Computational Research in Energetics

2011 National Capital Region Energetics Symposium (NCRES)

TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.

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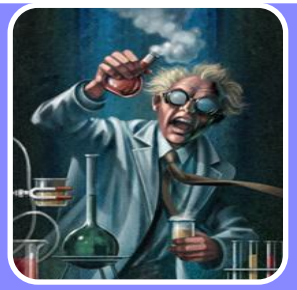
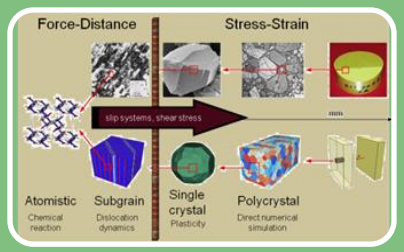
November 1, 2011

Computational Research in Energetics



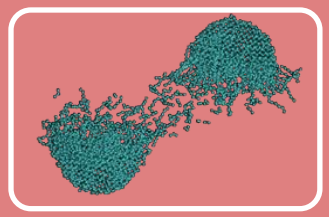
Virtual Design

- New Energetic Materials
- Energetic Formulations



Multiscale M&S in Energetic Systems Design

- development of meso-scale models of heterogeneous EM
  - Development of models relating hot spot dynamics to microstructure
  - Bottom-up meso-particle dynamics models
  - Virtual testing of EM in munitions



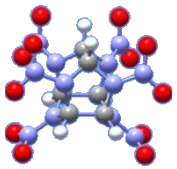
Exploring Novel energy releasing concepts using M&S

- QM characterization
  - Release of stored energy in ND
  - Dynamic response of shocked poly-N

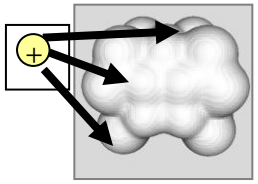
Virtual Design of New Energetic Materials

- **Using quantum mechanics, we have derived correlations to solid phase heats of formation and crystalline densities for both neutral and ionic energetic materials**
- **Correlations require calculations only on single molecule (*not* bulk material)**

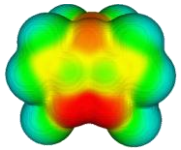
CL20

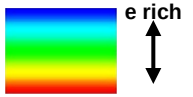


Mapping out e⁻ Density

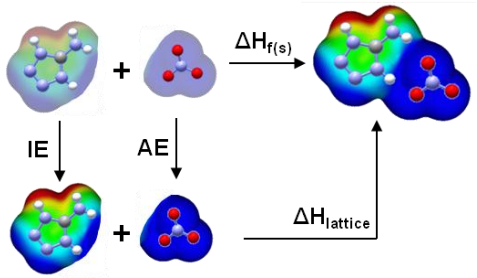


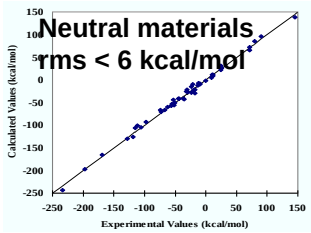
Electrostatic Potential

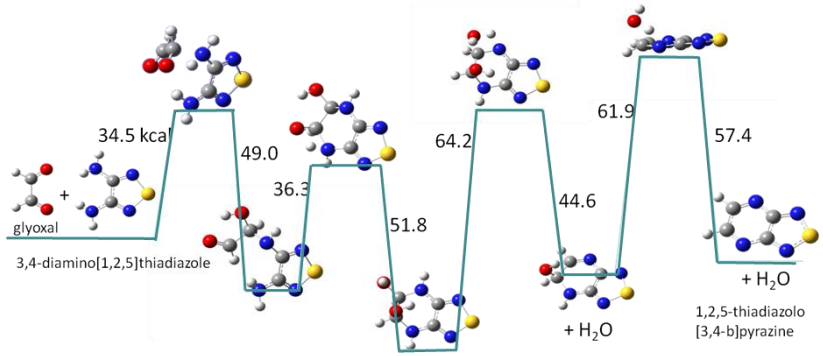




Heats of Formation

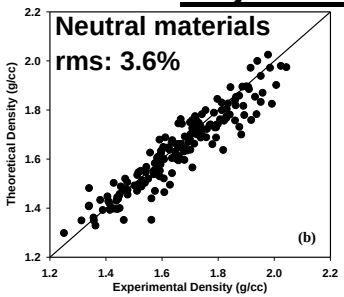


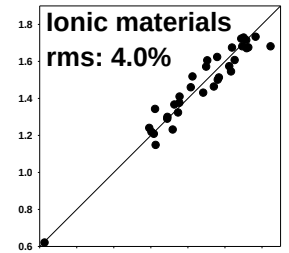




Reaction path mapping: Allows for exploration of synthesis steps, identification of intermediates

Crystal Densities



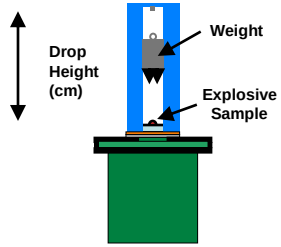


Neutral molecules refit to improve the RMS error to 2.9%!

