Air Force Research Laboratory

Integrity ★ Service ★ Excellence

Dynamic Materials and Interactions Portfolio

Seminar at Columbia University

May 12, 2015

Jennifer L. Jordan, Ph.D

AFOSR/RTA Team 1

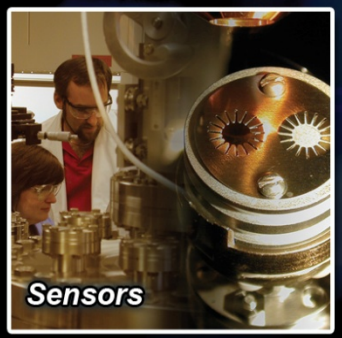
Air Force Research Laboratory

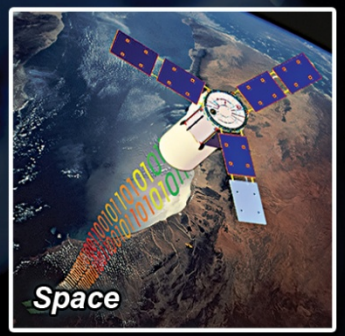
AFRL

Outline

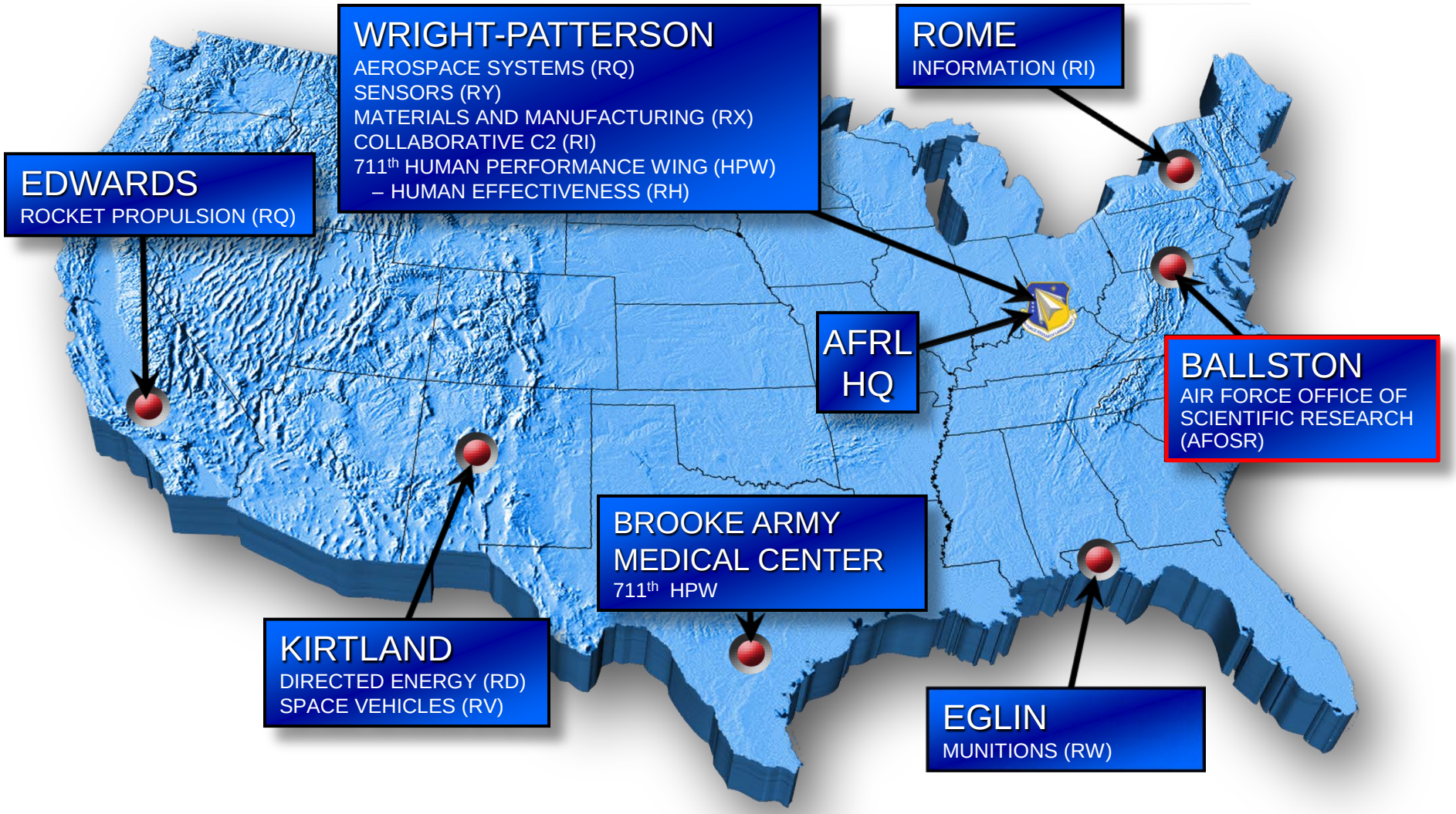
- AFOSR overview
- Portfolio Motivation and Investment Strategy
- Research Thrusts
  - Energetic Materials Science
  - Shock Physics of Heterogeneous Materials
  - Reactive Materials
- Summary

Air Force Research Laboratory





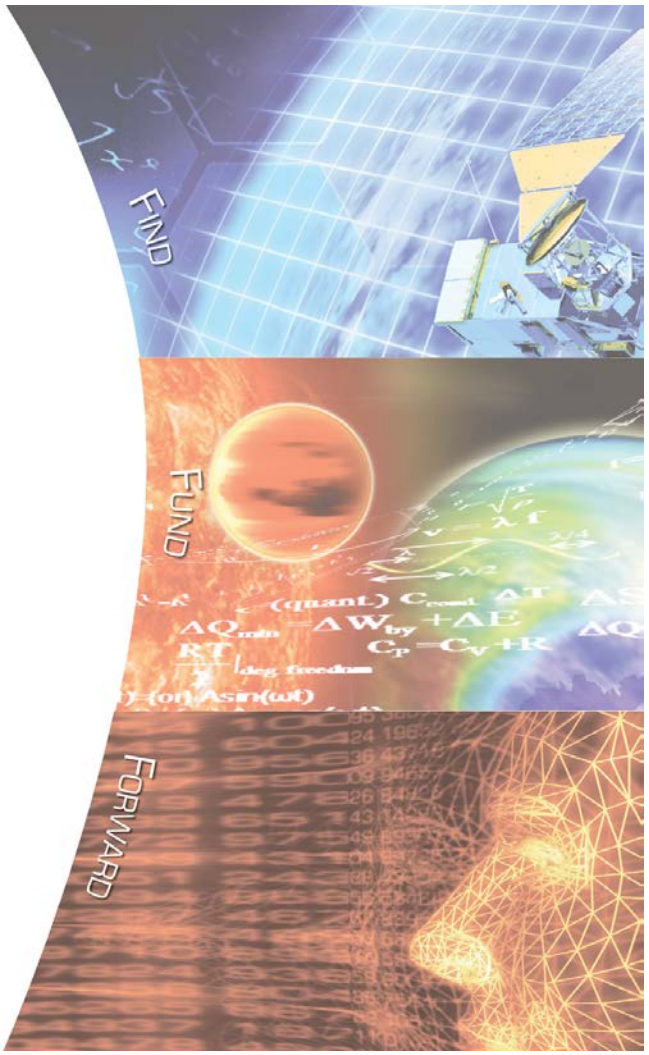
Major AFRL Facilities



40 Sites World-Wide

AFOSR

- **Manages the Basic Research Investment for the Air Force**
  - Basic Research is the foundation of all scientific discovery and progress
  - Advancement of science leads to revolutionary new concepts + technology
  - Discover, shape, and champion science that profoundly impacts the future Air Force
- **Find and fund the most dynamic + promising world-class researchers in academia, industry, + government**
  - Over 300 intramural research projects & 1300 research grants at more than 200 U.S. universities and 100 international institutions
  - Supporting over 1900 Principal Investigators, 3500 grad students, and 600 post-docs
- **Ensure timely transitions of research results**
  - Offer significant benefits to national warfighting and peacekeeping capabilities, and society at large



