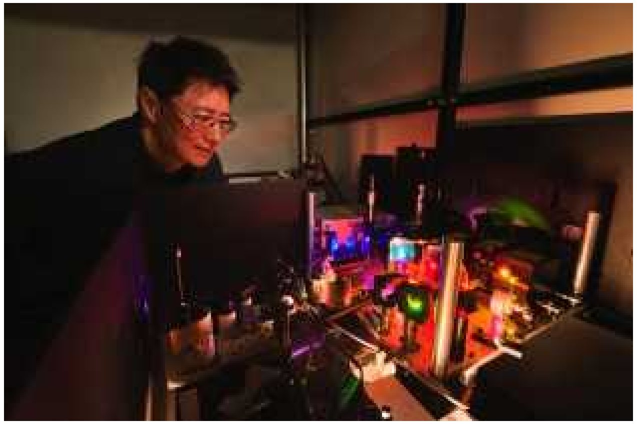
SAND2015-1194PE

Exceptional service in the national interest

Sandia National Laboratories



Sandia National Laboratories, the Materials Science and Engineering Center, and the Organic Materials Science Department

An Overview

Dr. James R. McElhanon
Brewer Science
February 24, 2015

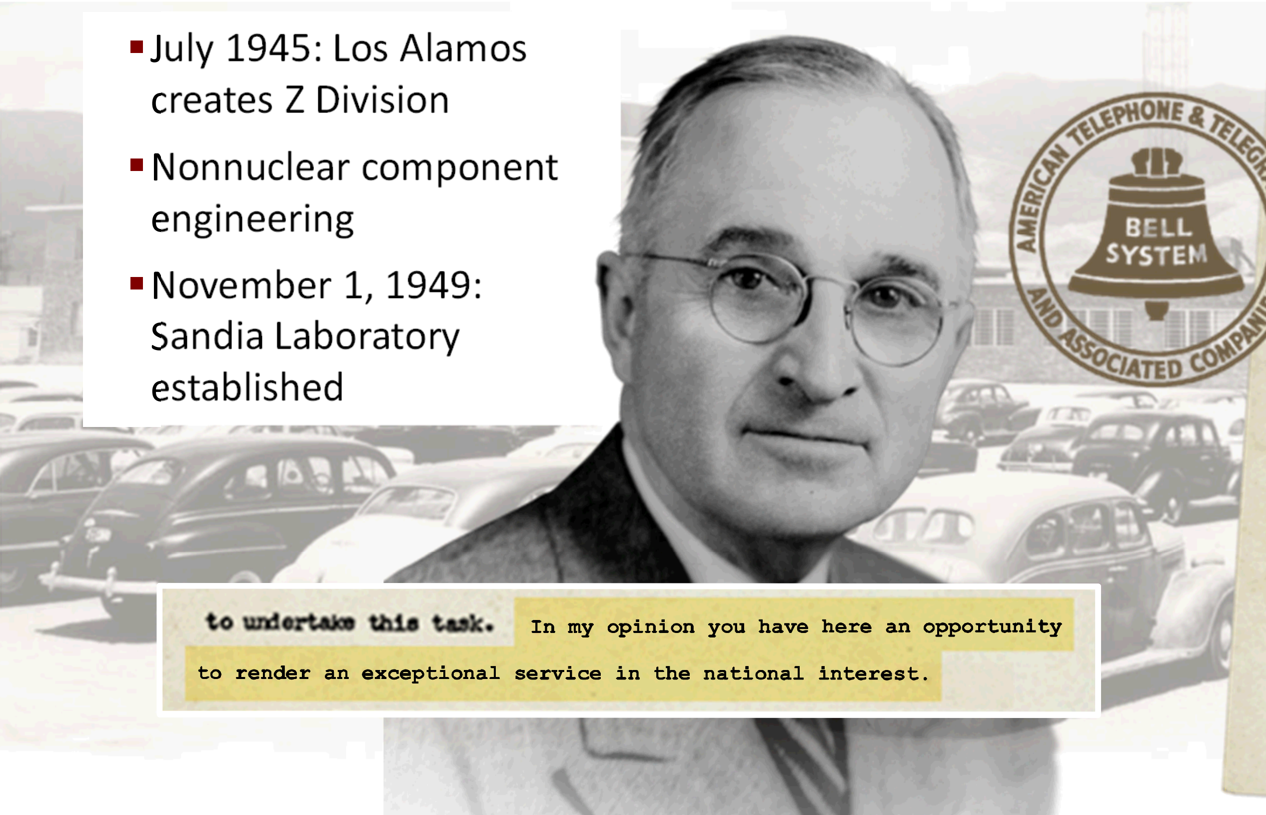
U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND No. SAND2014-17320 PE

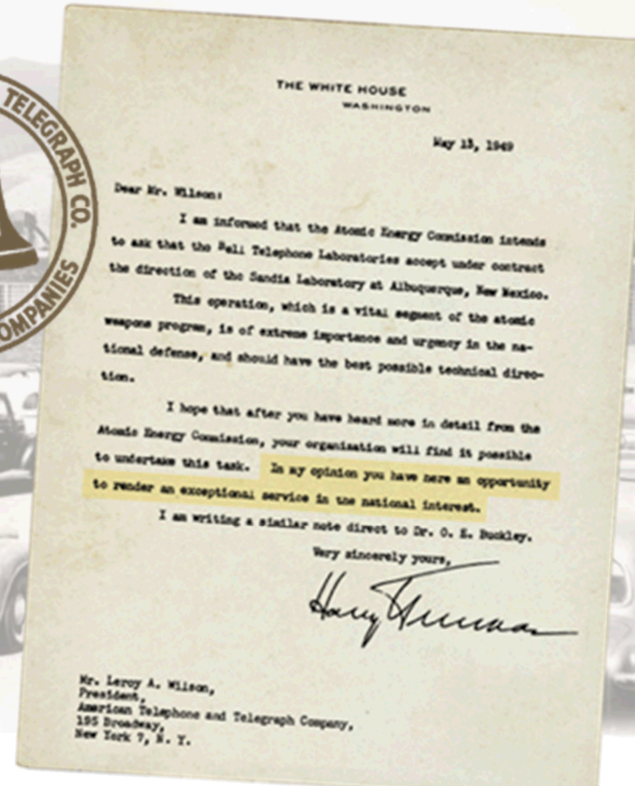
Sandia's History

Exceptional service in the national interest

- July 1945: Los Alamos creates Z Division
- Nonnuclear component engineering
- November 1, 1949: Sandia Laboratory established



to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.



THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely yours,

Harry Truman

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.

Outline

- History of Sandia National Laboratories
  - Add details
- Overview of the Materials Science and Engineering Center
  - Add details
- Capabilities and Science of the Organic Materials Science Department
  - Add details

Governance of Sandia Laboratories

Sandia Corporation

- AT&T: 1949–1993
- Martin Marietta: 1993–1995
- Lockheed Martin: 1995–present
- Existing contract expires: April 30, 2016, with a one-year contract extension option
- Government owned, contractor operated

Federally funded research and development center

Sandia Sites

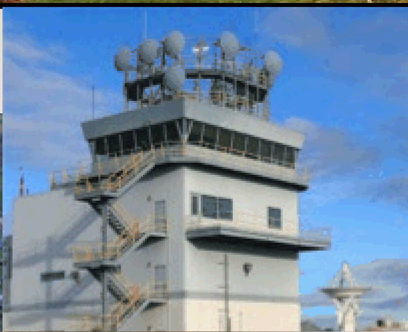
Albuquerque, New Mexico

Livermore, California

Kauai, Hawaii

Waste Isolation Pilot Plant, Carlsbad, New Mexico

Pantex Plant, Amarillo, Texas

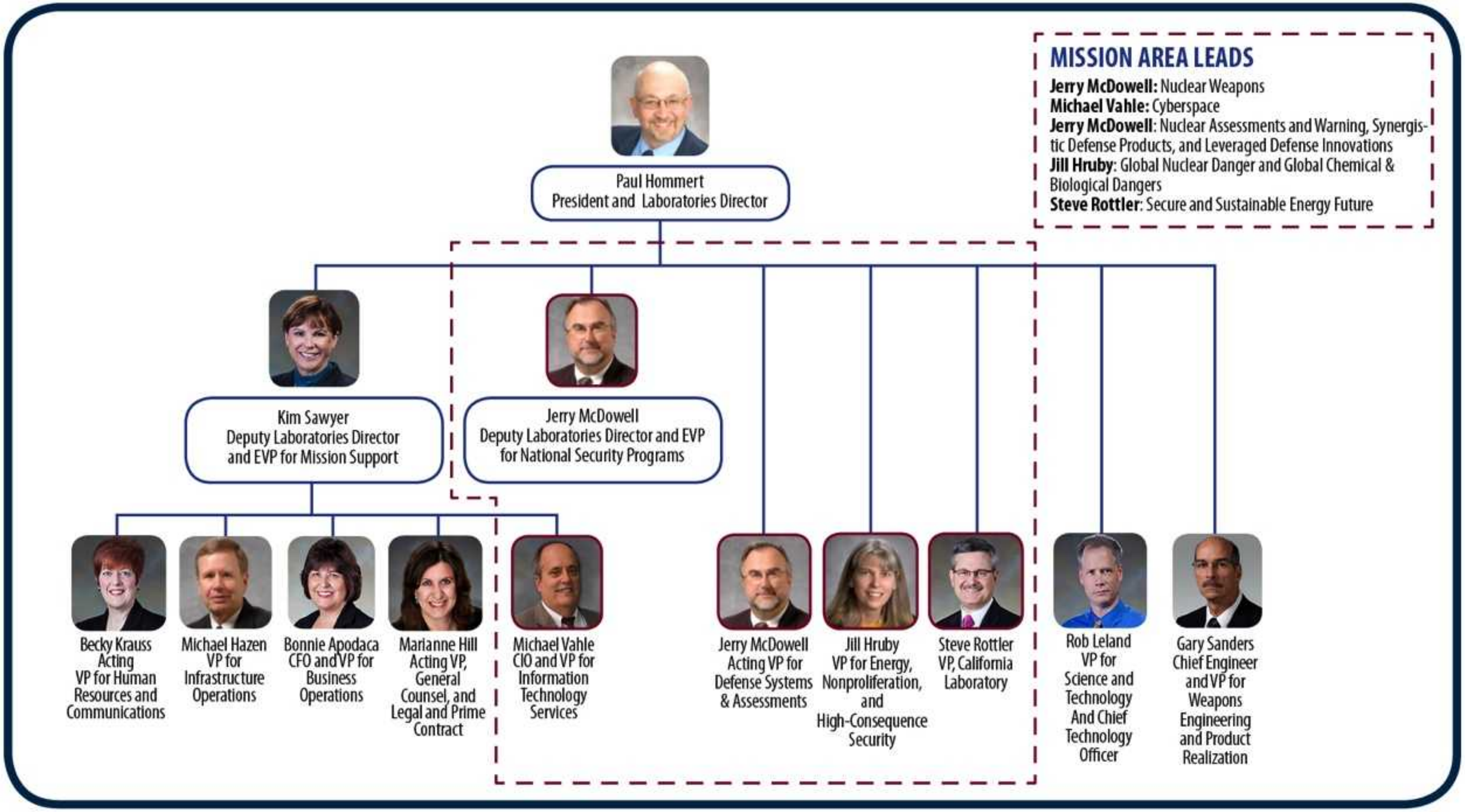


Tonopah, Nevada

Our Core Values

- Serve the nation
- Deliver with excellence
- Respect each other
- Act with integrity
- Team for great results