E. F. C. Byrd and B. M. Rice, "Improved Prediction of Heats of Formation of Energetic Materials Using Quantum Mechanical Calculations", Journal of Physical Chemistry A (2006) 110, 1005-1013; ibid (2009) 113, 5813.
B. M. Rice and E. F. C. Byrd, "Accurate predictions of crystal densities using quantum mechanical molecular volumes", Journal of Physical Chemistry A (2007) 111(42), 10874-1087

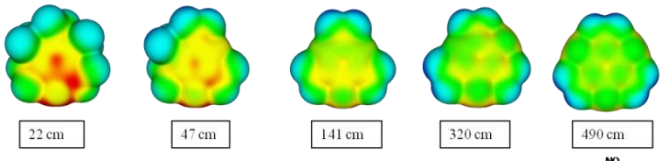
Predictions of Sensitivity

Previously developed tools capable of qualitative sensitivity predictive capability for neutral species.



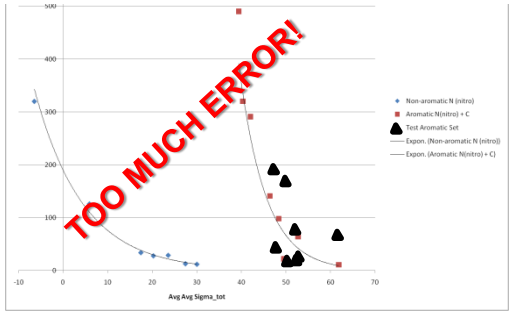
Drop Weight Impact Test

h_{50} value quantifies sensitivity

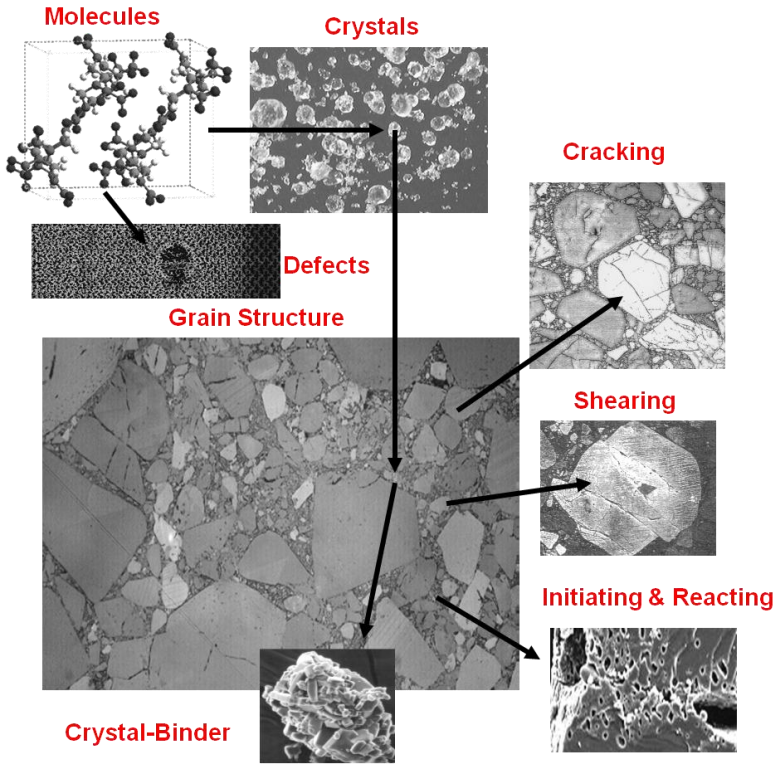


Charge Rich ↔ Charge Poor

Attempts at generating a quantitative correlation of electron density topologies (formally assessed through Bader's Atoms-In-Molecules [AIM]) to impact sensitivity has proven to be unsuccessful.