AFOSR (Arlington) Technical Departments

AFOSR/RT

Engineering and Information Science

Engineering and Complex Systems	Information and Networks
Multi-scale Structural Mechanics and Prognosis	Mathematical & Computational Cognition & Intelligence
Turbulence and Transition	Robust Decision Making
Test and Evaluation	Computational Security and Info Operations
Optoelectronics and Photonics	Trust and Influence
Energy Conversion and Combustion Sciences	Position, Navigation, and Timing
Multi-modal Sensing and GHz-THZ Electronics	Computational Mathematics
Low Density Materials	Systems and Software
Space Power and Propulsion	Complex Network Systems
Dynamic Materials and Interactions	Cognition, Decision, and Fusion
	Dynamics and Control
	Dynamic Data Driven Applications Systems

Physical and Biological Sciences

Physical Sciences	Chemistry and Biological Sciences
Atomic and Molecular Physics	Natural Materials & Systems
Space Sciences	Mechanics of Multi-Functional Materials & Microsystems
Ultrashort Pulse Laser-Matter Interactions	Robust Decision Making
Remote Sensing and Imaging Physics	Biophysics
Flow Interactions and Control	Human Performance & Biosystems
Aerospace Materials for Extreme Environments	Molecular Electronics Enabled Control of Cellular Systems
Quantum Electronic Solids	Molecular Dynamics and Theoretical Chemistry
Electromagnetics	
Plasma & Electro-Energetic Physics	
Laser & Optical Physics	

https://community.apan.org/afosr/default.aspx

Supporting World Class Research

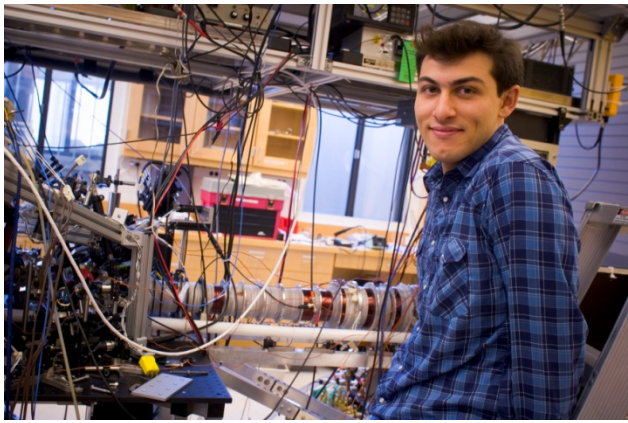
www.grants.gov

- Core Programs
  - Discipline-oriented portfolios that primarily support single investigator grants
  - Broad Agency Announcement (BAA) is open at all times – some portfolios may have review deadlines
- Young Investigator Program (YIP)
  - Designed to develop long term relationships with leading early career PIs (within 5 years of graduation)
  - Highly competitive; proposals due annually in Sept
  - 3 year grants, ~$120K/year
- Multidisciplinary University Research Initiative (MURI)
  - Multidisciplinary collaboration to achieve significant scientific advances
  - Up to $1.5 M/yr for five years
- Defense University Research Instrumentation Program (DURIP)
  - Supports acquisition of major equipment to augment current or develop new research capabilities
- Summer Faculty Fellowship Program (http://afsffp.sysplus.com/)
  - Opportunity to learn about AF research problems through collaborative research with AF researchers
  - 8-12 week research residencies for faculty at AFRL locations
  - Application process opens in September

Supporting Tomorrow's S&Es

National Defense Science and Engineering Graduate Fellowship (NDSEG)

- 3-year scholarship program to increase the numbers of PhDs in science and engineering fields
- Funds tuition, fees, etc. and $31K stipend/year
- No service commitments
- More info: http://www.asee.org/ndseg



David Kaz, Harvard
Physics PhD Candidate
2006 NDSEG AF Scholar

Science, Mathematics, and Research for Transformation (SMART)

- Career opportunity after graduation
- Funds tuition, fees, etc. and stipend
- Additional details at http://smart.asee.org/

Awards to Stimulate and Support Undergraduate Research Experience (ASSURE)

- Provide undergraduates with research opportunities in S&E fields of DoD interest
- http://www.wpafb.af.mil/library/factsheets/factsheet.asp?id=9333

Motivation

Enabling 6th Generation Aircraft

F-35 and Beyond –
Demands munition innovation

Internal Carriage	→	High energy density; Multifunctional; Insensitive
Survivable Penetrators	→	Mechanics of heterogeneous materials; Survivable energetics
Rapid Development Time	→	Energetic materials by design; predictive multi-scale modeling and simulation
High Temperature	→	Thermally stable energetic materials

Dynamic Materials and Interactions

Dynamic Materials and Interactions Portfolio

Description: Fundamental, basic research into the **dynamic** chemistry and physics of **complex materials**, particularly Energetic Materials (EMs).

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Energetic materials by design; predictive multi-scale M&S

Thermally stable energetic materials

Research Thrusts

- Energetic Materials Science

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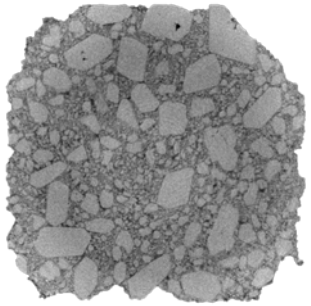
Thermally stable energetic materials

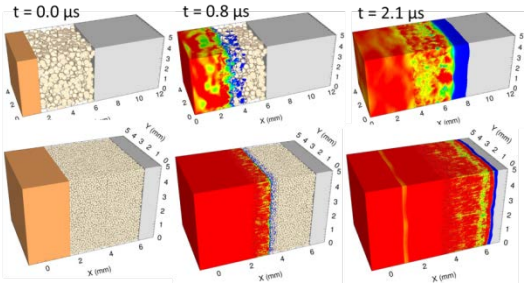
Research Thrusts

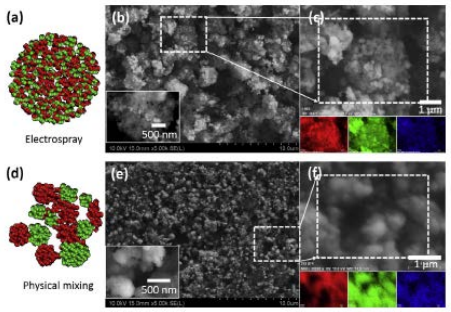
- Energetic Materials Science
- Shock Physics of Heterogeneous Materials
- Reactive Materials

Research Thrusts

- **Energetic Materials Science –** predictive processing-structure-property relationships in energetic materials
- **Shock Physics of Heterogeneous Materials –** understanding material structure-shock wave interactions
- **Reactive Materials** – enhancing energy content through new materials and improved efficiency