Executive Management Organization Chart

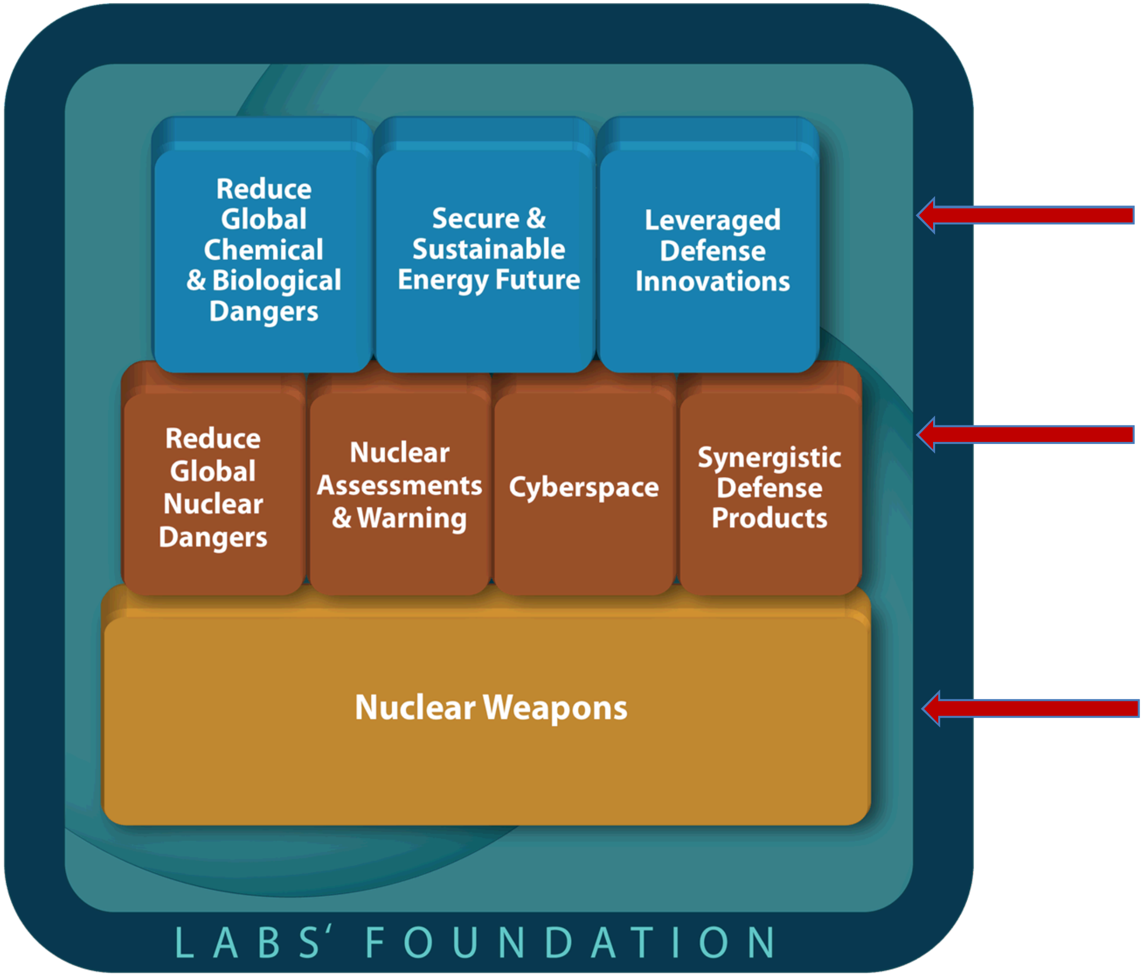


Strategic Plan

Strategic Objectives

- Deliver with excellence on our commitments to the unique nuclear weapons mission
- Amplify our national security impact
- Lead the Complex as a model 21st century government-owned contractor-operated national laboratory
- Excel in the practice of engineering
- Commit to a learning, inclusive, and engaging environment for our people

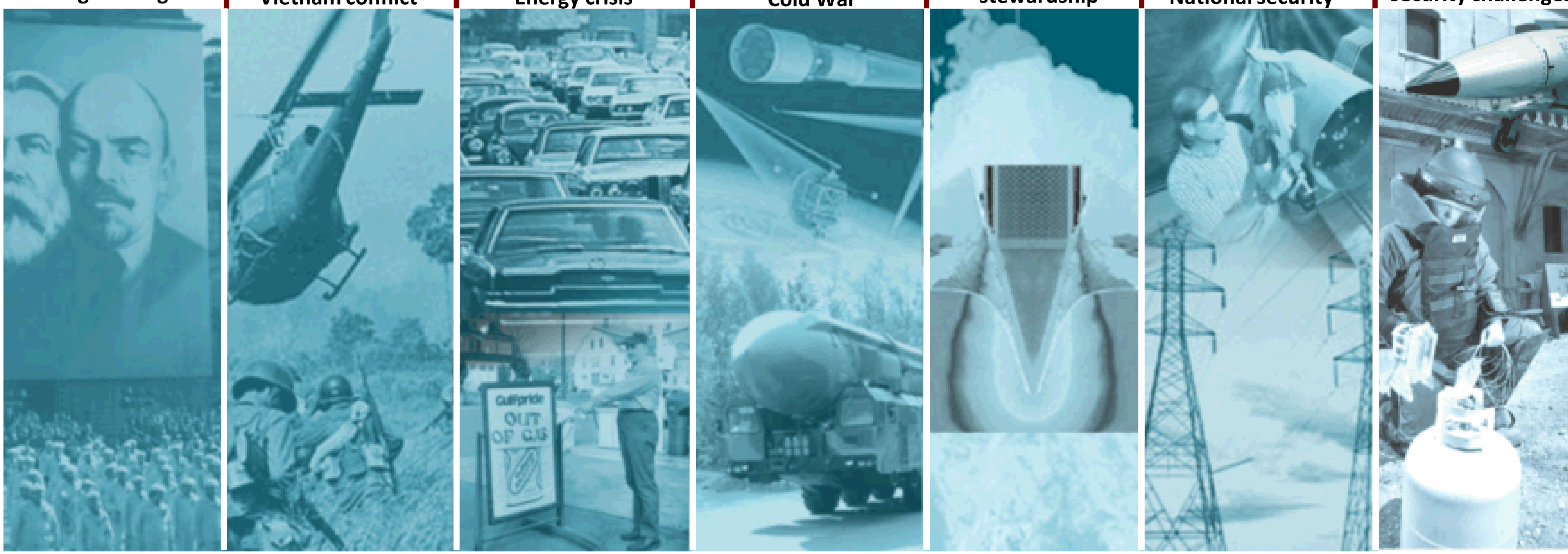
National Security Mission Areas



- Top row: Critical to our national security, these three mission areas leverage, enhance, and advance our capabilities.
- Middle row: Strongly interdependent with NW, these four mission areas are essential to sustaining Sandia's ability to fulfill its NW core mission.
- Bottom row: Our core mission, nuclear weapons (NW), is enabled by a strong scientific and engineering foundation.

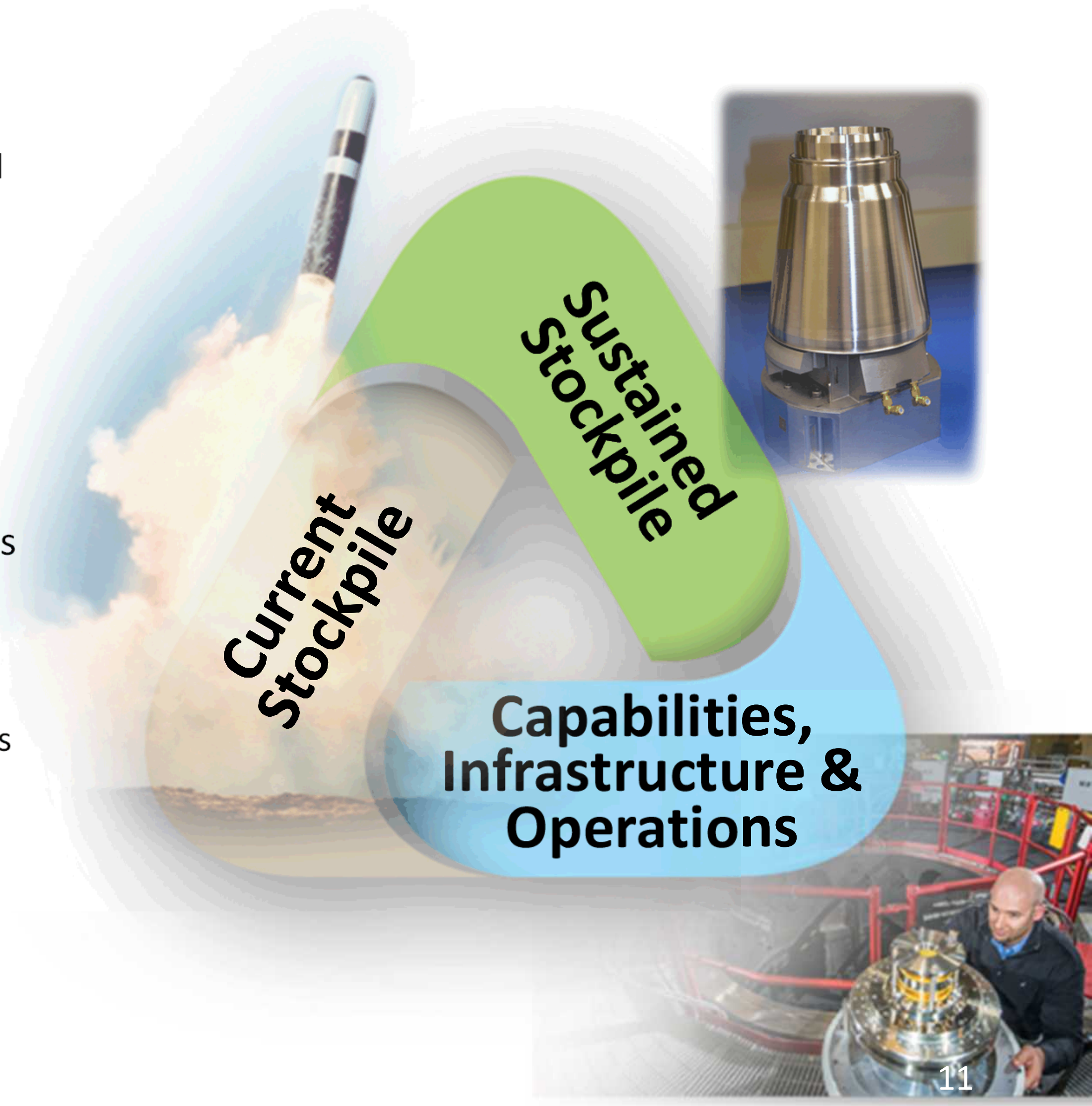
Sandia Addresses National Security Challenges

1950s	1960s	1970s	1980s	1990s	2000s	2010s
Nuclear weapons	Development engineering	Multiprogram laboratory	Missile defense work	Post–Cold War transition	START Post 9/11	LEPs Cyber, biosecurity proliferation
Production and manufacturing engineering	Vietnam conflict	Energy crisis	Cold War	Stockpile stewardship	National security	Evolving national security challenges



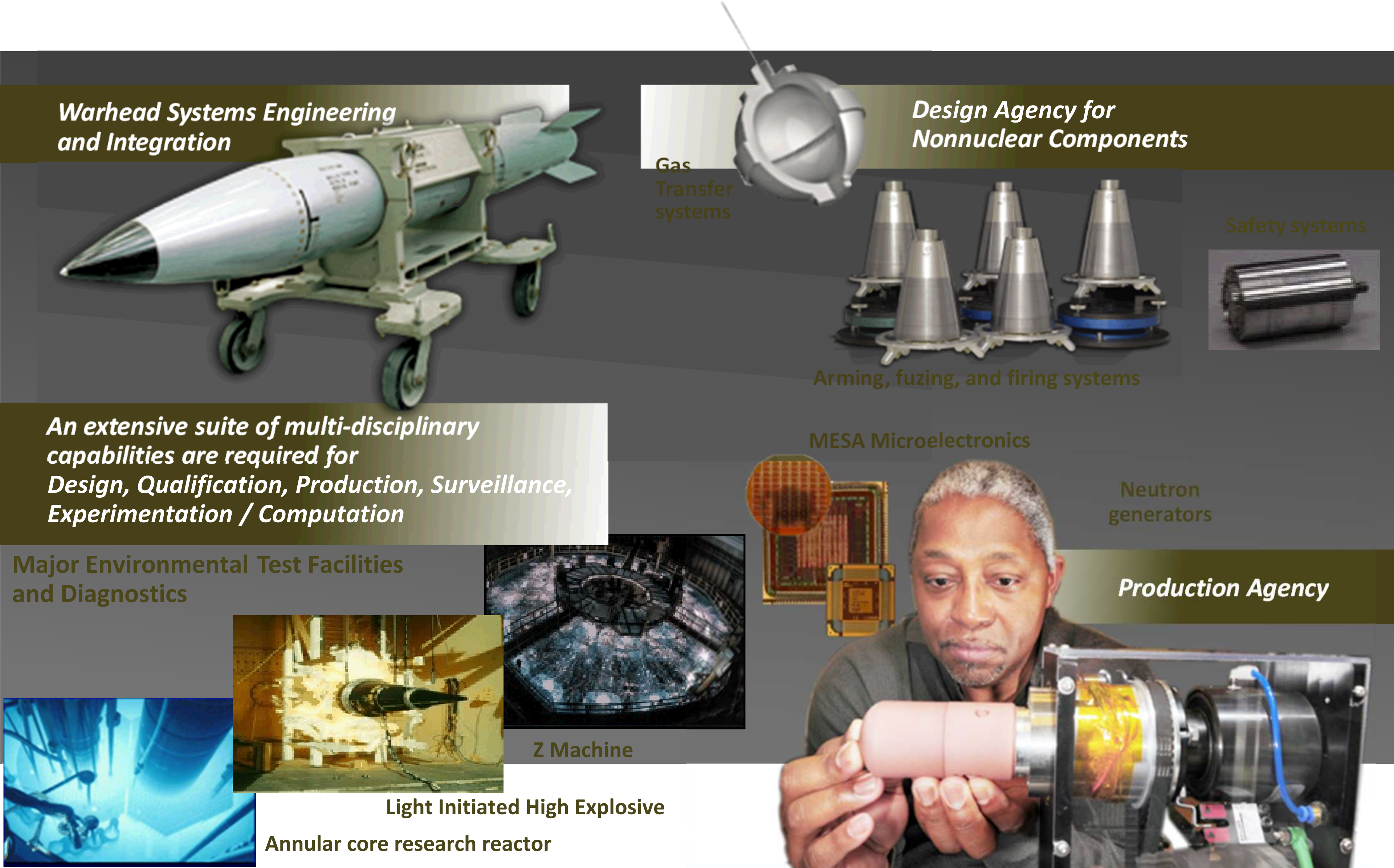
Sandia's Nuclear Weapons Mission

- Maintain the current U.S. nuclear weapons stockpile
  - Annual Assessment, Surveillance, Limited Life Component Exchanges, Significant Finding Investigations
- Sustain the stockpile into the future
  - Life Extension Programs, Alterations, technology maturation
- Steward the long-term vitality of our capabilities, infrastructure and operations
  - Persistent commitment to multi-disciplinary staff, state-of-the-art labs, equipment, facilities and safe/secure/quality/affordable operations