Microstructure has significant influence on EM response

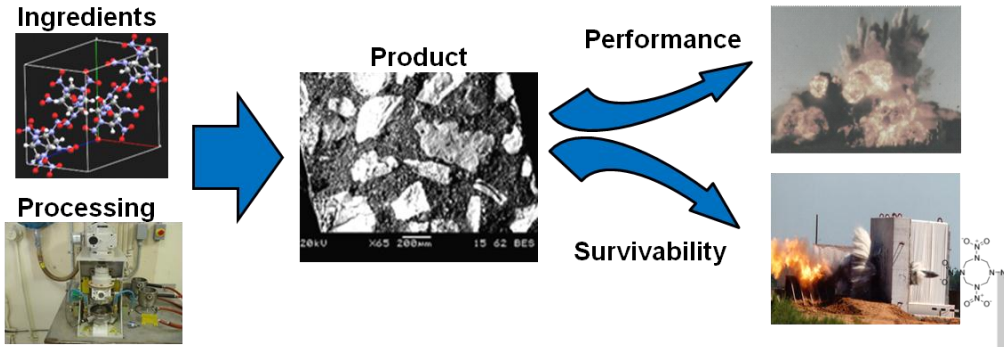


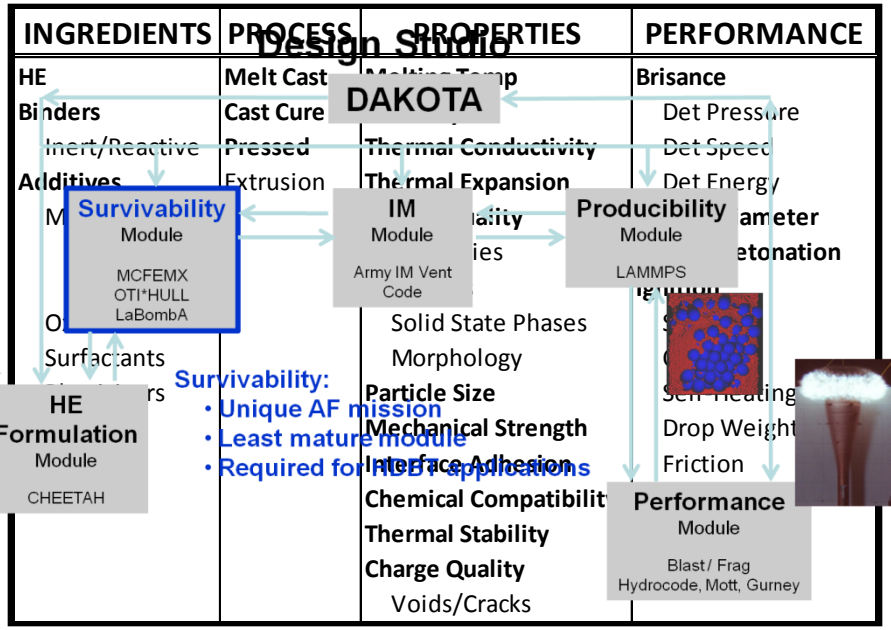
B. M. Rice and J. J. Hare, "A Quantum Mechanical Investigation of the Relation between Impact Sensitivity and the Charge Distribution in Energetic Molecules", the Journal of Physical Chemistry A (2002, 106, 1770-1783.

Anthony D. Yau, Edward F. C. Byrd and Betsy M. Rice, "An Investigation of KS-DFT Electron Densities used in Atoms-in-Molecules Studies of Energetic Molecules", The Journal of Physical Chemistry A 2009, 113 (21), 6166-6171

Virtual Design of Explosive Formulations

Energetic material development requires significant laboratory investment and breadth of knowledge/training





Virtual *Design Studio*
(software architecture: physics models + data-library)

- M&S formulation guidance
- Rapid design capability, from requirements to production
- Improved reliability/survivability of explosive fills
- Reduced learning curve

HE Formulation

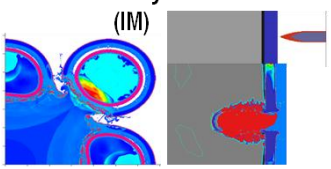
Performance (Blast, Fragmentation)