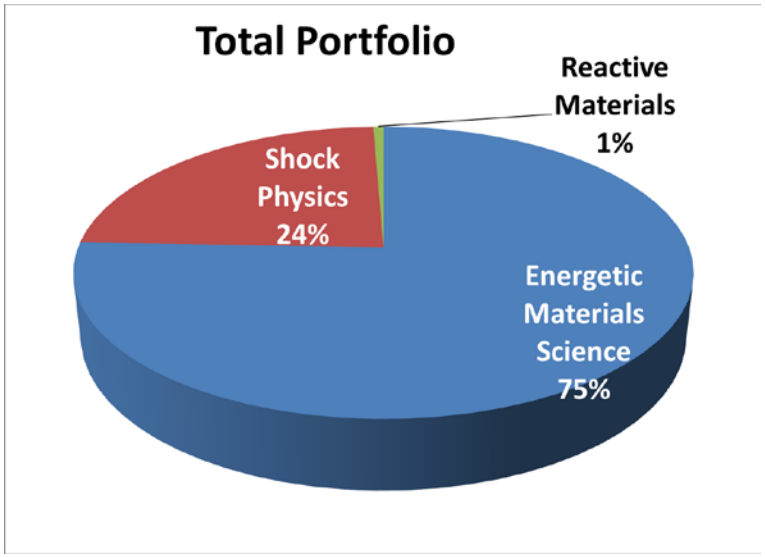






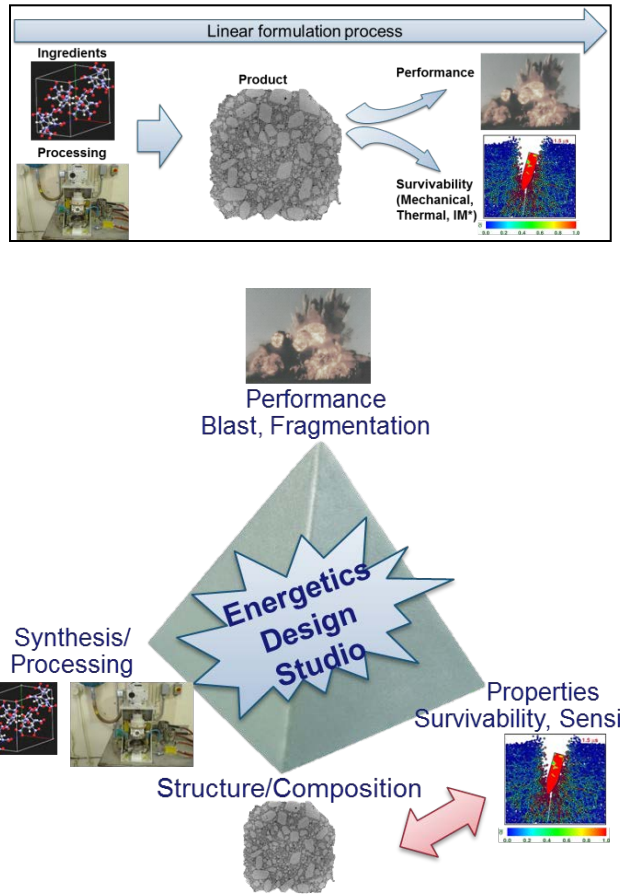
Portfolio Investment Strategy

- Discover
  - International collaboration through AOARD and EOARD
  - Cultivate Young Investigators
- Shape
  - Focus on key research gaps
  - Increase Academic – TD interactions
  - Working group for DoD basic research in energetic materials (ONR, ARO, DTRA and AFOSR)
- Champion
  - Fundamental research in energetic materials and shock physics
  - SBIR/STTR in collaboration with TDs to transition research



Energetic Materials Science

Challenge: Lack of predictive understanding requires long development times and large resource investment for new explosive formulation



Partners:

Coupling M&S with experimentation to transform energetic materials formulation from empiricism to predictive

*Insensitive Munitions

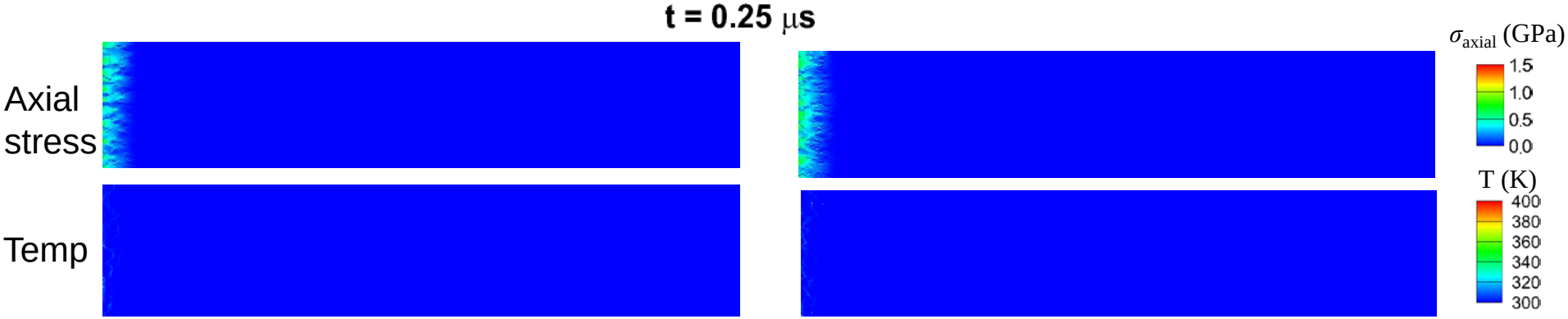
Energetic Materials Initiation

What mesoscale stress concentration features matter under what loading conditions?

Energetic Materials Initiation

HMX/Estane PBX

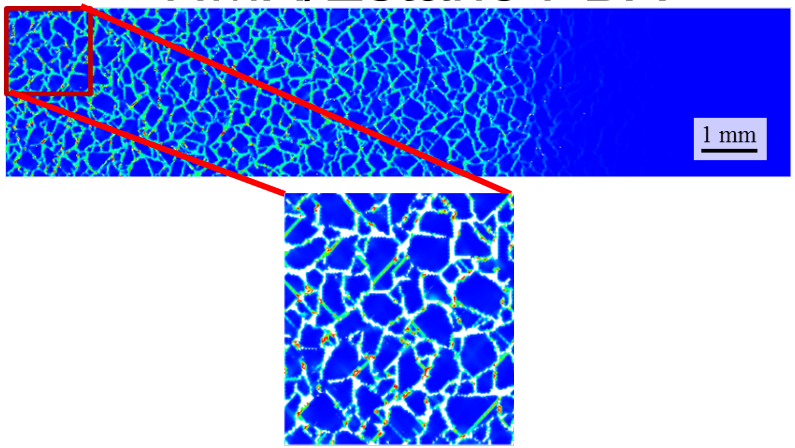
Aluminized HMX/Estane PBX



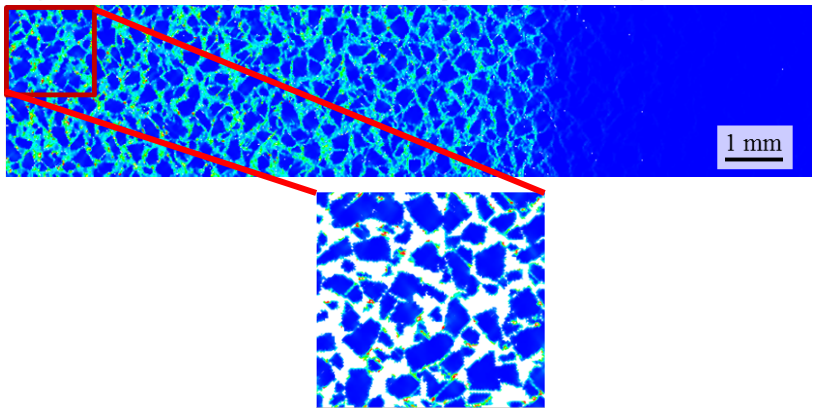
EM initiation key to increasing survivability & designing initiation systems → Mesoscale M&S advancing rapidly

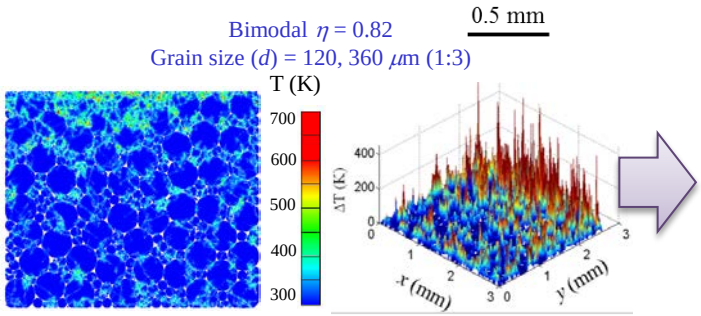
Energetic Materials Initiation

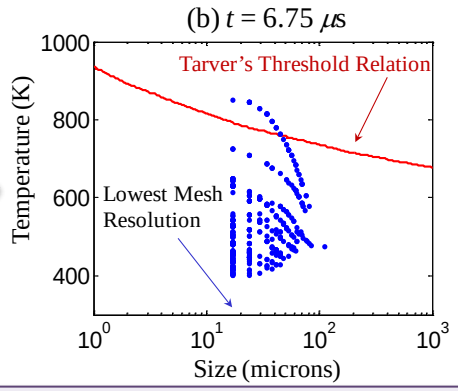
HMX/Estane PBX

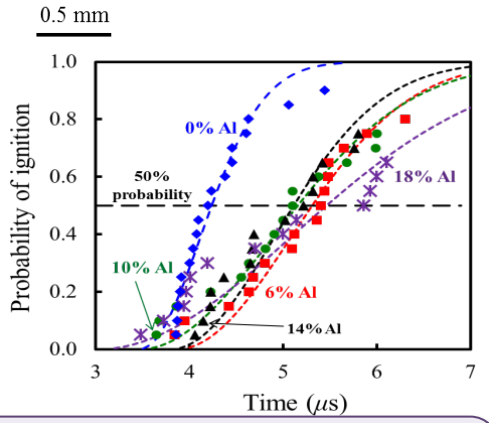


Aluminized HMX/Estane PBX





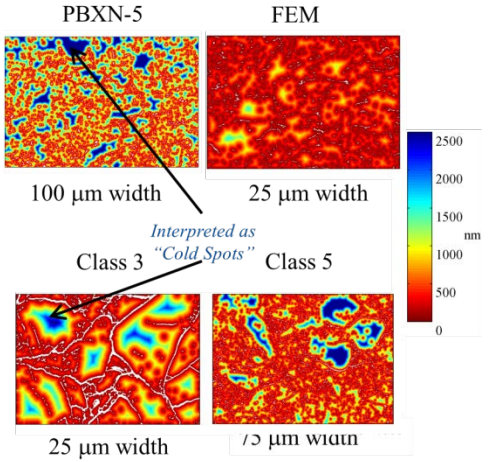




EM initiation key to increasing survivability & designing initiation systems → Mesoscale M&S advancing rapidly