Sandia's Current Nuclear Weapons Activities

Sandia National Laboratories

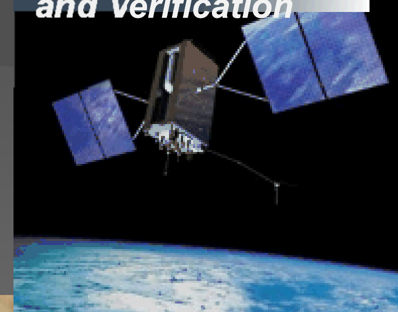


Defense Systems & Assessments Programs

Information Operations

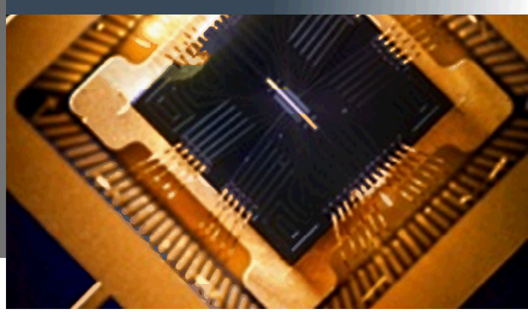
Surveillance & Reconnaissance

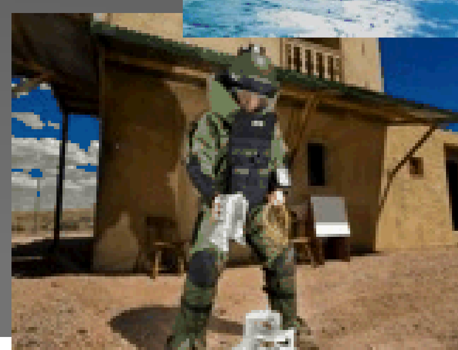
Remote Sensing and Verification



Space Mission

Science & Technology Products





Proliferation Assessment

Integrated Military Systems

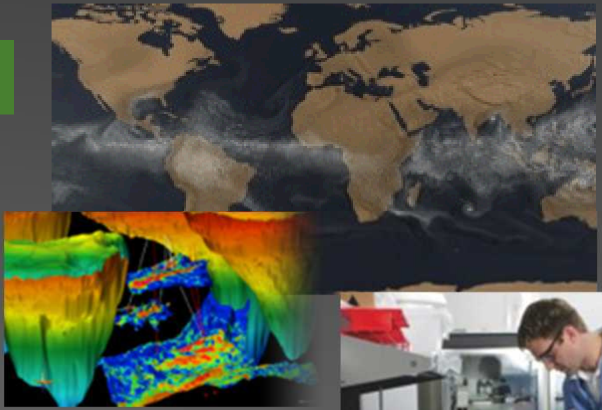
Energy & Climate

Energy Research

ARPAe, BES Chem Sciences, ASCR, CINT, Geo Bio Science, BES Material Science

Climate & Environment

Measurement & Modeling, Carbon Management, Water & Environment, and Biofuels



Nuclear Energy & Fuel Cycle

Commercial Nuclear Power & Fuel, Nuclear Energy Safety & Security, DOE Managed Nuclear Waste Disposal

Renewable Systems & Energy Infrastructure

Renewable Energy, Energy Efficiency,
Grid and Storage Systems

Transportation Energy & Systems

Vehicle Technologies, Biomass, Fuel Cells & Hydrogen Technology

International, Homeland, & Nuclear Security

Global Security

WMD Counterterrorism and Response

Homeland Security Programs

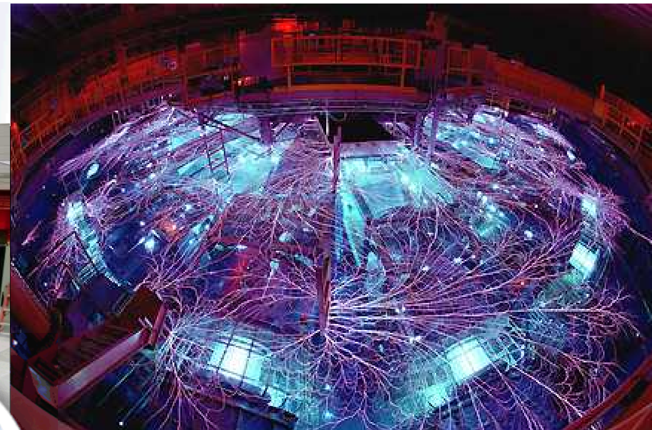
Homeland Defense and Force Protection

Cyber and Infrastructure Security

Our Research Framework

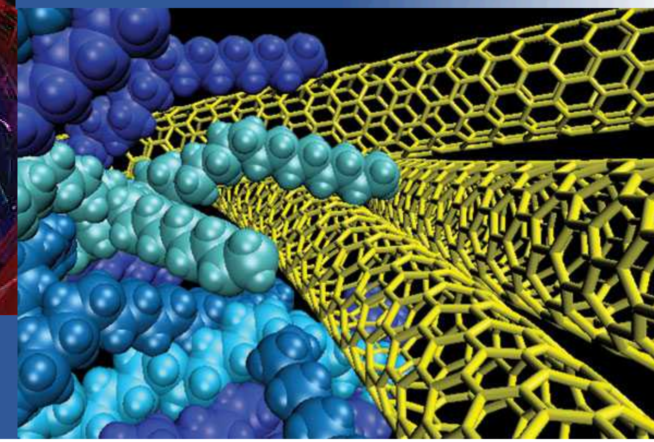
Strong research foundations play a differentiating role in our mission delivery

Computing & Information Sciences

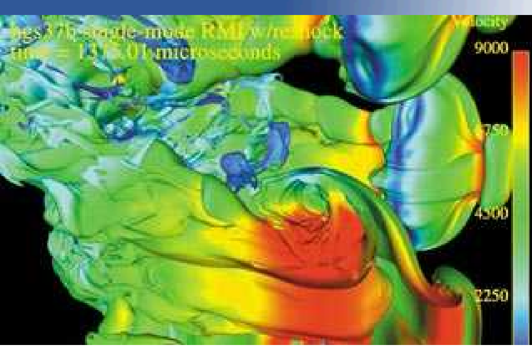


Radiation Effects & High Energy Density Science

Materials Sciences

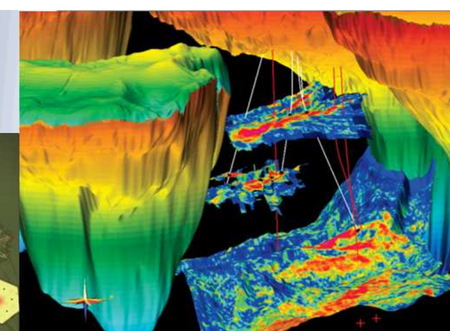


Engineering Sciences



Bioscience

Nanodevices & Microsystems

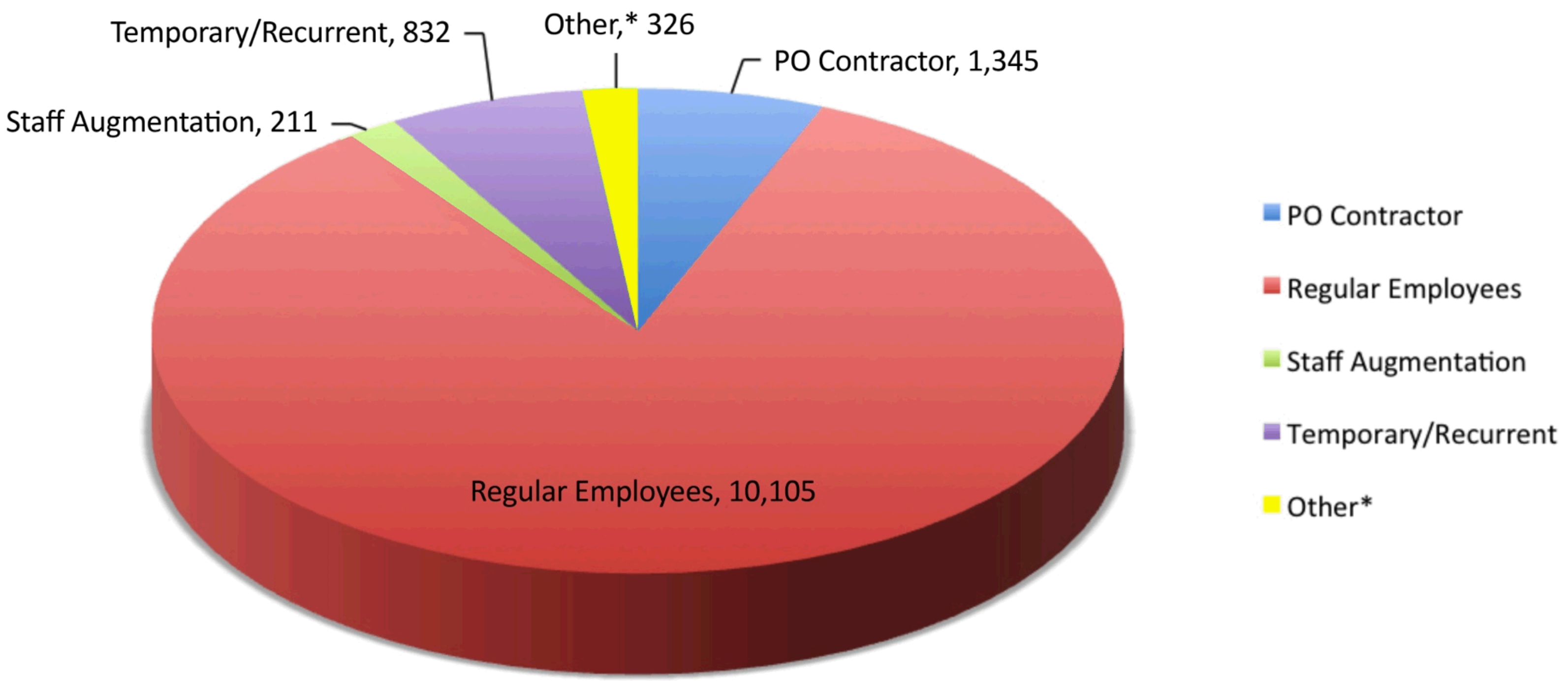


Geoscience

Our Workforce

- Total Sandia workforce: 12,819
- Regular employees: 10,105
- Advanced degrees: 6,054 (59%)

Data as of January 16, 2015



** Other badged personnel*

Materials Science and Engineering Center 1800

01810
Materials Science R&D

1814
Computational Materials & Data Science

1815
Advanced Materials Laboratory

1816
Electrical, Optical, and Nano

1819
Materials Characterization & Performance

01830
Materials Engineering and Manufacturing S&T

1831
Metallurgy & Materials Joining

1831
Coatings and Additive Manufacturing

1833
Packaging & Polymer Processing

01850
Materials Engineering and Manufacturing S&T

1851
Mechanics of Materials

1852
Materials Reliability

1853
Organic Materials Science

1854
Materials Aging and Surveillance

Center 1800 has 182 labs and 212 MOWs across our research facilities.