Survivability

Producibility

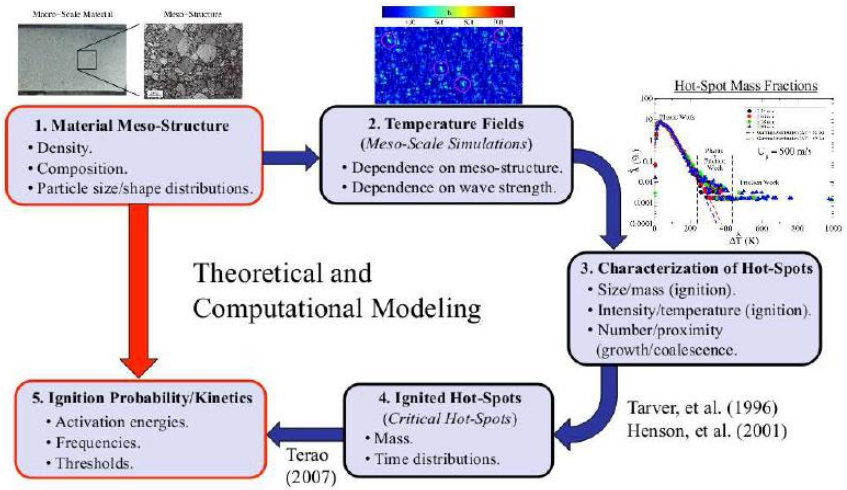
Life Cycle Costs:
Surety
Reliability
LAP
Shelf-Life
DeMil

Safety (IM)



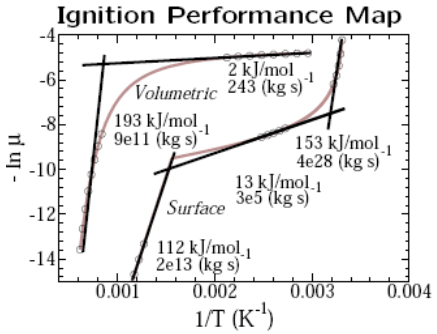
Framework for Relationship Between Applied Loads and Ignition Probability

- Examine how *meso-structure/wave strength* affect ignition probability.



- Analogous to statistical failure theory (Hahn and Shapiro, 1967).
  - *Time to failure* depends on distribution of activated defects/flaws.
  - *Time to ignition* depends on distribution of ignited hot-spots.

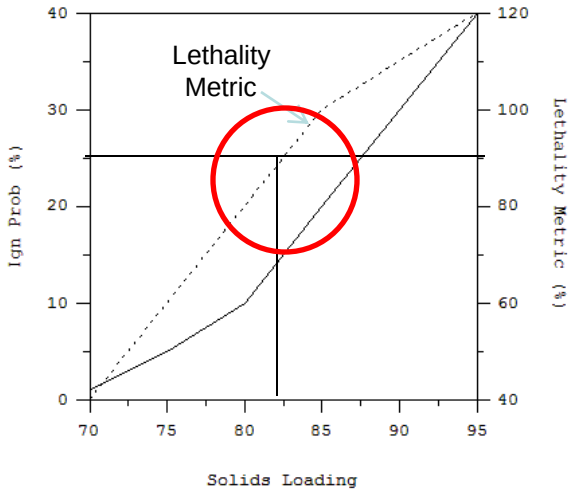
Ignition Performance Map for a given mesostructure



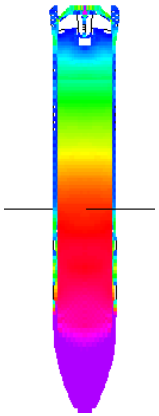
Correlate Meso Variables to Continuum Mechanics Variables (Pressure, Energy, Explosive Composition)

Implement Similar to Reactive Flow Model in Existing Hydrocodes

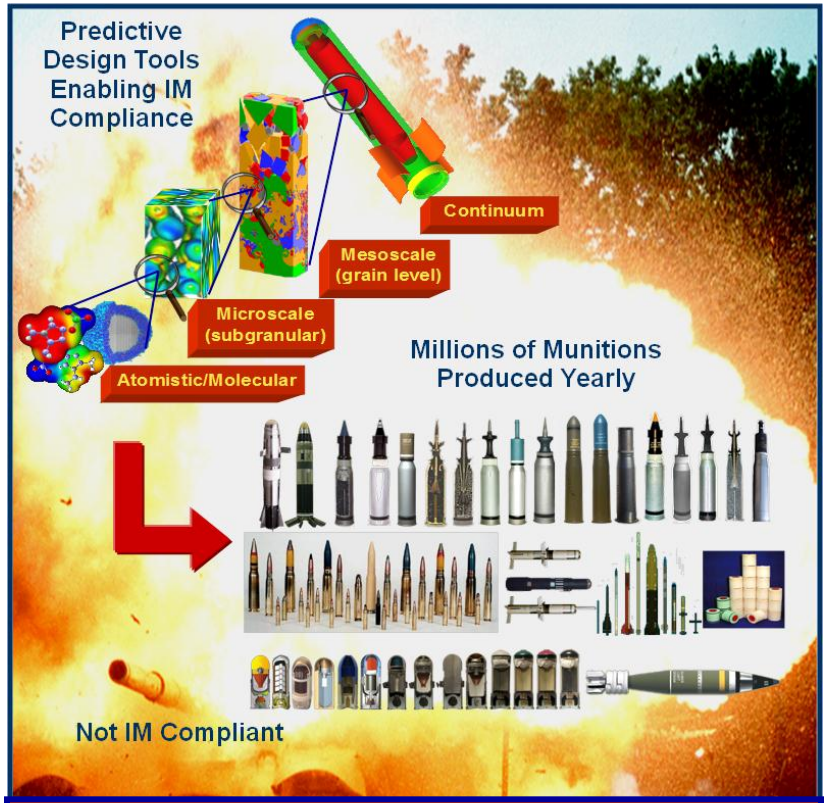
Clear Trade-offs Between Survivability and Performance



