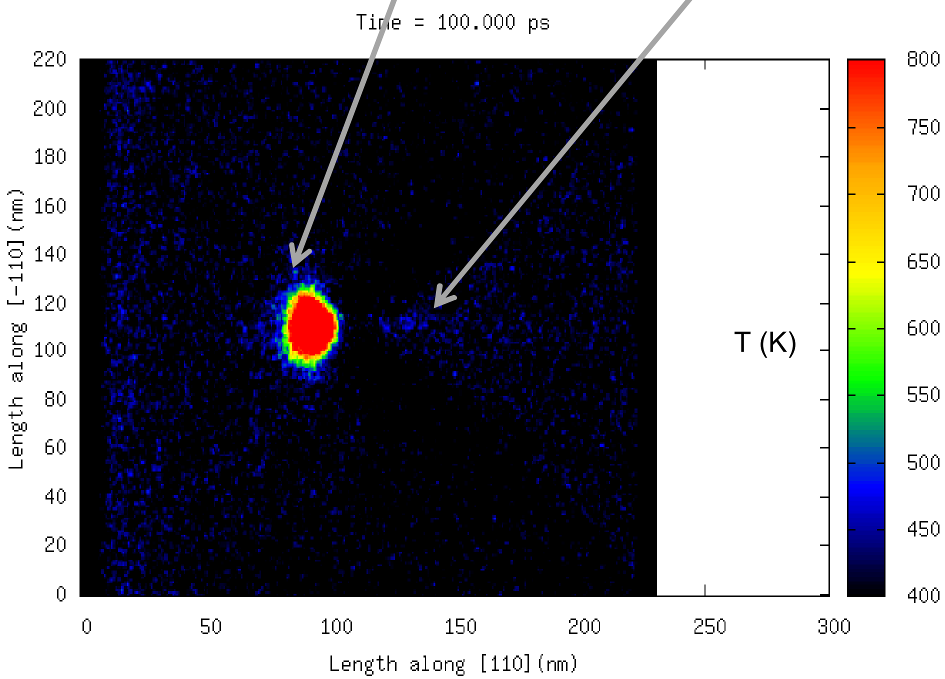
100 ps 200 ps 300 ps 400 ps 500 ps

- Asymmetry developed after 400 ps. How?

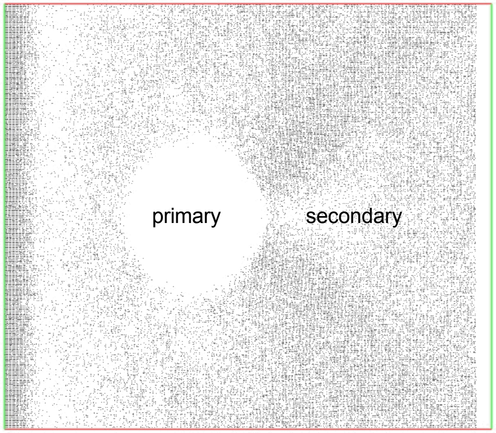
Results: hot spot morphology



- Asymmetry developed after 400 ps. How?
- Due to interaction between primary hot spot and secondary hot zone.