Major MS&T Facilities

Advanced Materials Laboratory (AML / Joint w Univ. of NM)

Center for Integrated Nano Technologies (CINT / Joint w LANL / DOE User Facility)

Integrated Materials Research Laboratory (IMRL)

Processing & Environmental Technology Laboratory (PETL)

Advanced Materials & Processes Laboratory (AMPL)

Ion Beam Laboratory (IBL)

Thermal Spray Research Laboratory (TSRL)

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Materials Science R&D is critical to Sandia's mission work

We *integrate* insightful theory, computational simulation tools and deliberate experiments in order to *deliver* predictive understanding of the performance of Sandia's current and future mission-critical materials in order to *provide* the solid technical basis for Sandia's engineering decisions

In the process of accomplishing this objective – we seek to advance the frontiers of materials science

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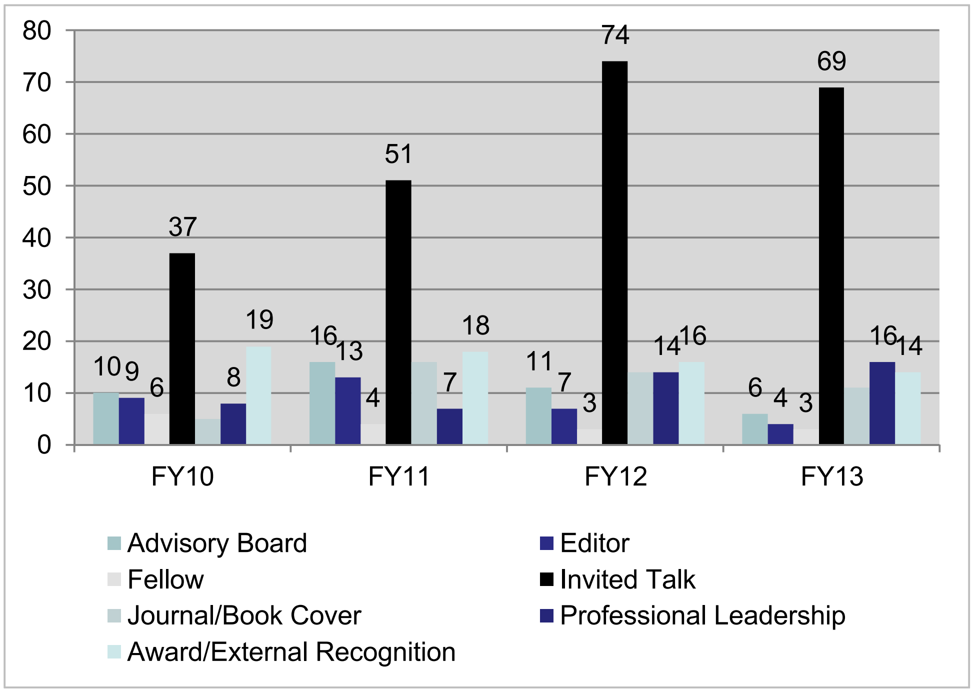
Staff external engagement and recognition



Our materials community has 73 fellows across 17 different professional societies

Organization	# of Fellows
American Physical Society (APS)	27
American Ceramic Society (ACerS)	10
American Association for the Advancement of Science	8
American Society for Metals/ASM International	7
American Vacuum Society (AVS)	5
Optical Society of America (OSA)	3
Institute of Electrical and Electronics Engineers (IEEE)	2
The American Society for Microbiology (ASM) International	2
Alpha Sigma Mu	1
American Academy of Arts and Sciences	1
American Chemical Society (ACS)	1
American Welding Society (AWS)	1
International Centre for Diffraction Data (ICDD)	1
Materials Research Society	1
National Academy of Engineering- Materials	1
Society of Tribology & Lubrication Engineers	1
Wilsmore Fellowship	1

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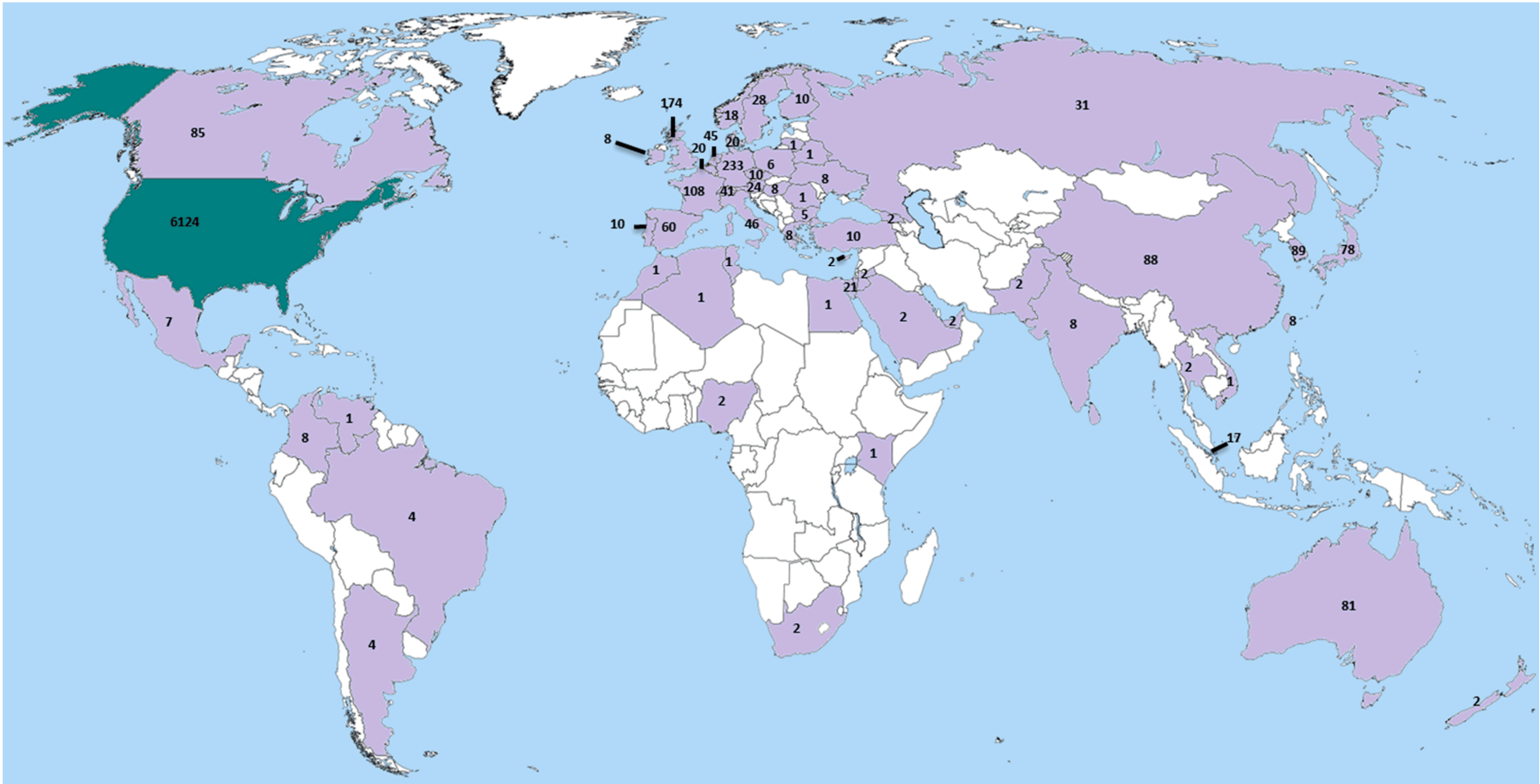
Publication Collaborations are World Wide

Sandia National Laboratories



All publication data: InCitesTM, Thomson Reuters (2014). Report Created:Mar 4, 2014 Data Processed Feb 28, 2013 5:34:23 PM Data Source: Web of Science ® This data is reproduced under a license from Thomson Reuters. You may not copy or redistribute this data in whole or in part without the written consent of the Science business of Thomson Reuters. Subject area baseline data processed Jan. 1, 1981->Dec. 31, 2013.

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Materials Scope

Provide fundamental understanding of the synthesis, processing, properties, and performance of materials.

- Fundamental understanding of mission critical materials and their processing
- Materials discovery and materials-enabled phenomena
- Materials performance in mission environments
- Materials aging and reliability
- Predictive materials behavior – atomic-to-continuum length scales
- Materials characterization, failure analysis, and forensics

Materials encompasses the breadth of the length scales – nano to continuum

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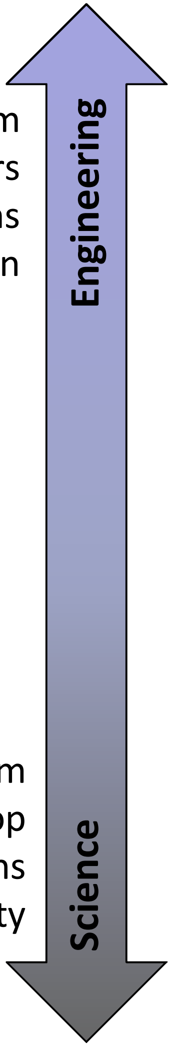
We address a spectrum of questions spanning engineering to science

Short-Term
Need fast answers
Use existing equations
Specific to Application



Long-term
Slow to develop
Derive new equations
Broad Applicability

- Will component X fail under a certain environment?
- How much margin exists between operation and failure?
- What is the probability that component X will fail in a certain environment?
- How consistent & homogeneous is the material and manufacturing processes?
- What is the mechanism by which failure occurs?
- What is the governing equation that dictates failure? Can the failure process be modeled, simulated, and predicted based on knowledge of the material & manufacturing processes?

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Materials

Provide fundamental understanding of the synthesis, processing, properties, and performance of materials

Competencies

Competencies – Facilities – Tools

Materials Synthesis & Processing
- Ceramics/glass synthesis & processing
- Joining/welding/brazing/soldering
- Surface characterization, analysis & engineering
- Metallography Nano-/meso-/micro-scale fabrication
- Organics synthesis & processing
- Electronic materials & synthesis
- Materials assembly
- Electrodeposition
- Thin film deposition (ALD, MBE, MOCVD, PVD, etc)
- Advanced semiconductor materials

Aging & Reliability
- Gas analysis & leak testing
- Environmental testing
- Materials compatibility testing
- Radiation effects characterization and defect analysis
- Plasma/surface interactions

Advanced Prototyping
- Vacuum system design & fabrication
- Electronic packaging
- Advanced machining & additive manufacturing
- Advanced electronic & optoelectronic devices
- Integrated nanotechnology platforms
- Advanced optical sensors
- Quantum devices

Materials Characterization, Analysis & Testing
- Surface analysis
- Optical & electron microscopy
- Ion beam effects & characterization
- Metallography Nano-/meso-/micro-scale fabrication
- Diffraction
- Mech/therm/elec/optical/magnetic properties meas & testing
- Tribology
- Plasma characterization
- Radiation effects microscopy
- Advanced materials diagnostic & characterization tools

Dynamic Materials Properties
- Shock physics
- Materials modeling & equation-of-state theory

Model-based Physics
- Atomistic, crystal and grain level materials and process models
- Quantum phenomena
- Plasma physics
- Defect physics

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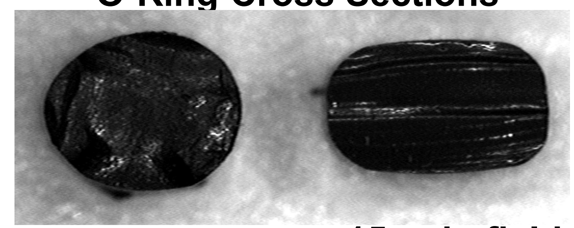
Organic Materials Science

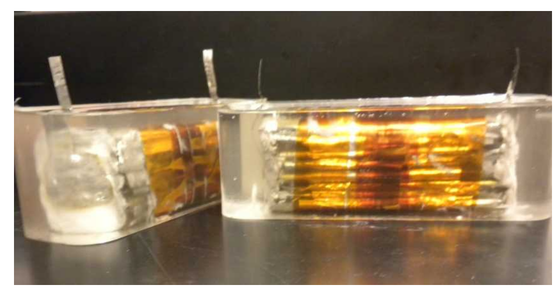
- Multi-Step Synthetic Organic Chemistry
- Polymer Synthesis
- Polymer Engineering
- Polymer Physics
- Polymer Characterization
- Aging and Degradation of Polymers
- Radiation Effects on Polymers
- Carbon-based Electronics
- Encapsulant Materials
- Thermal-Mechanical Testing of Organics
- Nanocomposites
- Adhesion Science
- Sensors

Spiropyran Light Activated Polymer

O-Ring Cross Sections



Unaged 15 yr in field



New Capacitor Dielectrics

Polymer Characterization

Full Spectrum of Characterization Capabilities for Polymers

- High Voltage Breakdown
- Oxygen Consumption
- Glove boxes and high vacuum lines for air and moisture control
- Rheology and Mechanical Analysis
- Thermal Characterizations (DSC, TGA, TMA, thermal conductivity)
- Structure determination by NMR, IR, UV, XPS, SIMS, chromatography
- X-ray/neutron scattering/diffraction and reflectivity