Calculate Fill Survivability Based Upon Weapon, Target Set, Fill Composition

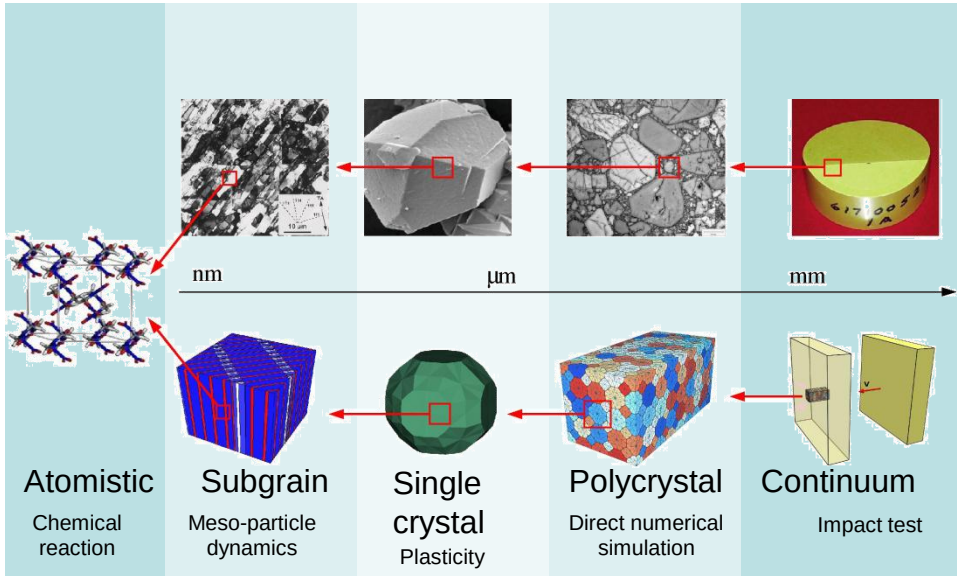


Complementary Modeling initiatives in realistic explosive formulations



Software Application Institute for Multiscale Reactive Modeling of IM

- Develop a science-based predictive capability to simulate munition response to insults.
- Implement a completely-coupled multi-scale M&S toolset used to
  - Develop and optimize new IM
  - Improve existing munitions to enable IM compliance.



Multiscale Response of Energetic Materials (core program, ARL)

Develop a science-based multiscale capability to simulate energetic material (EMs) response to insults through adequately capturing the effects that microstructural heterogeneities impose on macroscopic events.

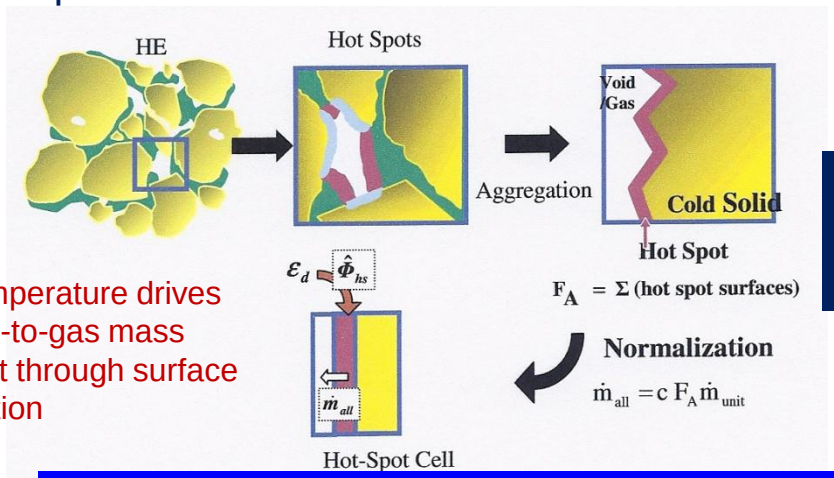
- Development of theories, methods, models at spatial and temporal scales ranging from atomistic up to continuum for multiscale coupling
- Advanced experimentation for verification and validation.