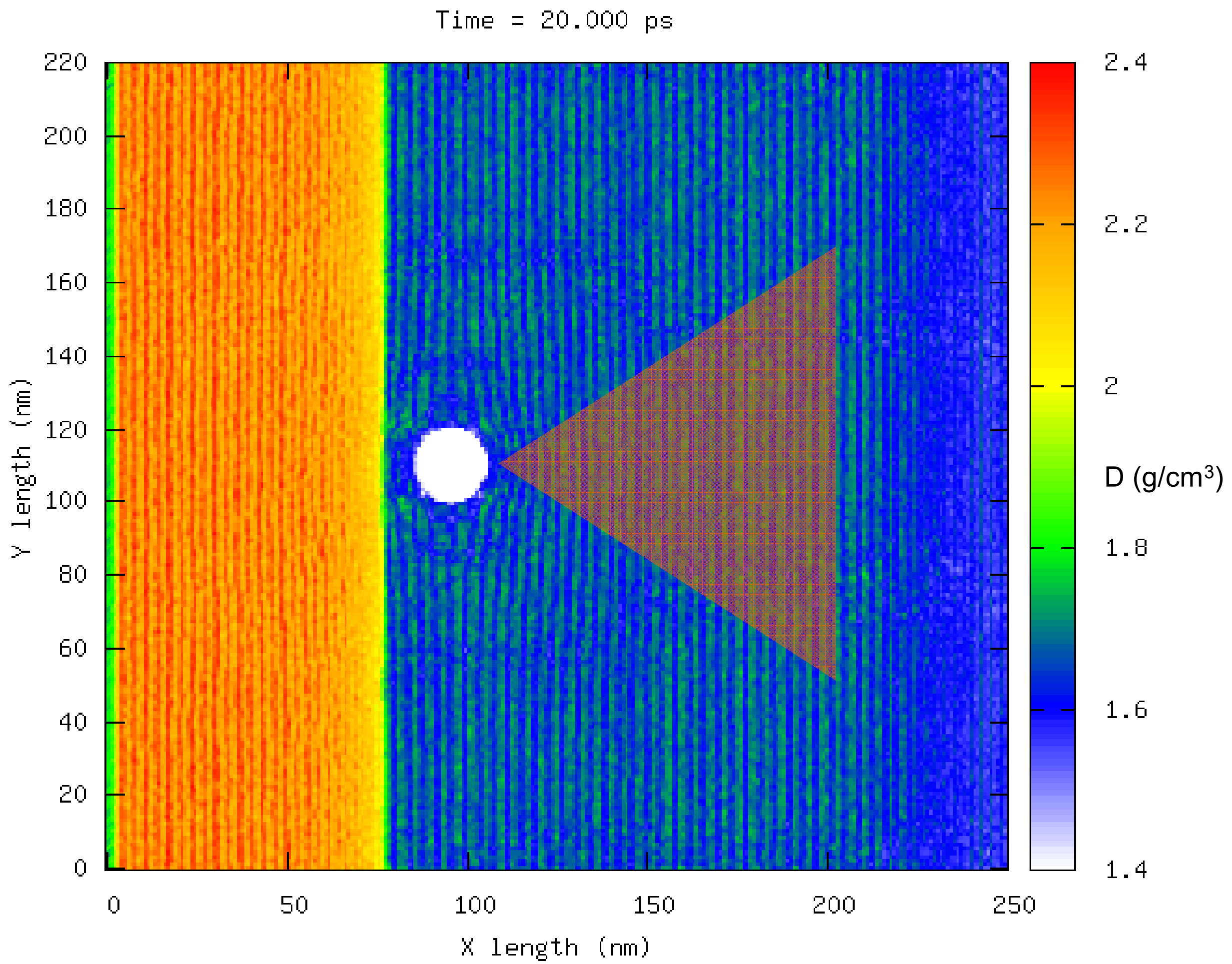


PETN @ 375 ps



Formation of secondary hot zone

- Due to secondary shock wave
  - Which occurs after void upstream/downstream collision
  - Forms a secondary hot zone as it fans out radially into uncompressed material



Conclusions

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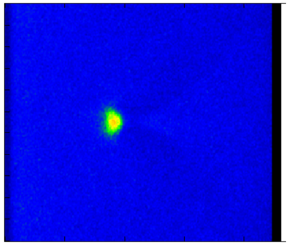
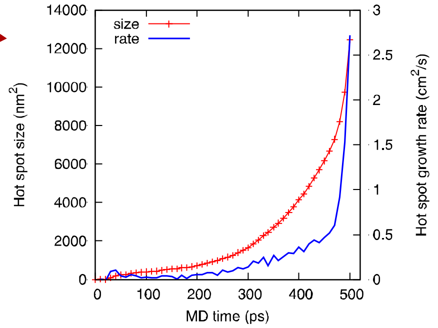
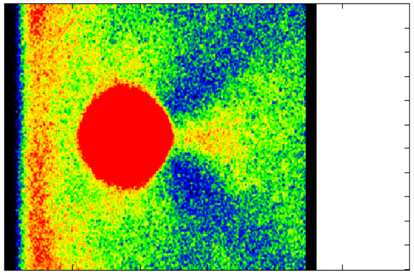
- Performed NEMD shock simulation of a 0.3 × 0.2 × 0.0013 µm3 PETN crystal containing a 20 nm cylindrical void
  - Observed void collapse-induced hot spot formation

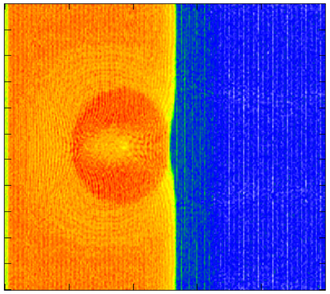


- Obtained an exponential growing hot spot
  - Hot spot growth coupled to exothermic chemical reactions
  - Asymmetry developed due to interaction between the primary hot spot and a secondary hot zone



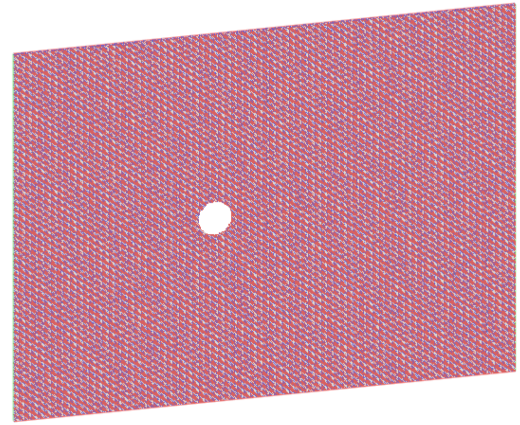


- Secondary hot zone resulted from secondary shock wave after collision between upstream void fragments and downstream void surface



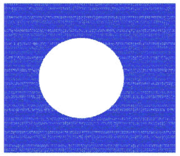
Ongoing work

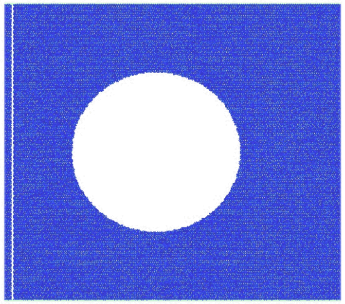
PETN
20 nm void



0.1 µm

HNS
50 & 100 nm void





Formation of
hot spots