TA ARES DMA

MTS load frame

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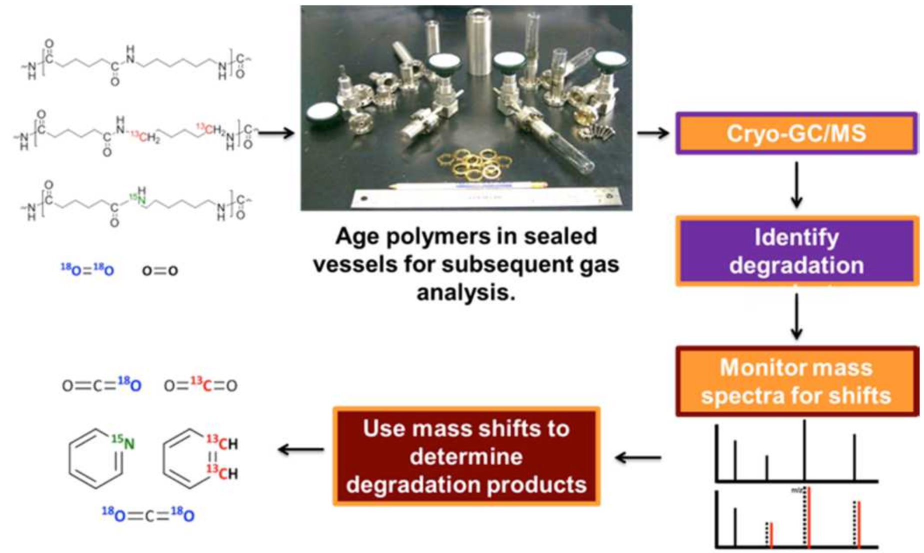
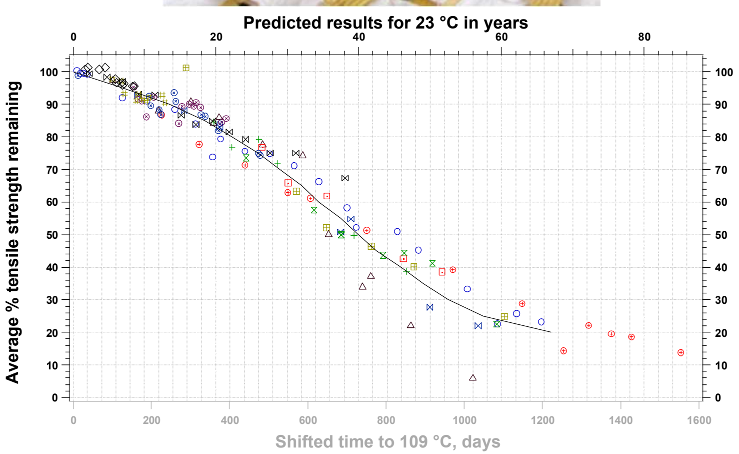
Organic Material Aging and Degradation

One primary objective of our work is to develop a fundamental understanding of the underlying degradation mechanisms that can be correlated to degradation in performance.

Bernstein, White

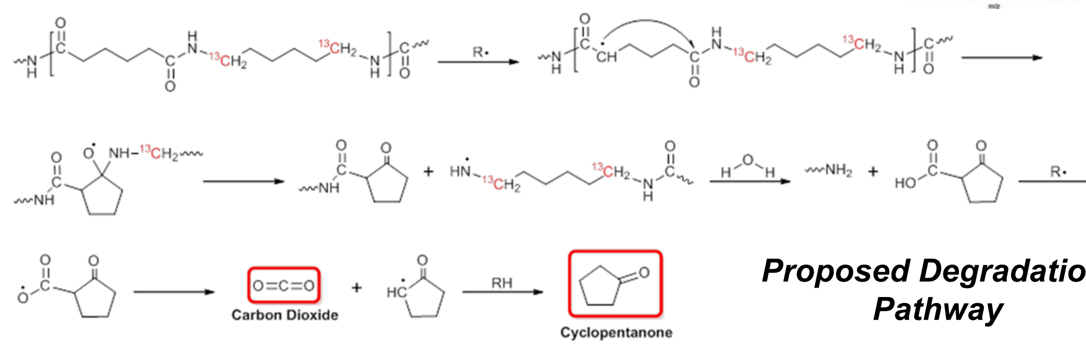
Nylon Mechanistic Studies





Lifetime Predictive Model for Nylon Strength

Bernstein R. et al. *Polym. Deg. Stab. 95, 1471-1479, 2010*



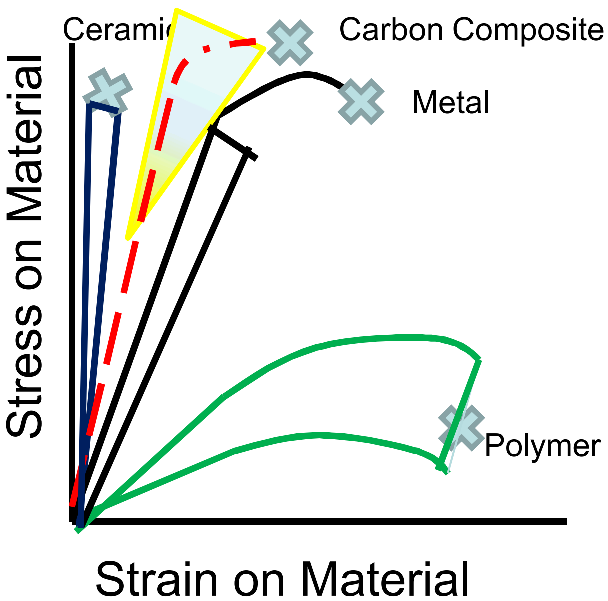
Proposed Degradation Pathway

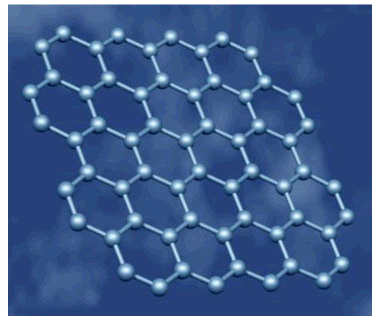
White II et al. *Poly. Deg. Stab. 97,1396-1404, 2012*
Smith et al. *J. Am. Soc. Spectr. 23, 1579-1592, 2012*

28

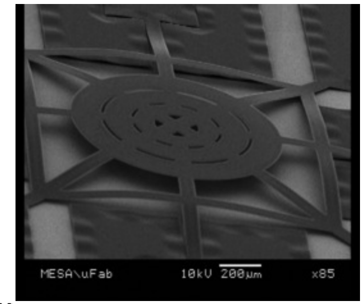
Carbon-Based Sensors

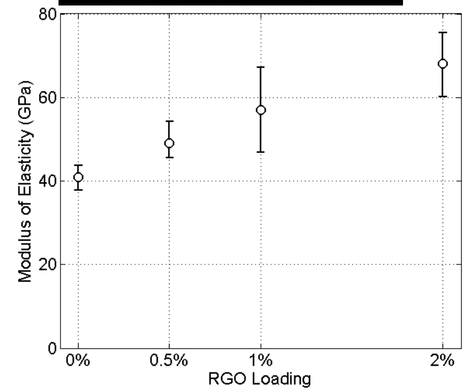
- **Pyrolytic Carbon needs stiffeners to be increase sensitivity towards an impedance based response mechanism.**





Graphene Sheet





Materials	Young's Modulus (GPa)
Pyrolzed Carbon (amorphous)	*20-40*
Graphene Sheets	*500-1000*
Single Crystal Silicon	175-195
Stainless Steel	180-225

Sensitivity

Washburn, Finnegan

2012 -X.Li – Multifunctional Graphene Woven fabrics, Nature Comm.

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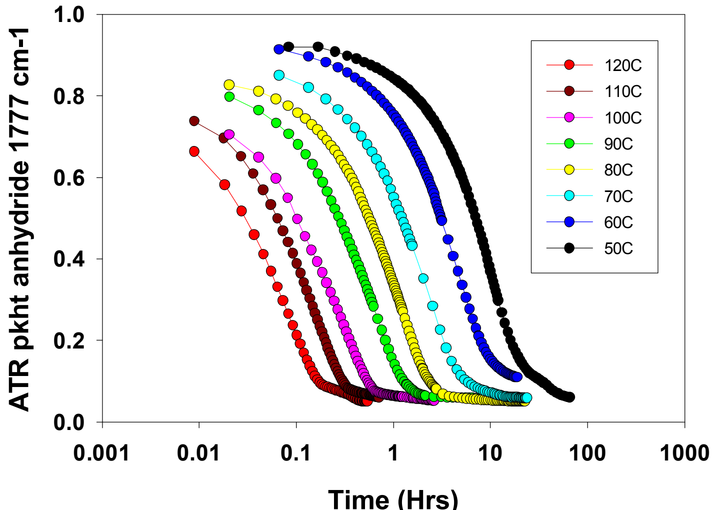
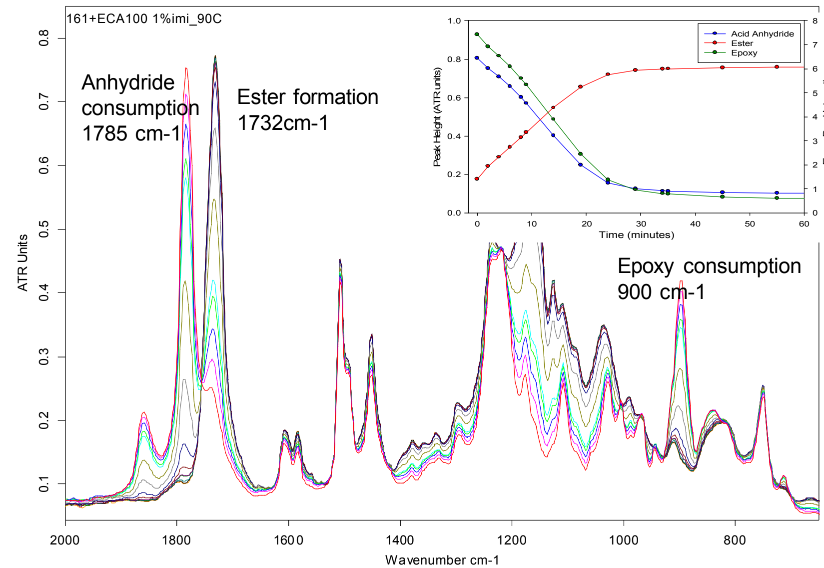
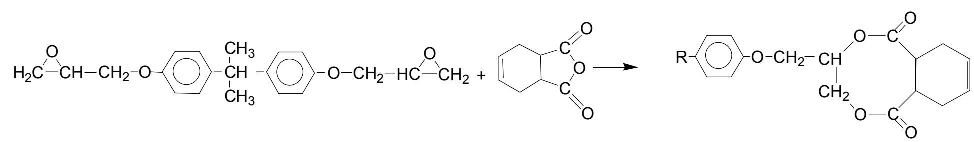
IR Spectroscopy – Thermo-set Cure Analysis

High temperature IR attachment

Cure kinetics of epoxy composite resin for energy storage applications





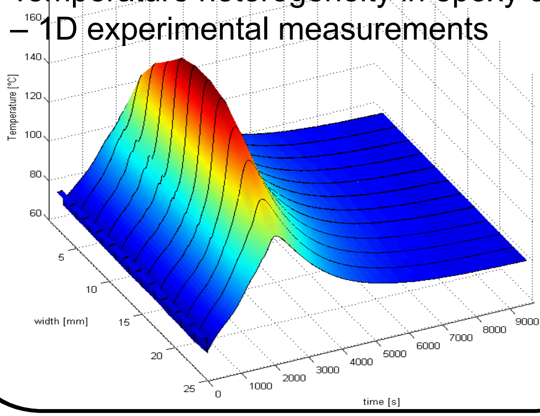


- **Characterization of polymerization and cure reactions**
- **Thermal reactivity of resin mixes**
- **Understanding catalysis**
- **Formulation development**
- **Input for kinetic cure models**

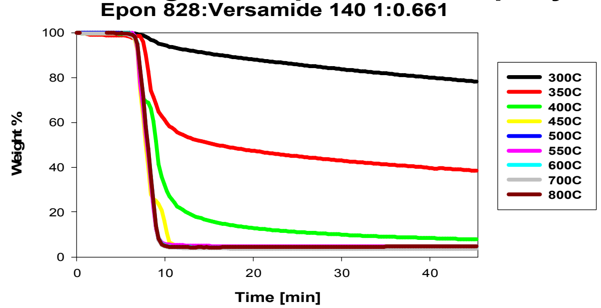
Characterization of Encapsulation Materials