Inputs to PBRB Model Derived from DPD-E

(Sunil Dwivedi*, UF-REEF & Yuki Horie, AFRL)

*Currently at School of Materials Science and Engineering, Georgia Institute of Technology

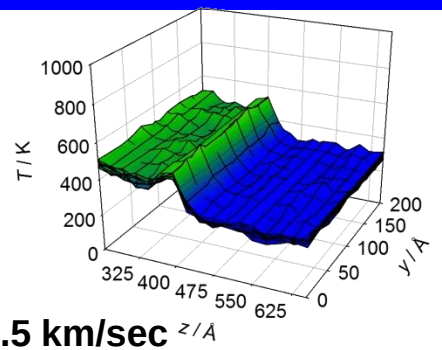
- Focuses on hot spot formation and growth in inhomogeneous HE composites
- Hot spot formation and resulting localized heating is the core mechanism modeled in the PBRB model for reaction initiation
- Model uses procedure of aggregating hot spots within hydrocell, then simplifying to a “super hot spot model”



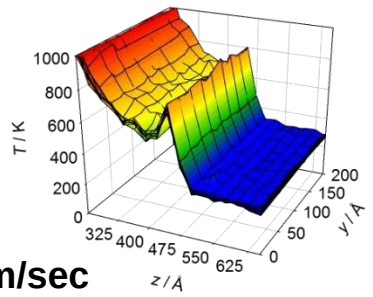
solid temperature drives the solid-to-gas mass transport through surface sublimation

Hot Spot Distribution is one of the Key Inputs to the PBRB Model

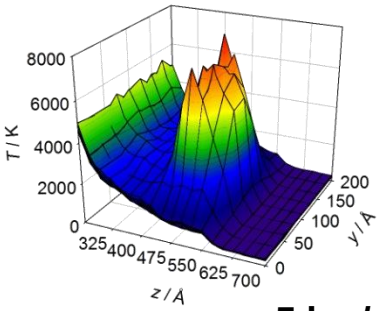
Example of temperature maps from meso-particle dynamics simulations



1.5 km/sec



3 km/sec



5 km/sec, 16 nm void

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US ARMY RDECOM

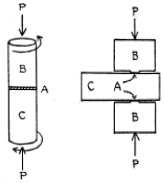
Exploring Structural Bond Energy Release (SBER) in Nano-Diamonds using Quantum Molecular Dynamics

ARL

SBER: The release of energy stored in structures through mechanical action.

First Observed by Bridgeman as Explosion of Common Substances Subjected to Pressure and Shear

Effects of High Shearing Stress Combined with Hydrostatic Pressure

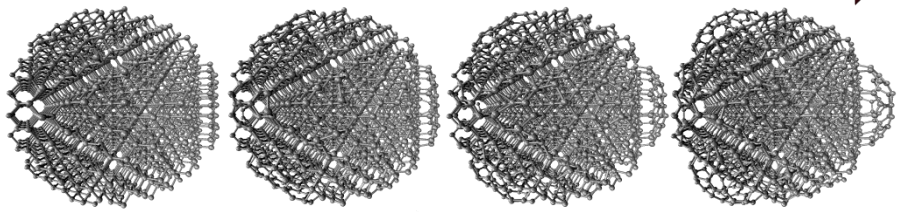


Physical Review, 48 (1935) 825-47

Extensive Russian efforts exploring this phenomena:
These focus on mechanically stressed solids producing *autowave behavior* such as

- Self-sustained failure waves (e.g. Prince Rupert's drops)
- Cold Detonation
- Rheological Explosion

