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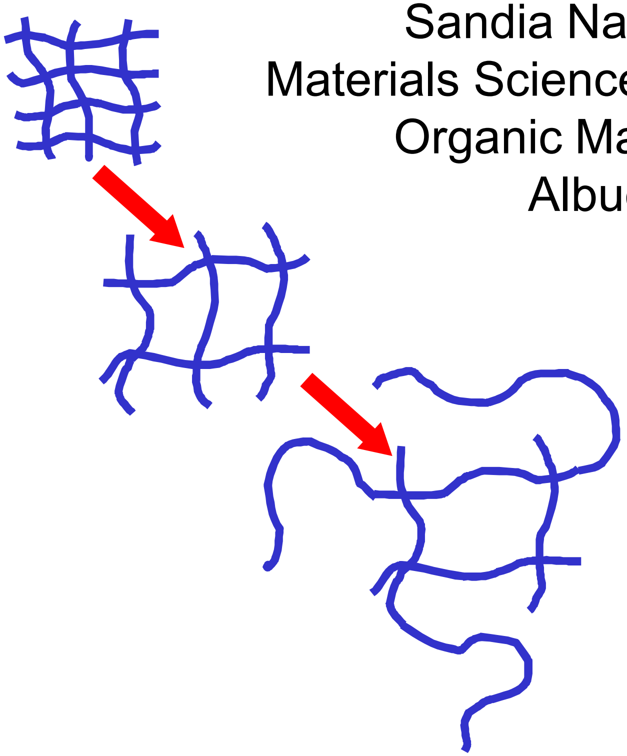
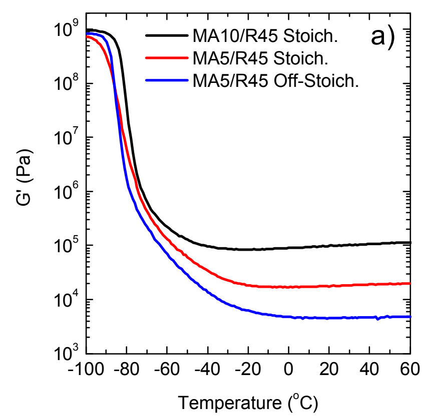
Materials Science at Sandia National Laboratories: Fundamental Understanding to Application

Joseph L. Lenhart
Sandia National Laboratories
Materials Science and Engineering Center
Organic Materials Department
Albuquerque, NM

Major strength is movement from fundamental science to practical implementation of materials technology in broad based applications.

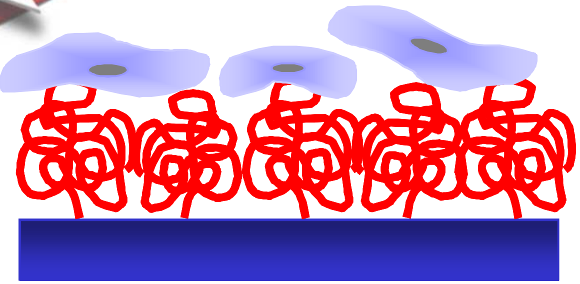


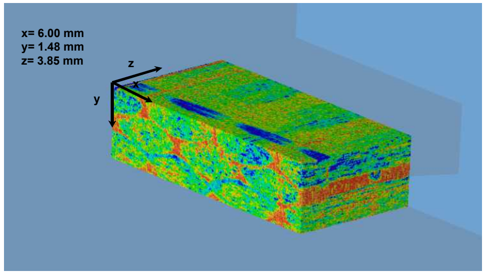


This work was performed at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Safety Administration under contract DE-AC04-94AL85000.