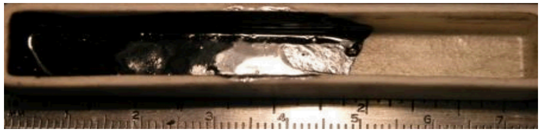
- Cure and degradation behavior
- Foam and thermoset formulations
- Composites with special needs
- High char foam materials
- Thermal performance of organics in strong link components and impact on nuclear safety

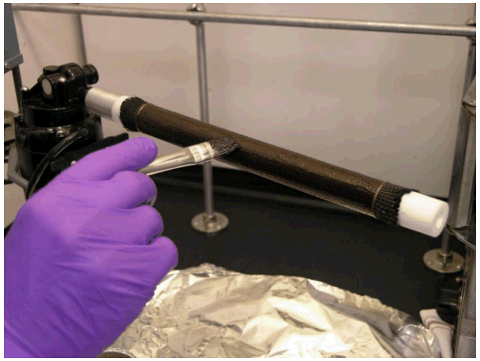
Temperature heterogeneity in epoxy cure – 1D experimental measurements



Charring/decomposition of epoxy







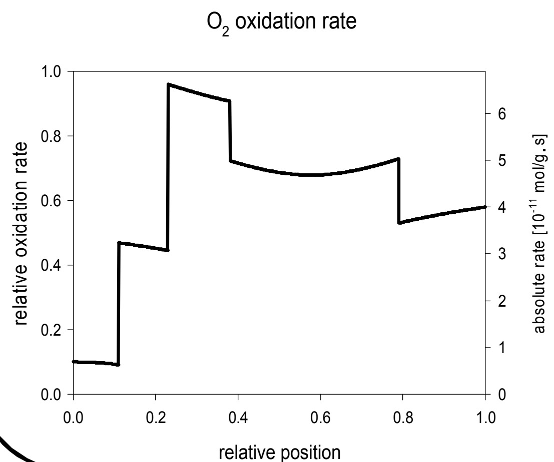
Application of 'special reactive' resin on rotating mandrel for carbon composites

Modeling of Polymer Degradation

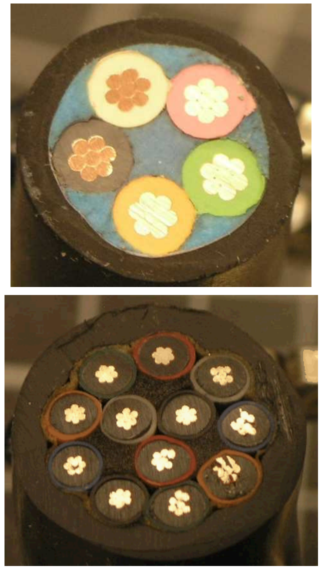
Polymer degradation is position-dependent as a function of local oxygen concentration

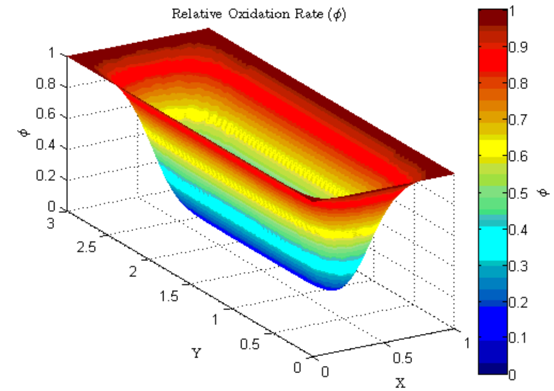
$$\frac{\partial[O_2]}{\partial t} = D\nabla^2[O_2] - \frac{k_1[O_2]}{k_2[O_2]+1}$$

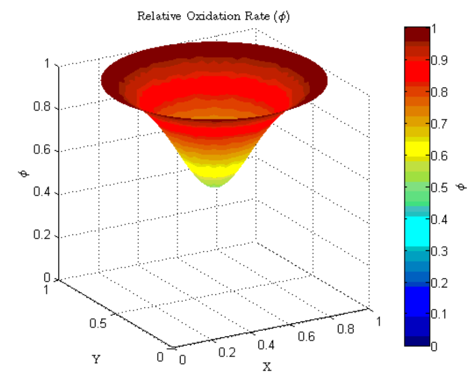
Predicted degradation rates in 5 layer elastomer composite



Complicated cable geometry







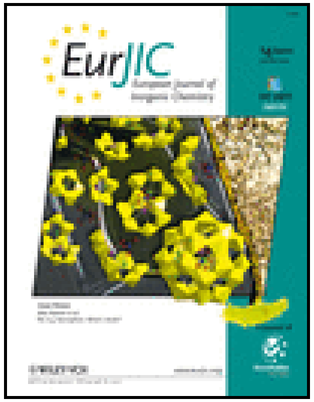
- **Polymer performance in aging nuclear power plants and for defense applications**
- **Oxidative degradation in thermal and radiation environments**
- **Characterization of DLO heterogeneity**
- **Development of modeling capabilities**
- **Measurement of oxid. rate and permeation**

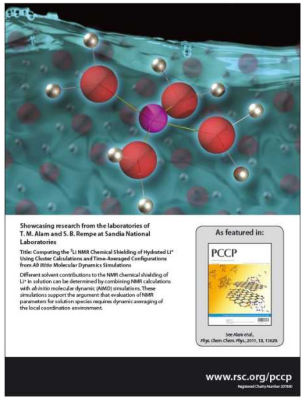
Celina

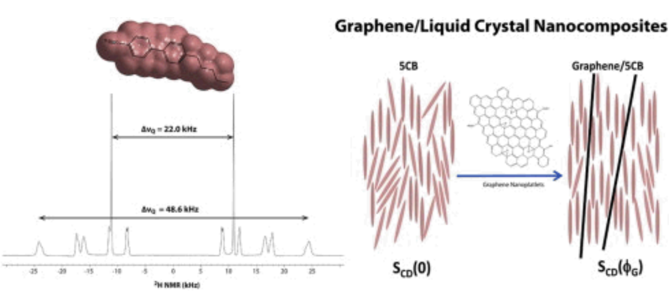
Sandia's NMR Spectroscopy Facility
Advanced Characterization Capabilities

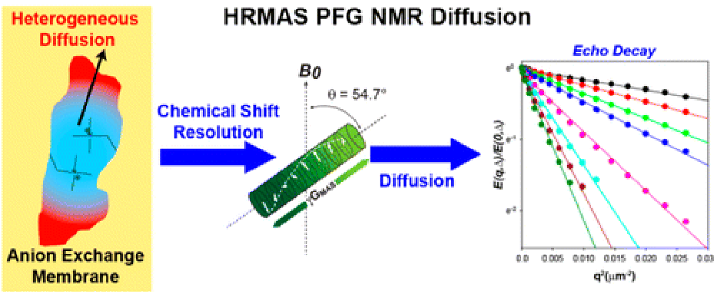
Sandia National Laboratories

- Maintain both high resolution solution and solid state capabilities for the characterization of chemical structure, reaction kinetics, morphology and dynamic properties
- Continue to develop and implement new and novel multi-dimensional and multi-frequency NMR capabilities
- Maintain an active research component linking computational simulations and NMR experimental results
- Recently developed combined high resolution magic angle spinning (HRMAS) NMR and pulse field gradient (PFG) NMR diffusion experiments for measuring transport of liquids and solvents in heterogeneous materials. Examples include water/methanol transport in polymer fuel cell membranes, water diffusion in thermo-responsive polymer gels and electrolyte transport in nano-porous carbons.







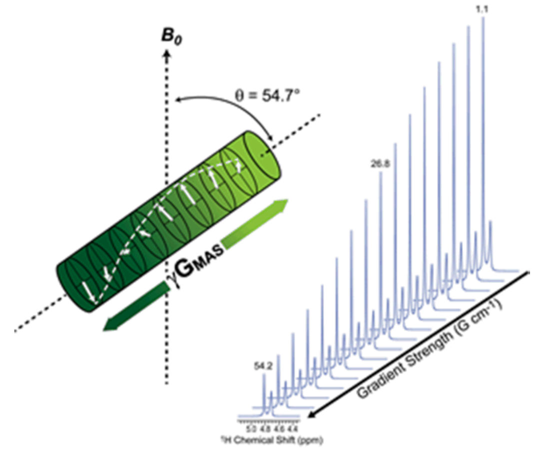


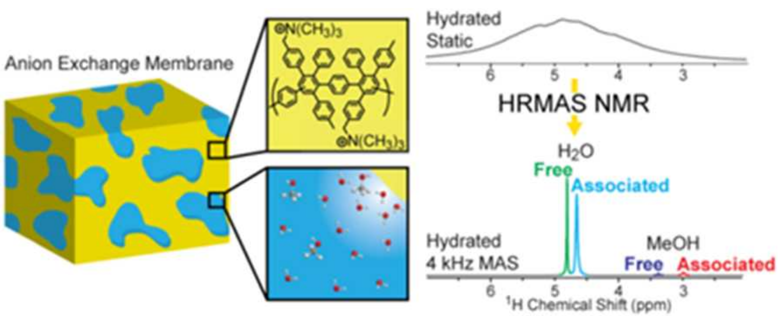
(see: http://www.sandia.gov/nmr_lab)

Diffusion Measurement Capabilities at Sandia's NMR Spectroscopy Facility

http://www.sandia.gov/nmr_lab

- Sandia has static pulsed field gradient (PFG) NMR capabilities for measuring diffusion of different chemical species in complex mixtures within materials including:
  - Polymers, composites and nanoporous carbons
  - Ceramics, Ionic liquids
- Water cooled high gradient strength (1250 G/cm) and 2500 G/cm (Summer 2015) for diffusion rates between 10^{-9} and 10^{-14} m^2/s.
- Multi-nuclear PFG NMR diffusion experiments
  - ^{1}H, ^{13}C, ^{31}P
  - ^{7}Li, ^{23}Na, ^{19}F (Expanded, Summer 2105).
- Recently developed combined high resolution magic angle spinning (HRMAS) NMR and pulse field gradient (PFG) NMR diffusion experiments for measuring transport of liquids and solvents in heterogeneous materials. The MAS allows increased resolution of different solvent environments.





http://www.intechopen.com/books/advanced-aspects-of-spectroscopy/hr-mas-nmr-spectroscopy-in-material-science

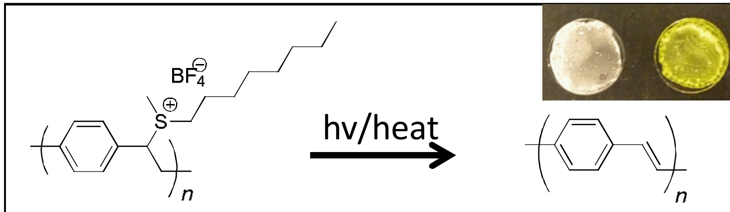
Switchable Anti-biofouling Polymer Coatings

Michele L. Denton, Shane J. Stafslien, Shawn M. Dirk

Non-toxic anti-fouling and fouling release marine coatings are a billion dollar market and serve to increase the efficiency of marine energy-harvesting technologies and sea faring vessels.

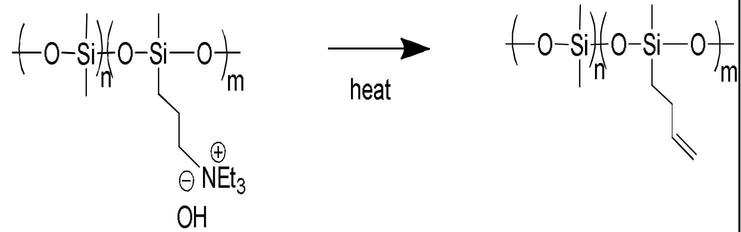
Our goal is to produce a non-toxic coating that is anti-fouling and can be “switched” to fouling release. Such a coating would be effective to address both anti-fouling and fouling adhesion issues.

Our laboratory has produced three such coatings. These coatings have performed well during initial fouling tests and two coatings are currently undergoing open water testing at Pacific Northwest National Labs.