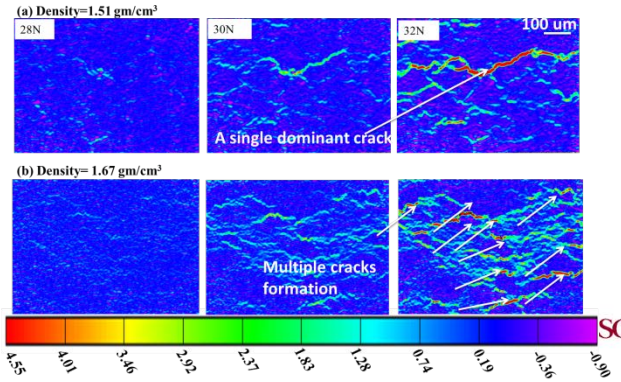
Mesoscale Initiation Experiments

Microstructural Characterization



PIs: Chris Molek, Eric Welle, Mario Fajardo (Lab Task)

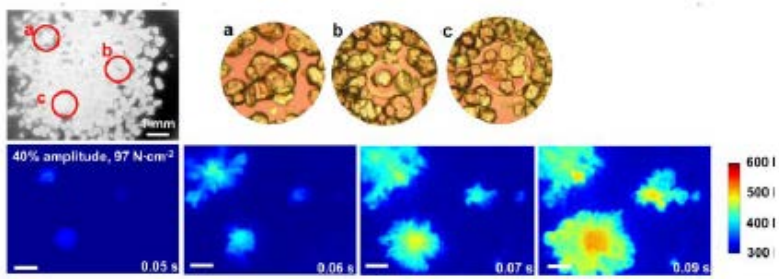
Micromechanical Characterization



UNIVERSITY OF SOUTH CAROLINA

PI: Addis Kidane (YIP)

Microfunctional Characterization

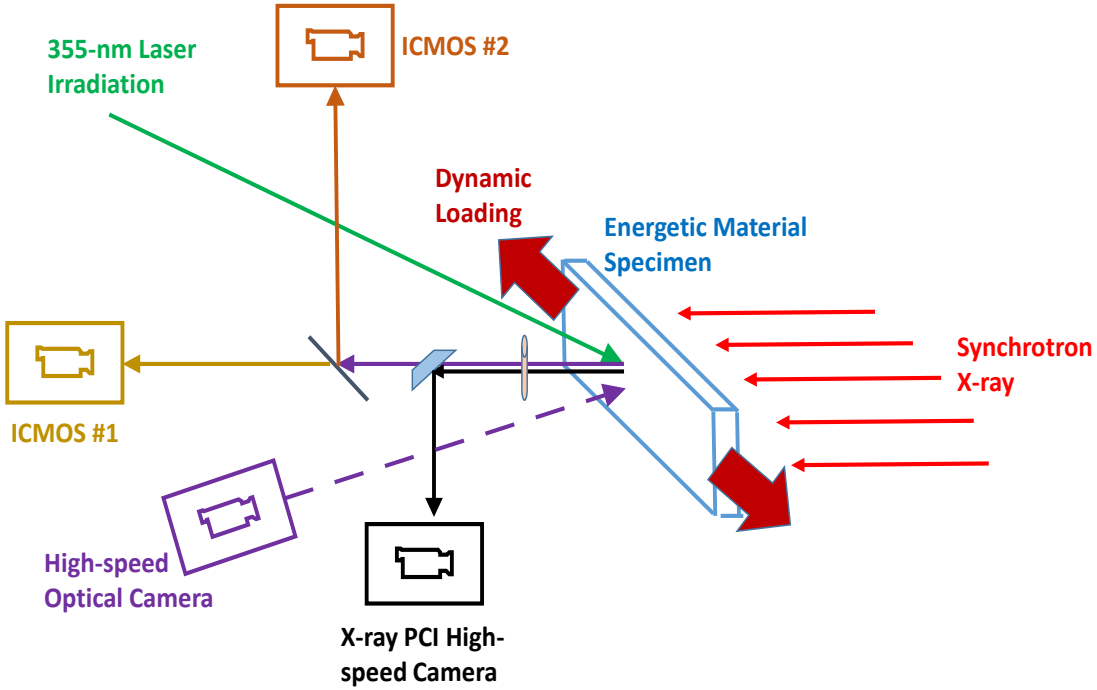


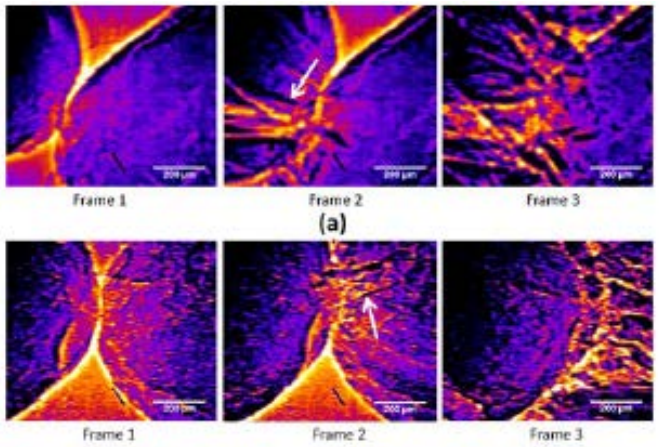
ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

PI: Dana Dlott

Real time, mesoscale experiments to capture EM initiation

Micromechanical and Microfunctional Experiments



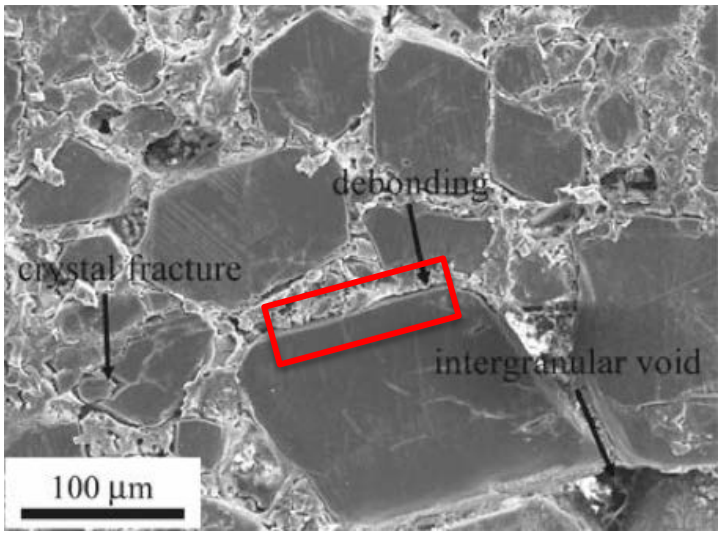


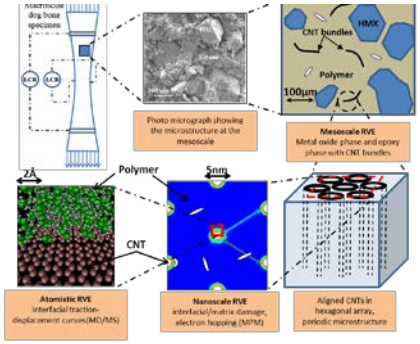
PURDUE UNIVERSITY

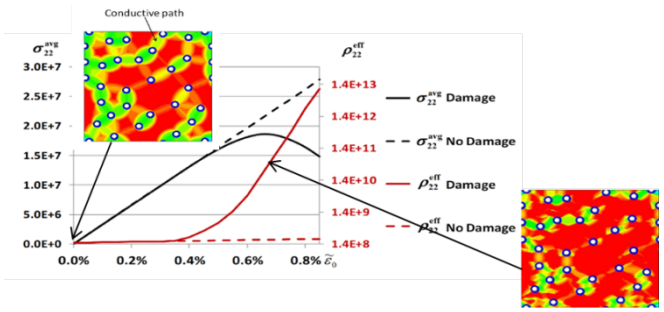
PIs: Wayne Chen, M. Gonzalez, M. Koslowski, Jeff Rhodes, Steve Son