Joseph L. Lenhart; jllenha@sandia.gov; 505-284-9209

My Research Background (Pre Sandia)



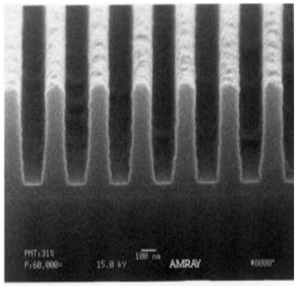


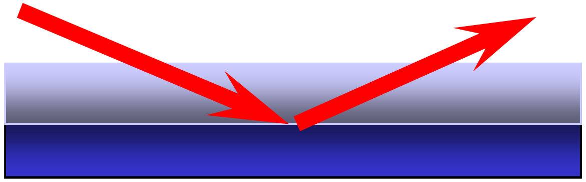
BS Chemical Engineering (University of Maryland)

- Bio-polymer chitosan
- Processing development
- Enzymatic reaction / chitosan absorption for water purification

PhD Chemical Engineering (Johns Hopkins University)

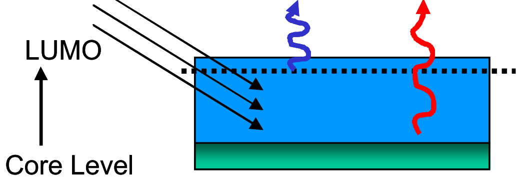
- Polymer composites
- Fluorescently labeled coupling agent
- Epoxy / silane / glass interface
- Fiber optic sensor





Neutron and X-ray reflectivity

- Thermal properties of ultrathin crosslinked polymer films

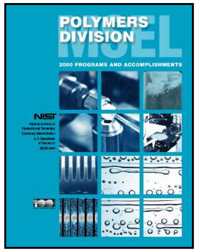


Interfacial phenomena in photolithography

- Led CRADA with Brewer Science
- Part of NIST / IBM team
- Resist-air interface
- Resist-BARC interface
- BARC thin film and surface characterization

Synchrotron Interfacial Science

- Polymer surfaces
- Interfacial chemistry of lithographic materials



National Research Council Postdoctoral Appointee in Polymers Division at the National Institute of Standards and Technology

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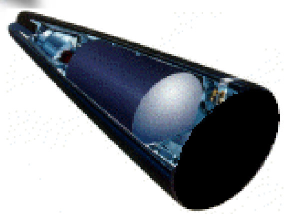
Sandia National Laboratories

Sandia Mission Areas



Nuclear Weapons Complex

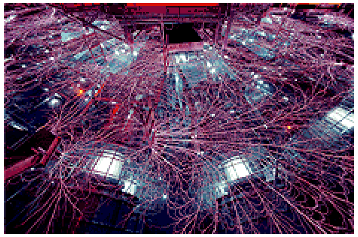
- Los Alamos
- Lawrence Livermore
- Sandia (NM, CA)
- Pantex Plant
- Kansas City Plant
- Oak Ridge Y-12
- Savanna River Site

1) Nuclear Weapons

- Weapons surveillance
- New technology
- Maintain safe, secure, reliable stockpile
- Update weapons

2) Non-proliferation

- Treaty verification
- WMD detection capability
- Physical security
- Nuclear materials management



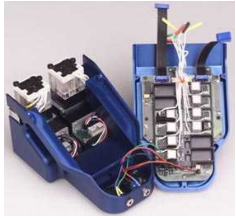
Science, Technology, Engineering

- Physical, chemical, nano-science (CINT)
- Materials science
- Science in extreme environments (radiation, voltage)

National Security Laboratory

Defense Systems and Assessment

- Science and technology development
- Missile defense
- System level simulation / computation
- Robotics
- C3ISR (Command, Control, Communication, Intelligence, Surveillance, Reconnaissance)



Homeland Security and Defense

- External partnerships
- Technology development ie. detection, first responders, clean-up
- Manufacturability and commercialization

Energy and Infrastructure Assurance

- Renewable energy
- Safe, secure, reliable infrastructure
- Safe, secure, sustainable water supply