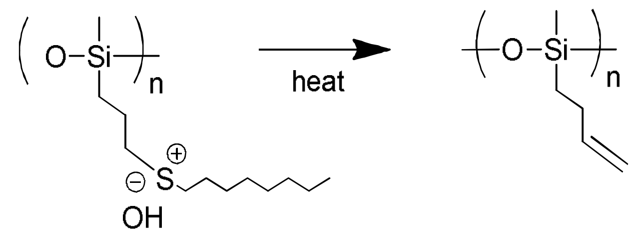


5 1

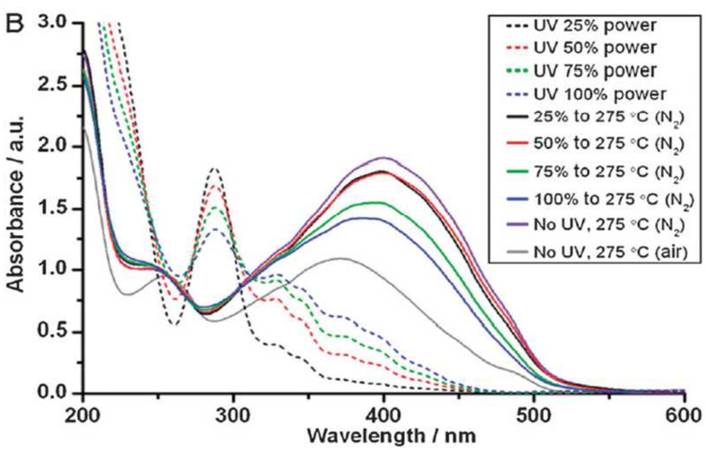
Sulfonium Polyphenylene Vinylene (PPV) Polymer



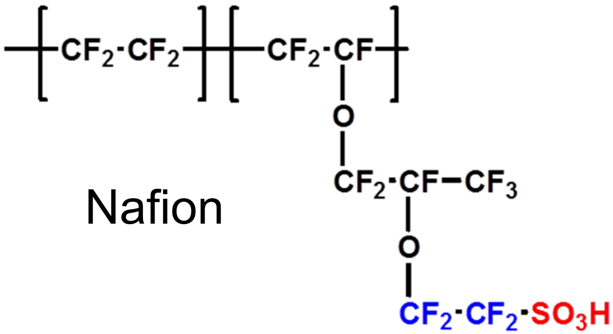
Ammonium Silane Polymer and Copolymer



Sulfonium Silane Polymer



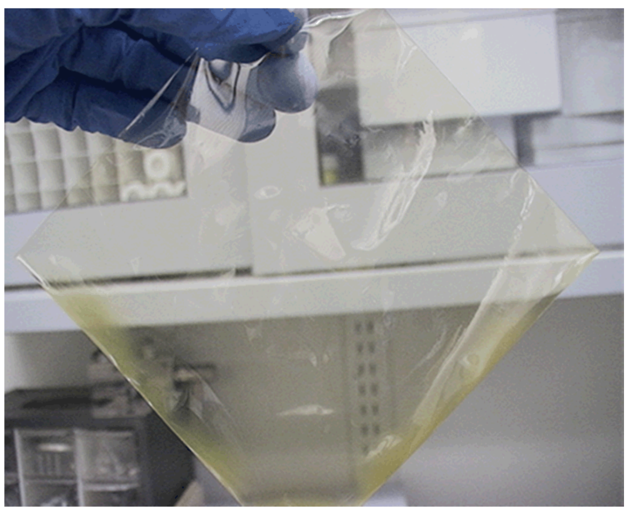
Electrochemical Membranes for Alternative Energy

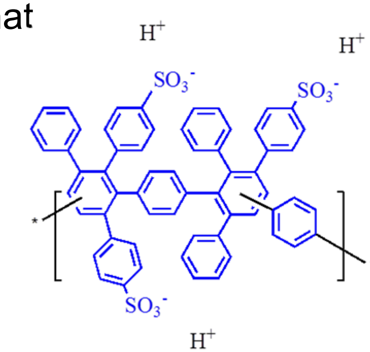


Nafion

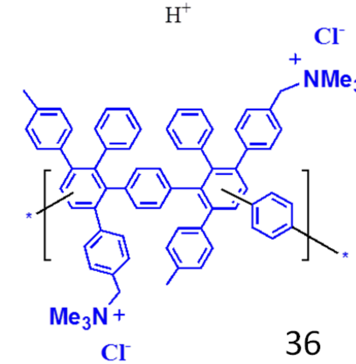
Dupont's Nafion is currently the state of the art for developing electrochemical systems (flow batteries, fuel cells, and water electrolysis) since it provides good performance and durability. However, the high cost ($\$400/m^2$) of this material is pushing development for less expensive alternatives.

Sandia has developed and patented a series of drop and drag replacement membrane that are cheaper to manufacture, while offering the same or better performance to Nafion.





- The materials are poly(phenylene)s, chemically and thermally stable
- Flexible synthesis allows for both acid or base functionalization depending on application use

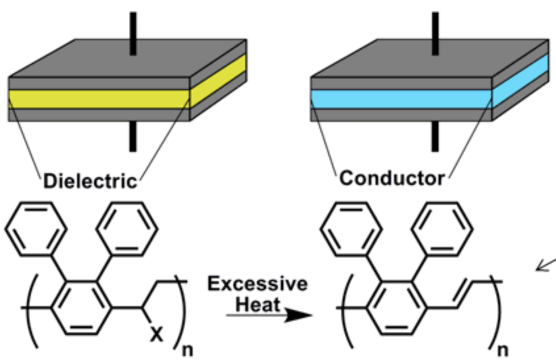


 poly(phenylene) film

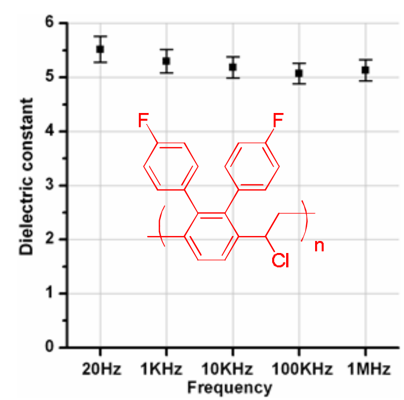
Fujimoto

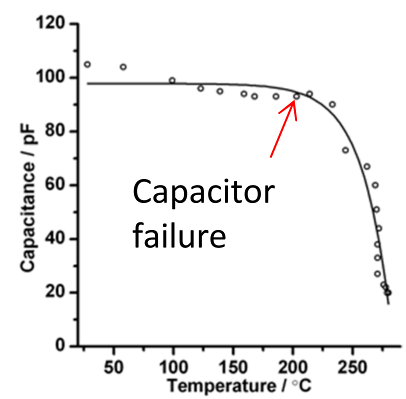
Switchable Polymer Dielectrics

- Switchable dielectric materials
  - Conjugated polymer precursors can be used as high energy density dielectrics
  - Upon heating to predetermined controlled temperature the dielectric *irreversibly switches* to a conjugated semi-conducting polymer bleed resistor
  - Increased dielectric constant relative to Mylar while maintaining similar breakdown strength leads to a calculated a higher energy density of 1.29 J/cm^3 for the PPV precursor dielectric relative to Mylar based capacitors (0.35 J/cm^3).



Conducting polymer acts as a controlled bleed resistor

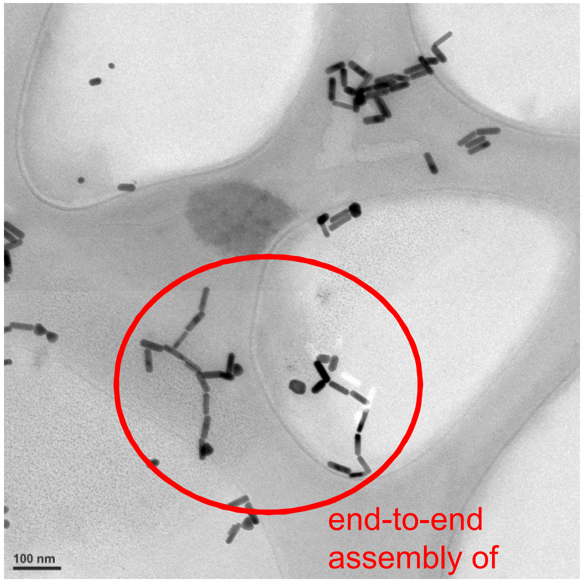


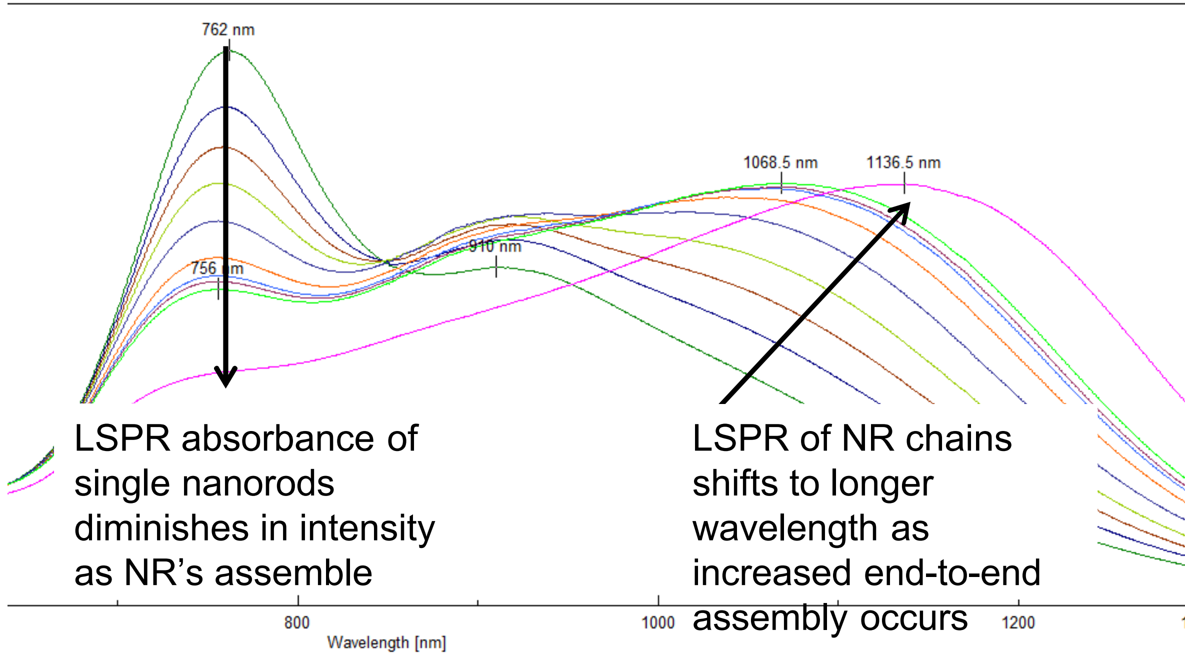


Dirk, Johnson

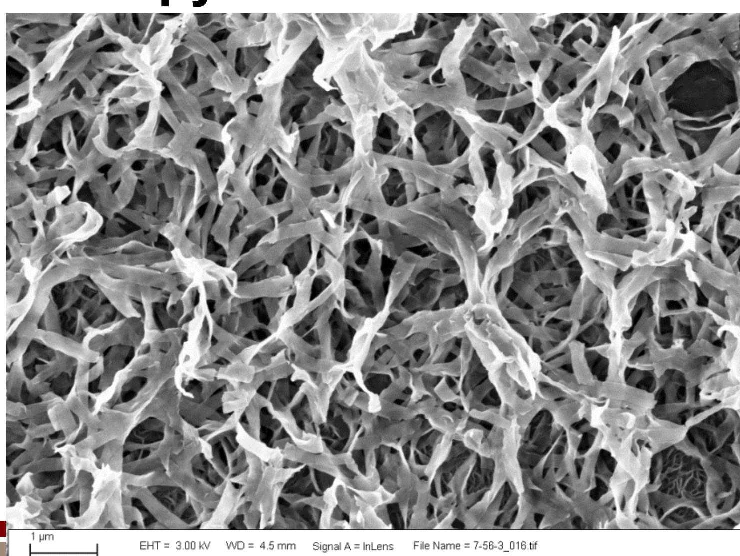
Understanding and Controlling Supramolecular Assembly