QM Diamond Surface Reconstruction with Buckyball Features

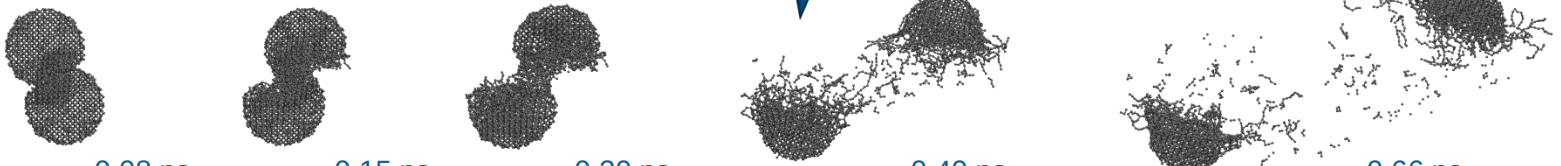


- Quantum simulations of smaller ND clusters show surface reconstruction to fullerene arrangement, core maintains diamond structure
- Calculations show tensile stress on the surface. Our calculations suggest core pressure in excess of 50GPa.

Sudden Disruption of ND Surface will Release Energy Stored in the Compressed Core

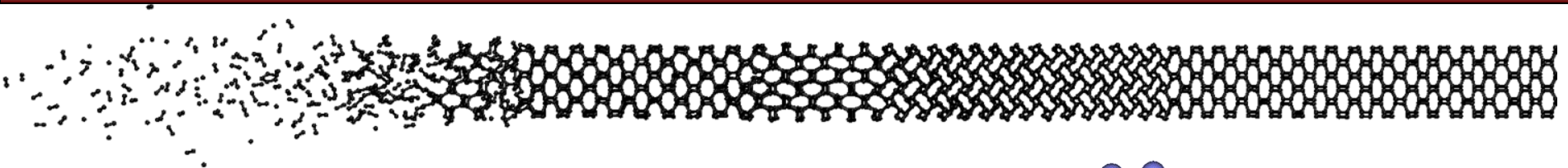
Testing the Hypothesis: Hypervelocity Collisions of ND