Mesoscale temperature measurements present technical challenge

Damage and Interfaces

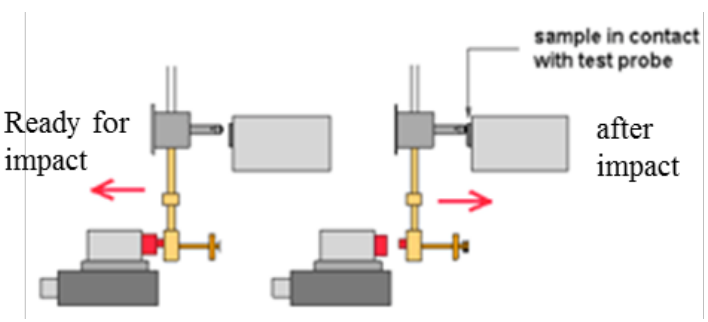


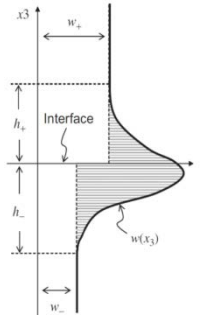




VirginiaTech
Invent the Future

PI: Gary Seidel (YIP)





VANDERBILT UNIVERSITY
PURDUE UNIVERSITY

PIs: Caglar Oskay, Vikas Tomar, Emre Gunduz

Understanding damage evolution and interfaces in EM critical for accurate prediction of response

Way Ahead

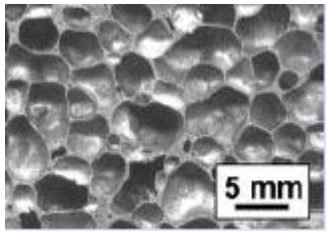
- Mesoscale processing-structure-property relationships focus for DMI portfolio
- Collaborations with RW to impact Energetics Design Studio

Shock Physics of Heterogeneous Materials

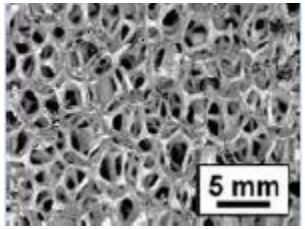
Challenge: Shock wave interactions with heterogeneous materials are complex and continuum response depends on the stochastic mesostructure

Heterogeneous Materials

Closed Cell Foam

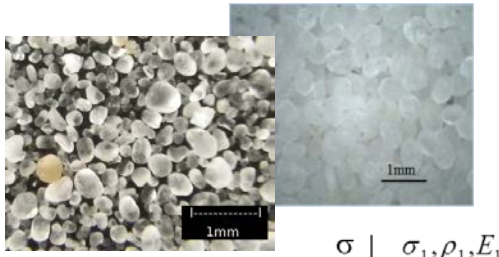


Open Cell Foam

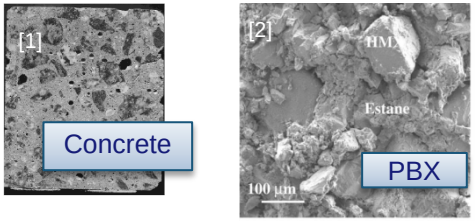


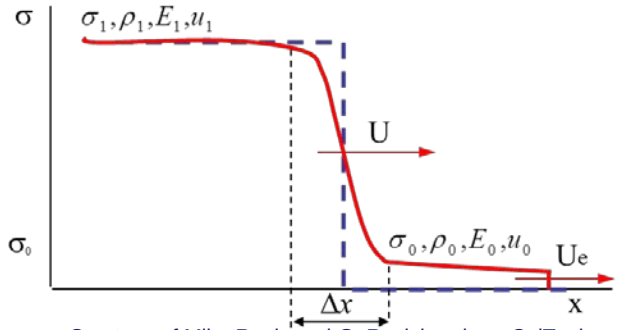
Courtesy of John Borg, Marquette

Granular



Multi-Constituent





Courtesy of Mike Rauls and G. Ravichandran, CalTech

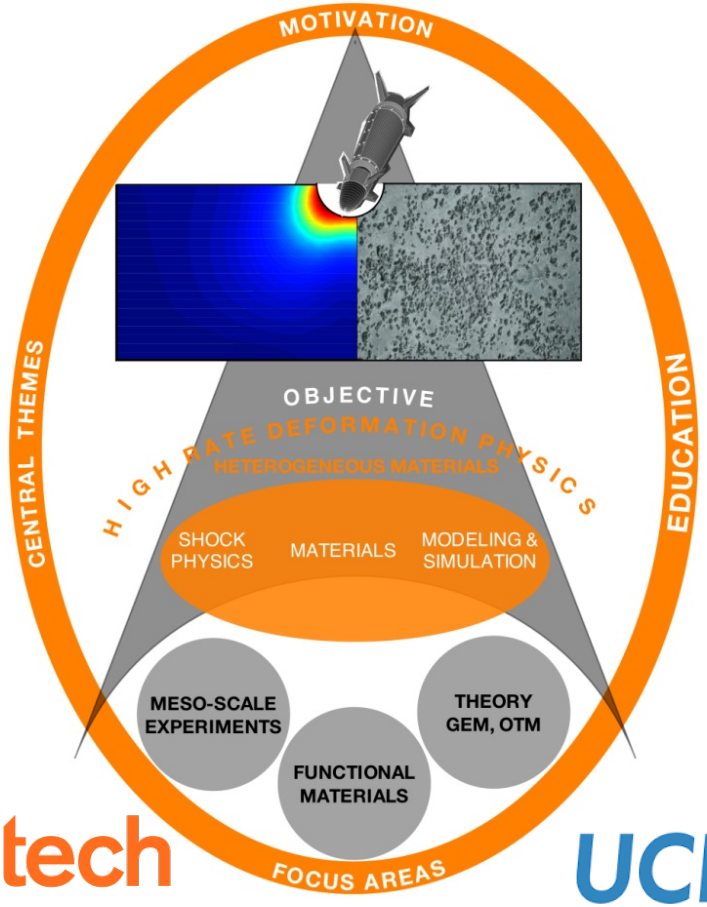
Partners:

Controlling shock wave interaction by microstructural manipulation; Create metastable materials with dynamic high pressure

[1] http://www.fhwa.dot.gov

[2] M.R. Baer, *Thermochimica Acta*, 2002

Center of Excellence



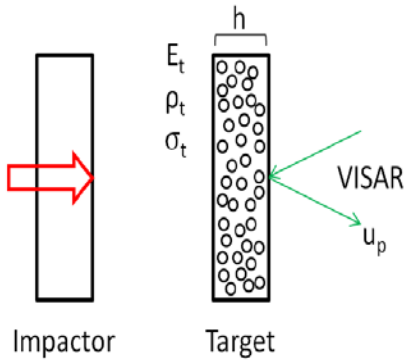
Caltech UCLA

PIs: G. Ravichandran, J.E. Andrade, K. Bhattacharya, G.P. Carman, C. Daraio, C.S. Lynch, and M. Ortiz

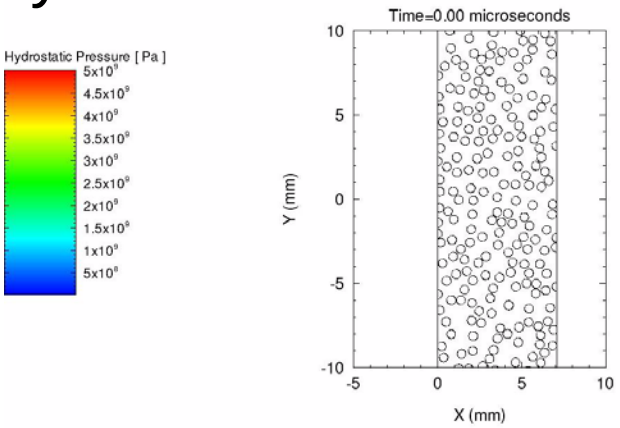
- Develop fundamental understanding of physics of heterogeneous materials at high strain rates (10^5-10^7 /s) and pressures (1-100 GPa)
- Develop engineered microstructures and functional materials for mitigating shock and damage
- Use innovative methods for educating and training next generation of scientists and engineers