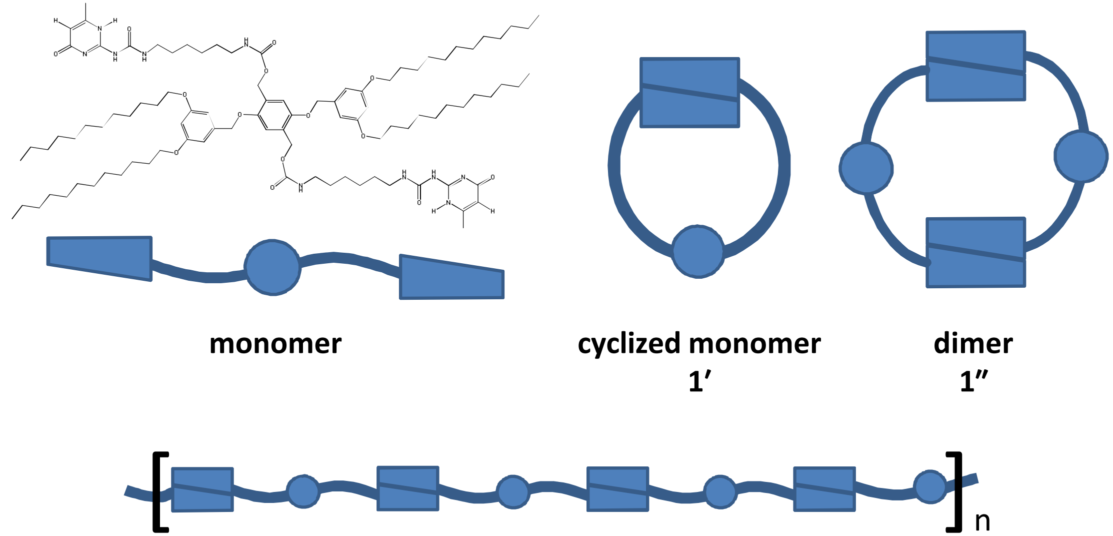
Gold Nanorods





Ureidopyrimidinones

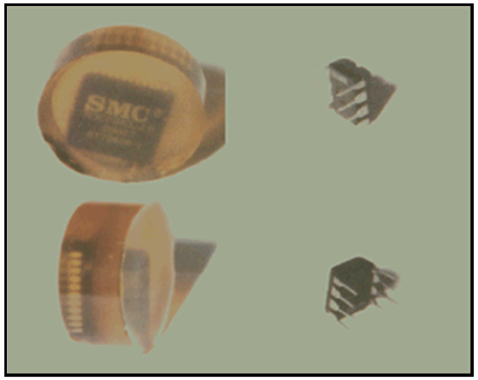




polymer

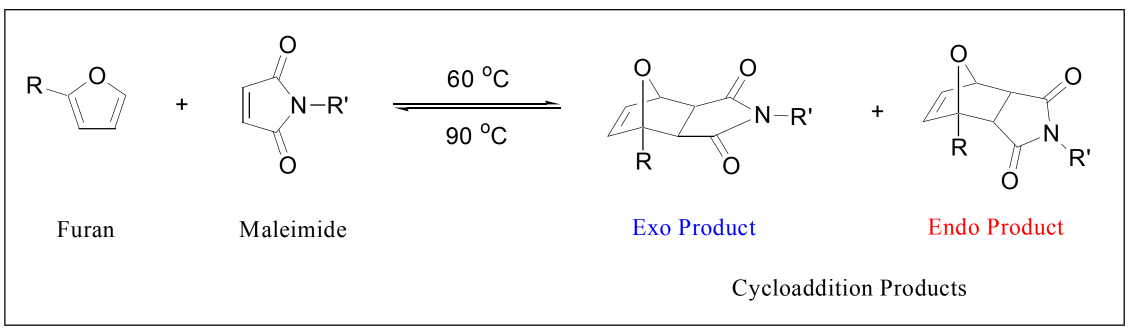
Sandia History of Thermally Degradable Materials

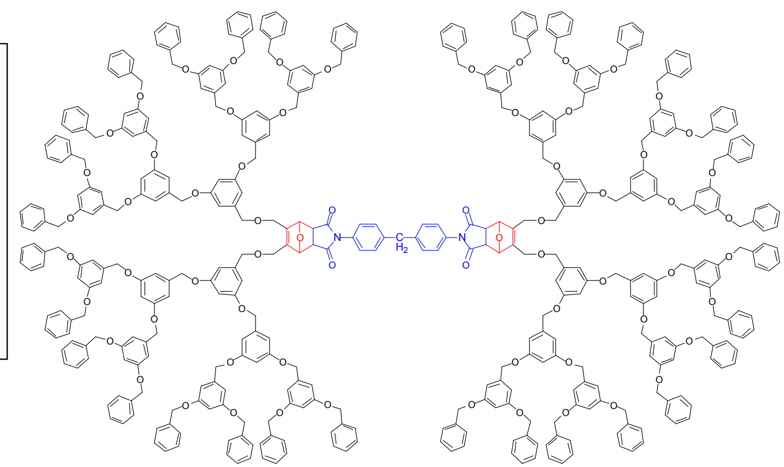
Removable Solid Encapsulants



Removable Adhesives

Cleavable Surfactants





Thermally Reversible Dendrimers

McElhanon, J.R; Wheeler, D.R. *Org. Lett.* **2001**, *3*, 2681-2683.
Aubert, J.H. *J. Adhes.* **2003**, *79*, 609-616.
McElhanon, J.R. et. al. *Langmuir* **2005**, *21*, 3259-3266.
Szalai, M.L; McGrath, D.V.; Wheeler, D.R.; Zifer, T.; McElhanon, J.R. *Macromolecules* **2007**, *40*, 818-823.
Small, J.H.; Loy, D.A.; Wheeler, D.R.; Russick, E.M; McElhanon, J.R.; Sanders, R.S. U.S. Patent 6271335 B1, 2001, 8 pp.
McElhanon, J.R. et. al. U.S. Patent 7022861 B1, 2006, 19 pp.
Aubert, J.H. US Patent 4116272 A1, 2003, 10 pp.

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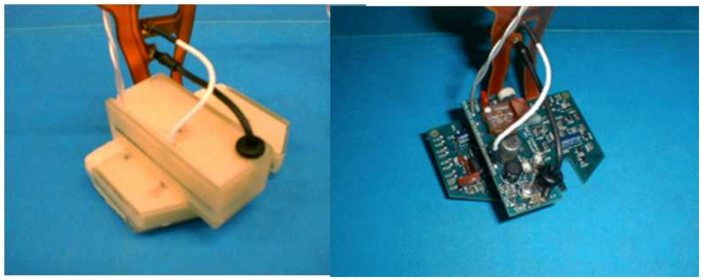
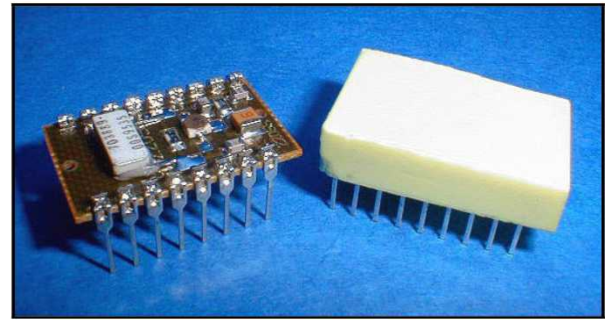
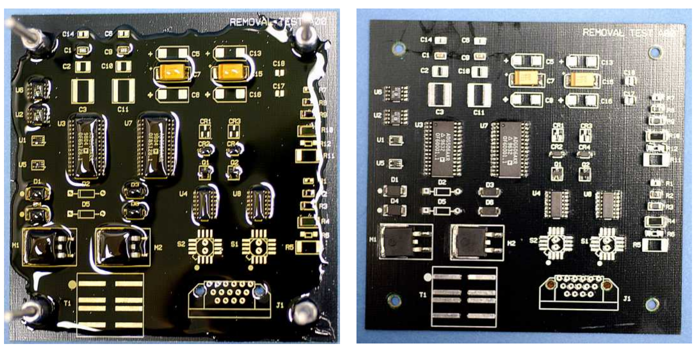
Thermally Removable Encapsulants



Removable Epoxy Foam (REF) 308 and 320



Removable Syntactic Foam (RSF)



Removable Conformal Coating (RCC)

Wheeler, Loy, McElhanon, Aubert, Russick, Sawyer, Celina, lots of others

McElhanon, J.R.; Russick, E.M.; Wheeler, D.R. Loy, D.A.; Aubert, J.H. *J. Appl. Polym. Sci. Chem. Soc.* **2002**, *85*, 1496-1502.
Loy, D.A.; Wheeler, D.R.; Russick, E.M; McElhanon, J.R.; Sanders, R.S. U.S. Patent 6337384 B1, 2002, 7 pp.
Loy, D. A.; Wheeler, D.R.; McElhanon, J.R.; Durbin-Voss, M.L. U.S. 6403753 B1 2002, 13 pp.

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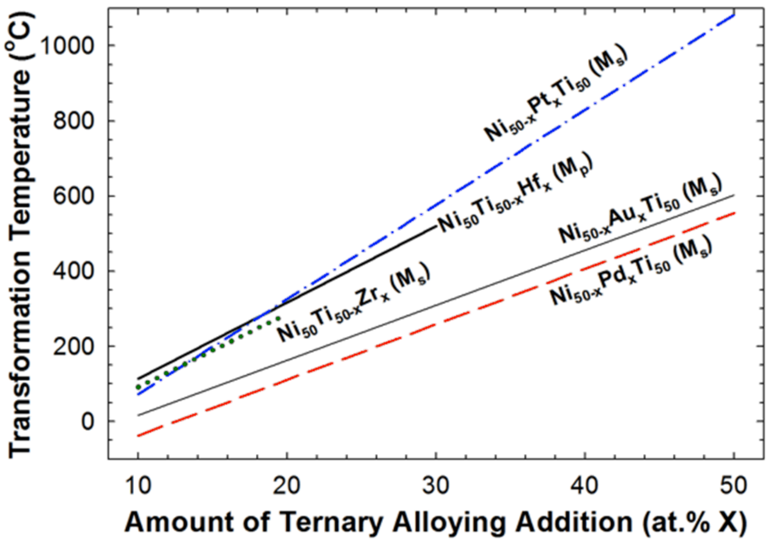
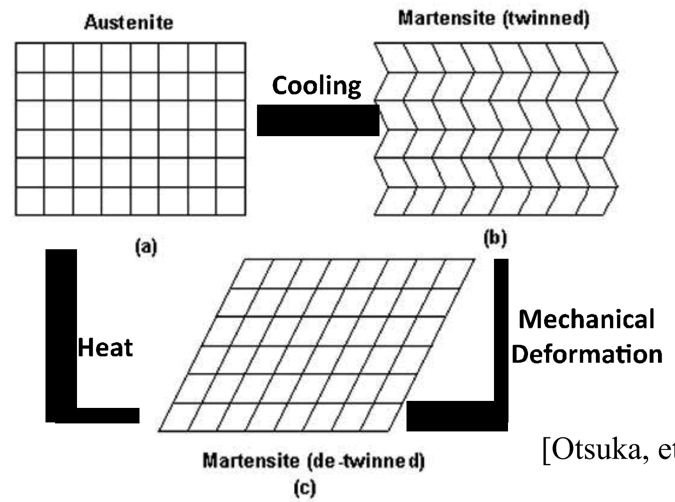
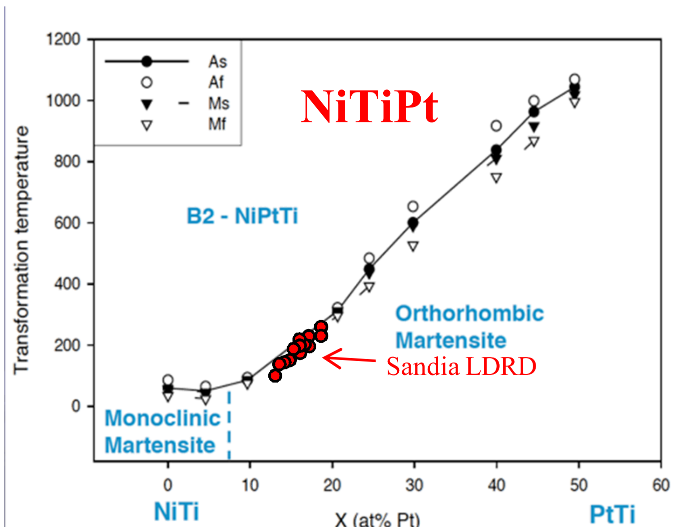
High Temperature Shape Memory Alloys

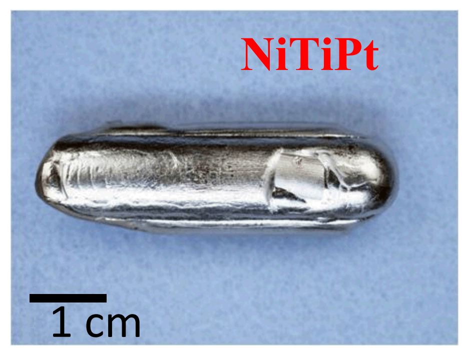


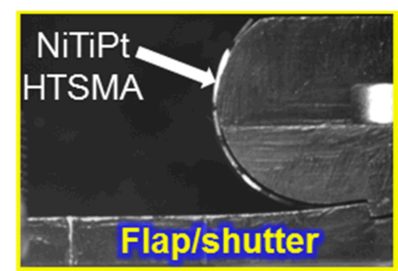
THE SHAPE MEMORY EFFECT (SME)



[Otsuka, et al.]







41 Susan, Buchheit, Debassige, Massad, Reece, Bradley, McElhanon

Questions?

We have a diverse set of capabilities

- **Materials Engineering Support**
  - Problem solving, program support (LEPs, ALTs, WFO)
  - Application of existing expertise (SFIs, production support)
  - Point solutions
- **Materials & Process Advanced Development**
  - Advanced & exploratory materials & process development
  - Production process development & tech transfer
  - Understanding the margins
- **Fundamental Materials & Process Science**
  - Develop/integrate theoretical insights, computational simulation tools, and experiments to provide foundational, predictive understanding (BES, LDRD)
  - Develop innovative new materials and process technologies