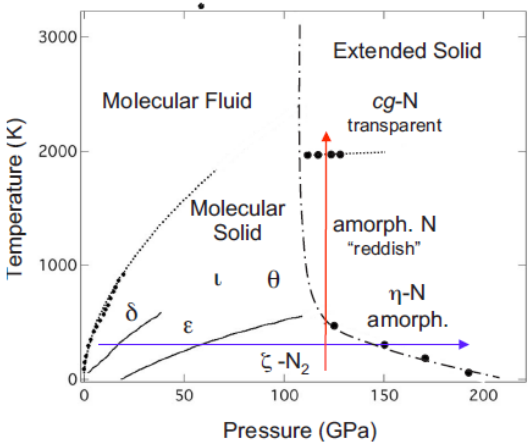
Perpendicular to Axis of Collision

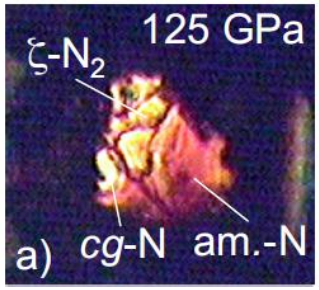


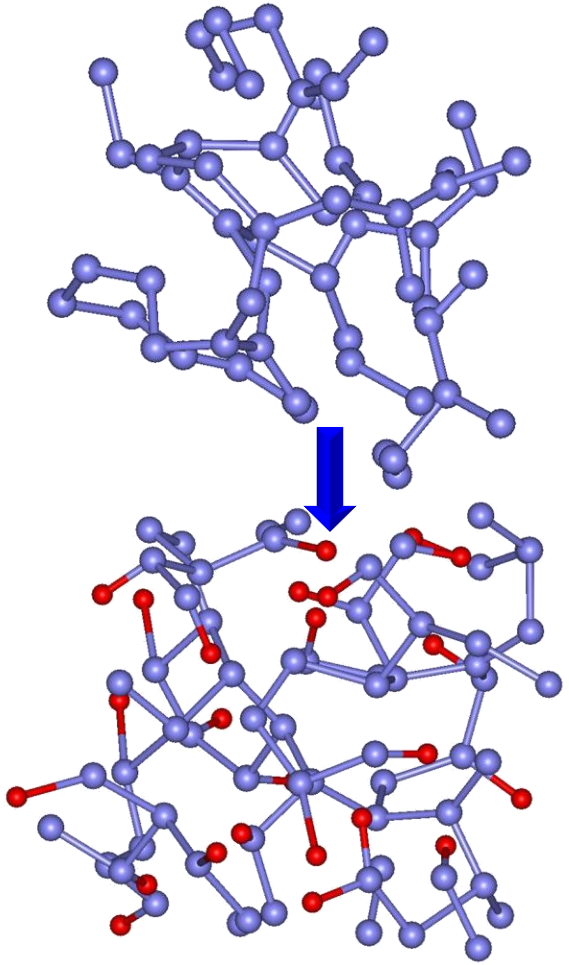
Along Axis of Collision

Polymeric Nitrogen



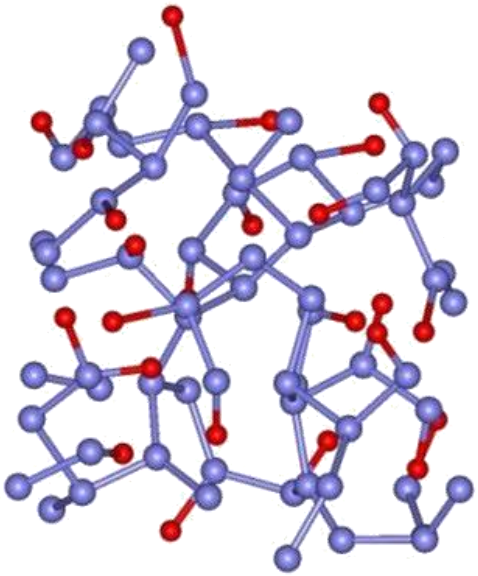


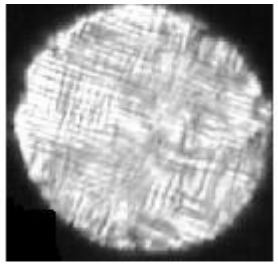




- Early Experiments show highly sensitive amorphous polymeric nitrogen.
- Simulation show initiation starts with unpassivated nitrogen atoms.
- Simulation with hydrogen passivated nitrogen atoms are more stable.

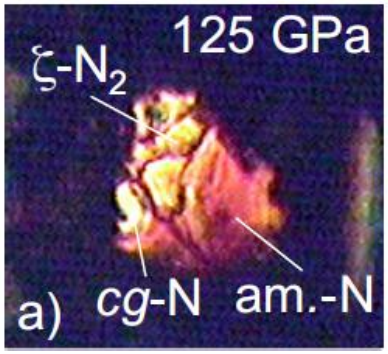
Nitrogen/Hydrogen Mixtures – Novel Precursors to Polynitrogen?





6 GPa

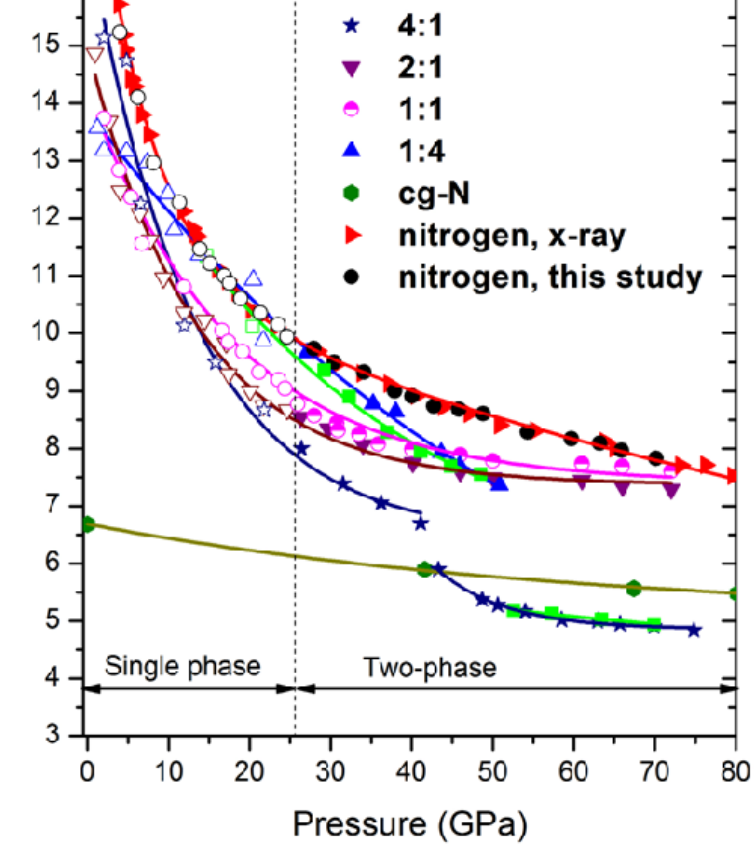
30 GPa



Lipp et al., Phys. Rev. B 76, 014113 (2007).

80 GPa

0.5 GPa



Concluding remarks

Thanks for your attention! Questions?

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