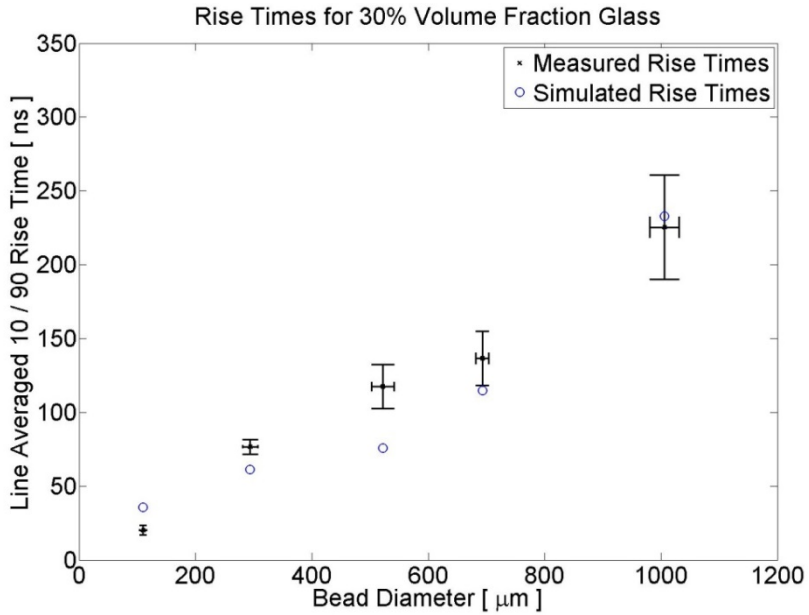
AFRL

Physics of Heterogeneous Materials



Hydrocode simulation



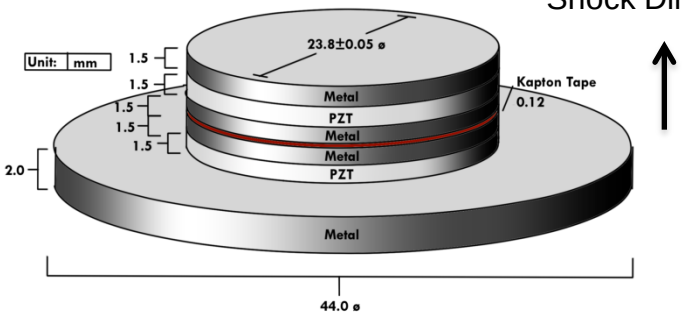


Caltech

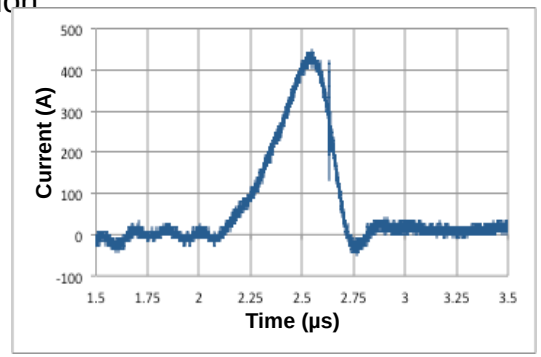
PI: G. Ravichandran

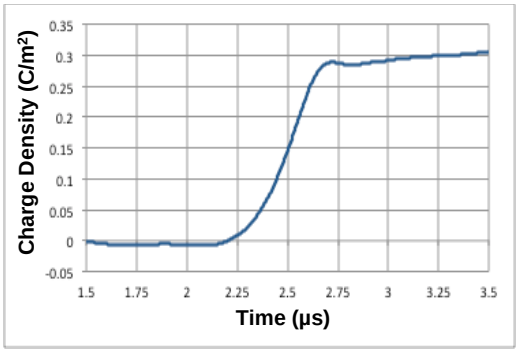
Interface scattering increases rise time of shock wave and effective viscosity of composite

Functional Materials to Mitigate Shock and Damage



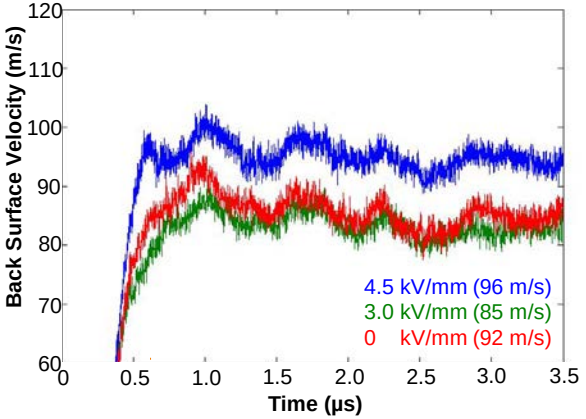
Depolarization Current and Charge



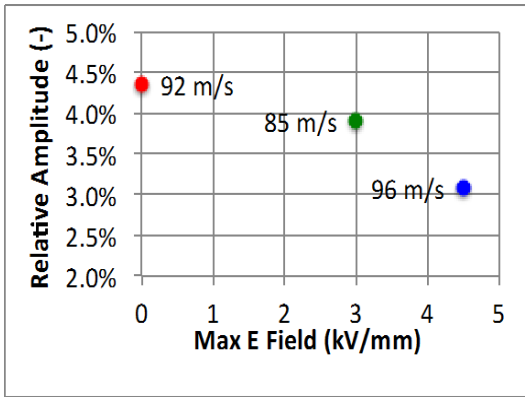


- Shock wave induces ferroelectric – antiferroelectric phase transformation
- Wave scattering modified by electrical boundary conditions

VISAR Results



Wave Scattering vs. E Field



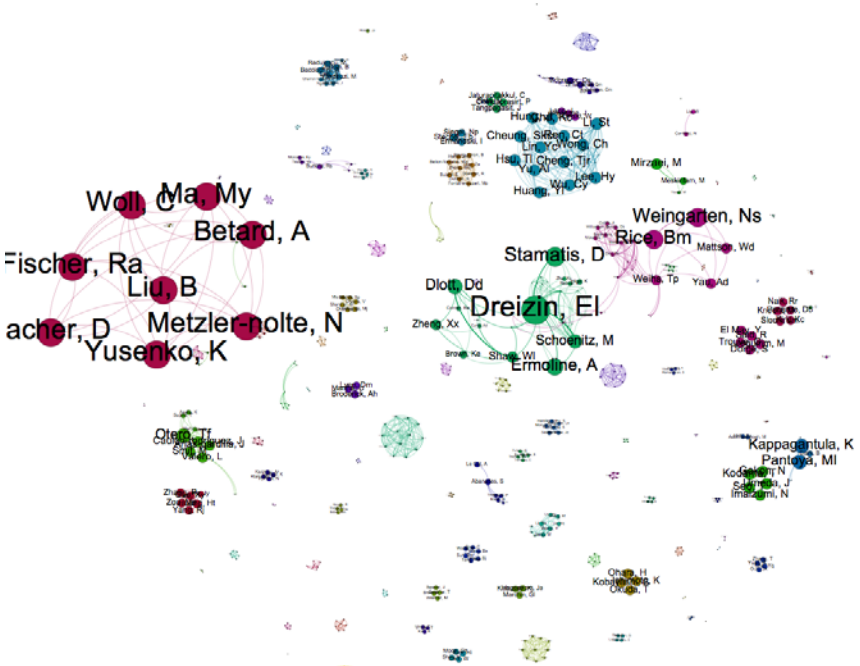
Smart composite material changes acoustic impedance through pressure driven phase transformation

Investment and Way Ahead

- Center of Excellence (COE) ends in FY17
- Planning Particulate Mechanics Workshop
  - Current state-of-the-art
  - Technical gaps
  - Clarify way forward for FY17+

Reactive Materials

Challenge: Reactive materials provide promise of increased energy density that has not been realized



Partners:

Discovery Strategy

- Survey community using science analytics tools
- Survey literature to develop research areas

Research Areas

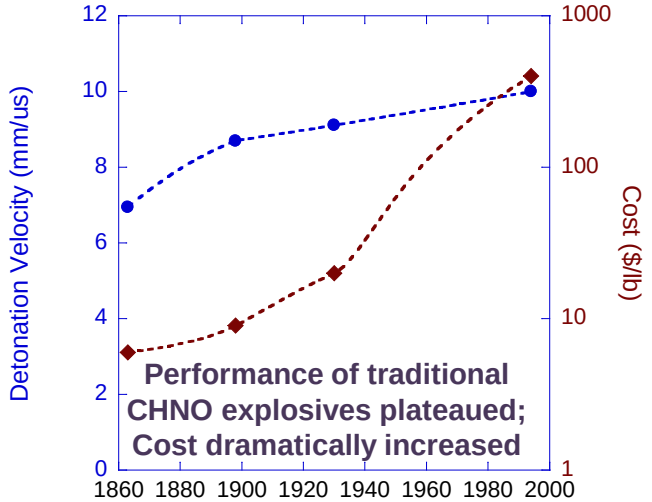
- Bottom up material design
- Reactive multi-phase flow
- Bridging length scales

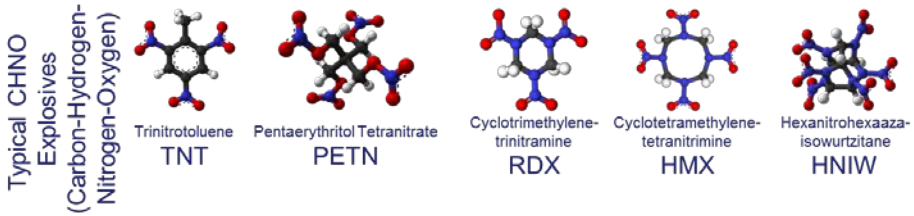
Area of Future Investment

Reactive Materials

Monomolecular Energetics

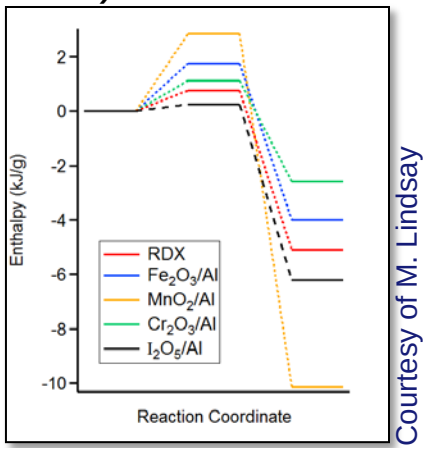
- Fuel and oxidizer on the same molecule
- Kinetics controlled by bond energy
- Heat and gas production → volumetric work





Reactive Materials

- Thermites, intermetallics, metal+polymer
- Fuel and oxidizer separate → mass transport
- Diffusion limited
- Heat + little or no gas (some exceptions)



Courtesy of M. Lindsay

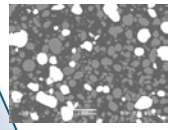
Energy content is comparable to CHNO explosives.
Reaction time can be significantly longer.

Reactive Materials
Bottom Up Material Design

Top Down

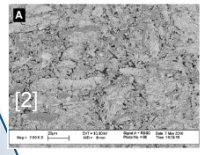
Bottom Up

Mixing μ-sized powders (with binder)

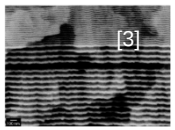


Mixing nano-sized powders

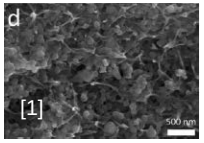
Arrested Reactive Milling



Nano-foils

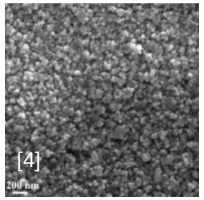


Electrospray

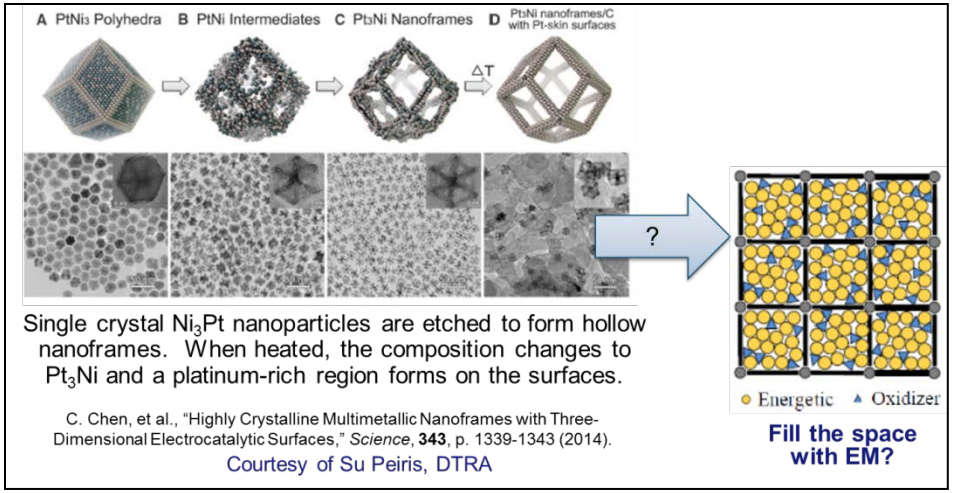


Functionalized Nano-Particles

Core-Shell Particles



Clusters

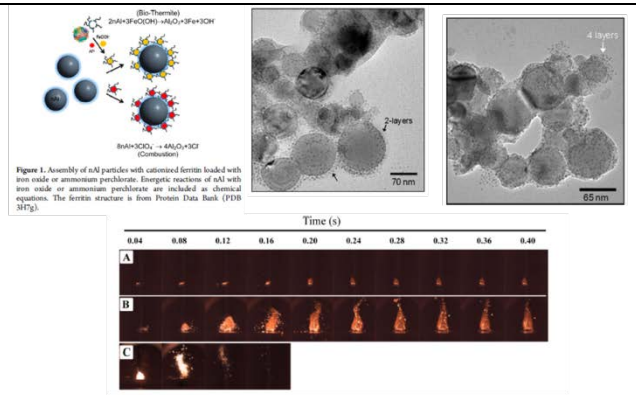


Single crystal Ni_3Pt nanoparticles are etched to form hollow nanoframes. When heated, the composition changes to Pt_3Ni and a platinum-rich region forms on the surfaces.

C. Chen, et al., "Highly Crystalline Multimetallic Nanoframes with Three-Dimensional Electrocatalytic Surfaces," *Science*, **343**, p. 1339-1343 (2014).

Courtesy of Su Peiris, DTRA

Fill the space with EM?



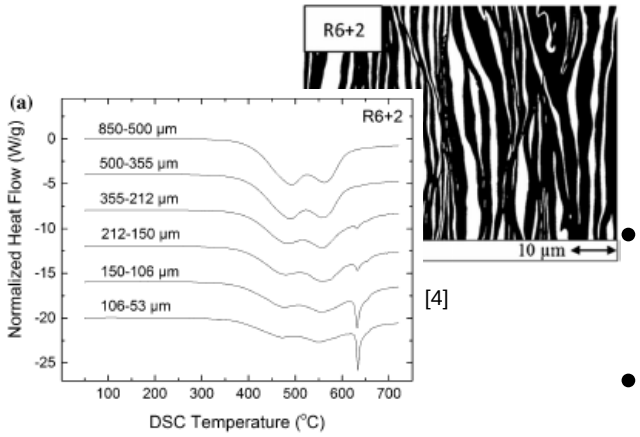
Biologically inspired assembly of AP or Fe_2O_3 loaded ferritin protein cages onto the surface of Al nanoparticles. Ability to tailor layers of protein cages → optimize reactivity

J.M. Slocik, et al. "Biologically Tunable Reactivity of Energetic Nanomaterials Using Protein Cages," *Nano Letters*, **13**, p. 2535-2540 (2013).

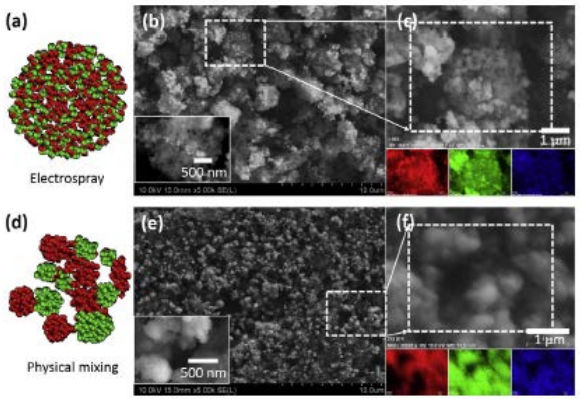
[1] C. Huang, G. Jian, J. DeLisio, H. Wang and M.R. Zachariah, *Adv Engr Mat* 10.1002/adem.201400151 (2014).
[2] D. Stamatis, X. Zhu, M. Schoenitz, E.L. Dreizin, and P. Redner, *Powder Tech*, **208**, 637-642 (2011).
[3] R. Knepper, M.R. Snyder, G. Fritz, K. Fisher, O.M. Knio, and T.P. Weihs, *JAP*, **105**, 083504 (2009).
[4] Picture courtesy of C. Ridge, S. Emery, K. Rider, and C.M. Lindsay

Bridging Length Scales

Powder Scale

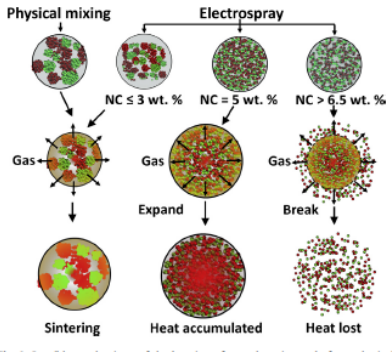


[4]

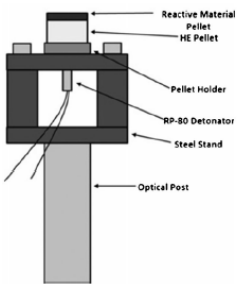


[3]

- Slow, thermal initiation, e.g. DSC vs. dynamic initiation
- Effect of morphology on reaction mechanisms
- **Prediction of behavior**



Laboratory Testing Scale



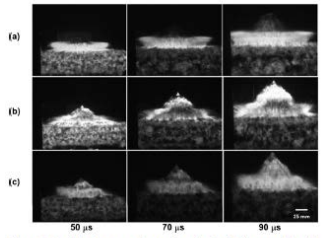
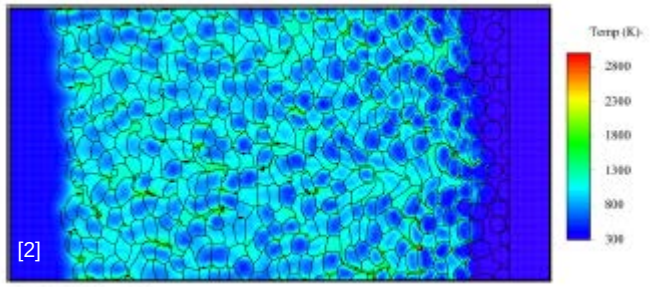


Figure 7. Qualitative comparison of mechanical alloy reactivity. (a) UIUC Mechanical Alloy #1, (b) UIUC Mechanical Alloy #2, (c) NJIT Mechanical Alloy.

[1]

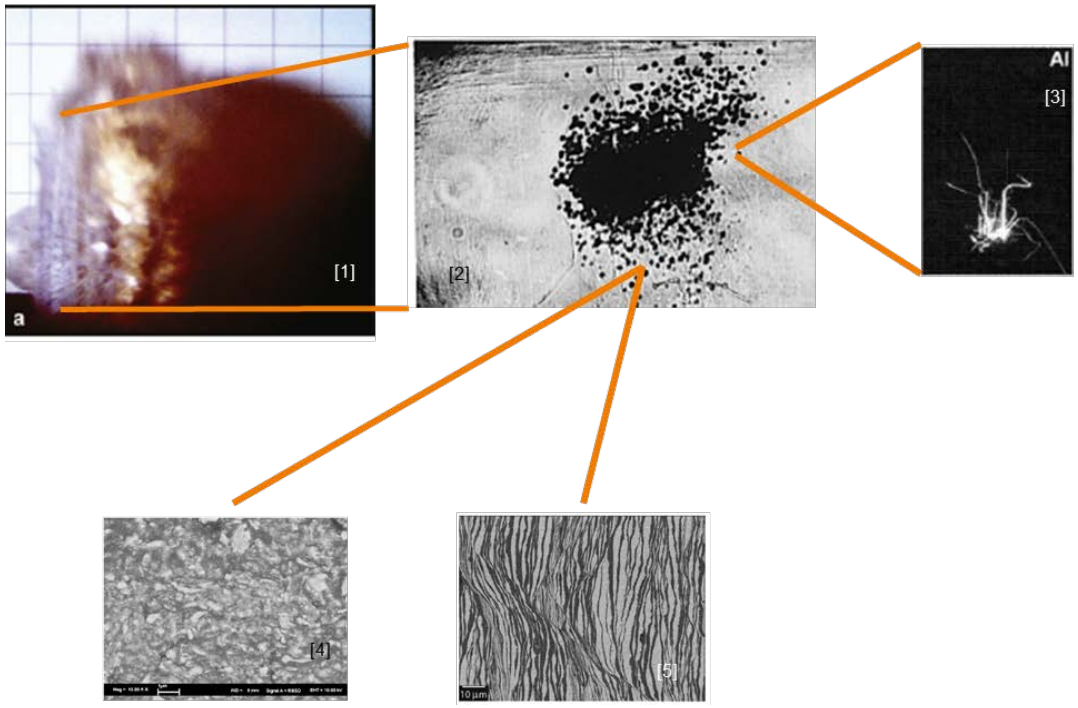


Understanding Heterogeneous Reaction Mechanisms

[1] M.D. Clemenson, S. Johnson, H. Krier, and N. Glumac, *Propellants Explos. Pyrotech.*, **39,** 454-462 (2014).
[2] R.A. Austin, D.L. McDowell, and D.J. Benson, *JAP*, **111**, 123511 (2012).
[3] H. Wang, G. Jian, G.C. Egan, and M.R. Zachariah, *Combustion and Flame*, **161**, 2203-2208 (2014).
[4] A.K. Stover, N.M. Krywopusk, J.D. Gibbins, and T.P. Weihs, *J Mater Sci*, **49**, 5821-5830 (2014).

Reactive, Multi-Phase Flow

- Reaction mechanism of complex particles
- Interactions with shock wave driven by detonation
- Models for reaction included in multi-phase flow models – including complex particles



[1] C.M. Jenkins, R.C. Ripley, C.-Y. Wu, Y. Horie, K. Powers, and W.H. Wilson, *Intl J Multiphase Flow*, **51**, 73-86 (2013).
[2] V.M. Boiko, V.P. Kiselev, S.P. Kiselev, A.N. Papyrin, S.V. Poplavsky, V.M. Fomin, *Shock Waves*, **7**, 275-285 (1997).
[3] E.L. Dreizin, C. Badiola, S. Zhang, and Y. Aly, *Intl J Energetic Matls Chemical Propulsion*, **10** [4], 297-319 (2011).
[4] E.L. Dreizin, *Progress in Energy and Combustion Science*, **35**, 141-167 (2009).
[5] R. Knepper, M.R. Snyder, G. Fritz, K. Fisher, O.M. Knio, and T.P. Weihs, *JAP*, **105**, 083504 (2009).

Investment and Way Ahead

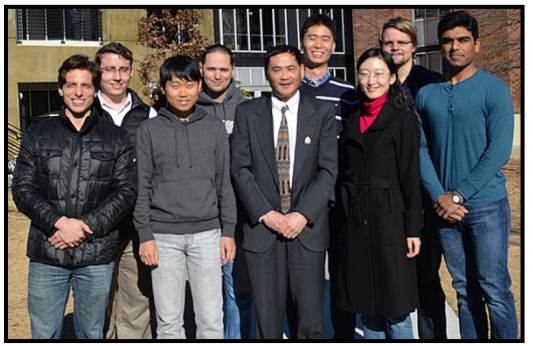
- Engaging with community → invited presentation at Materials Research Society Meeting
- Planning for future leveraging ONR and DTRA work

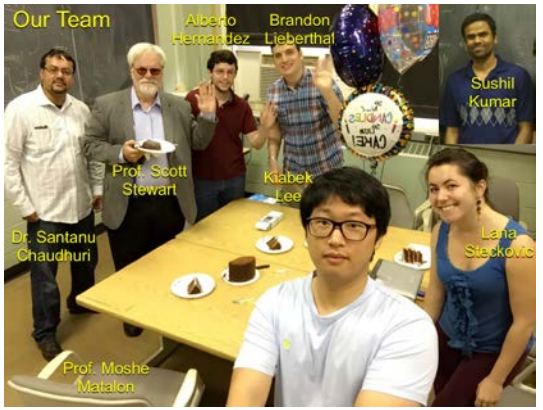
Summary

- DMI portfolio focused on dynamic chemistry and physics of complex materials, particularly EM
- Energetic Materials Science
  - FY15 investment in understanding mesoscale initiation
- Shock Physics of Heterogeneous Materials
  - High-Rate Deformation Physics of Heterogeneous Materials Center of Excellence
- Reactive Materials
  - Future area of emphasis for portfolio

Acknowledgements

- Jordan Comins, BRICC, for science analytics
- PIs and graduate students of the DMI portfolio





Contact Information

Dr. Jennifer Jordan

Email: jennifer.jordan.6@us.af.mil

Phone: 703-588-8436

APAN: http://tinyurl.com/AFOSR-DMI

2015 Review:
August 11-13, 2015, Doolittle Institute, Fort Walton Beach, FL