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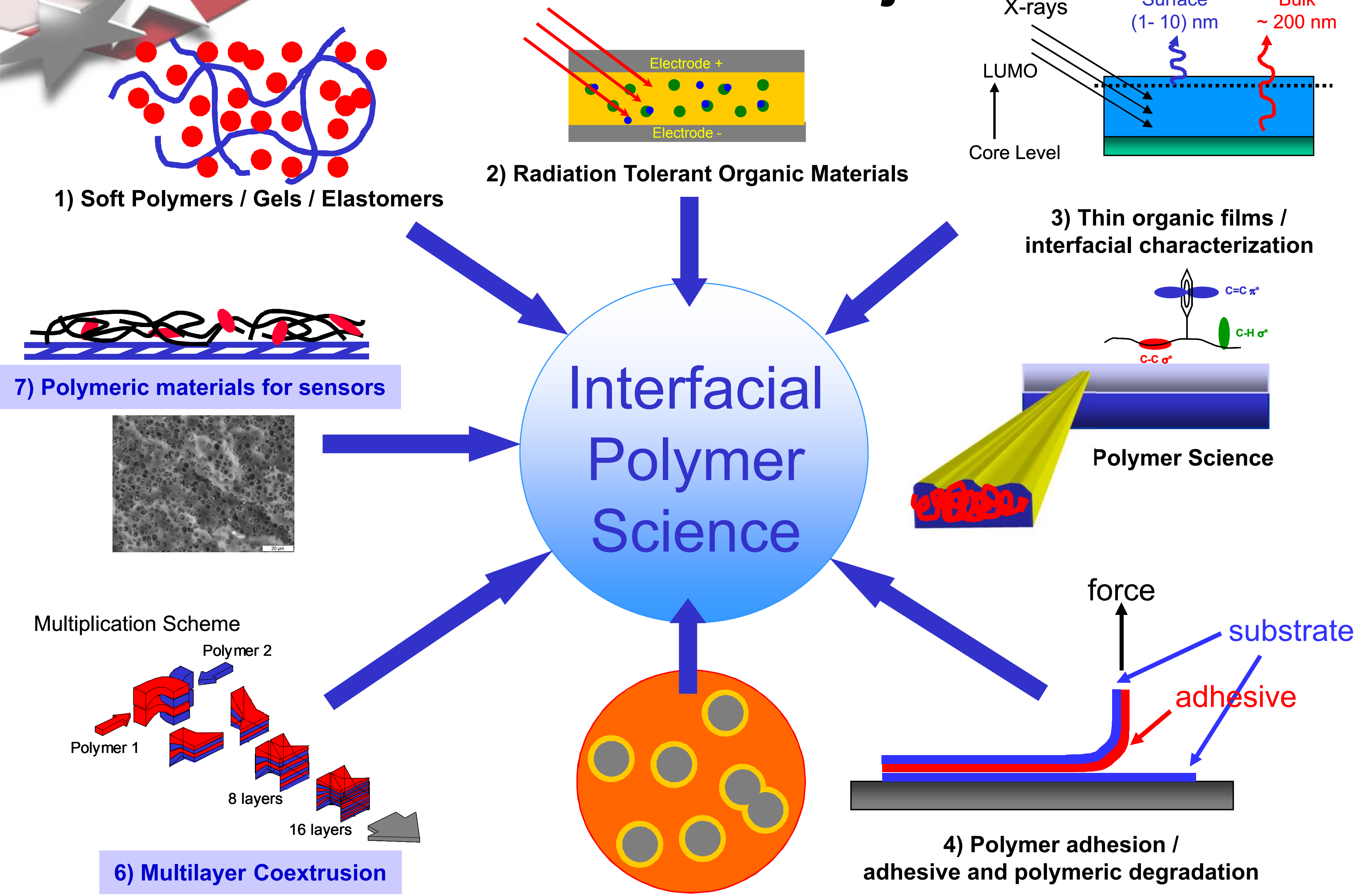
Current Sandia Projects



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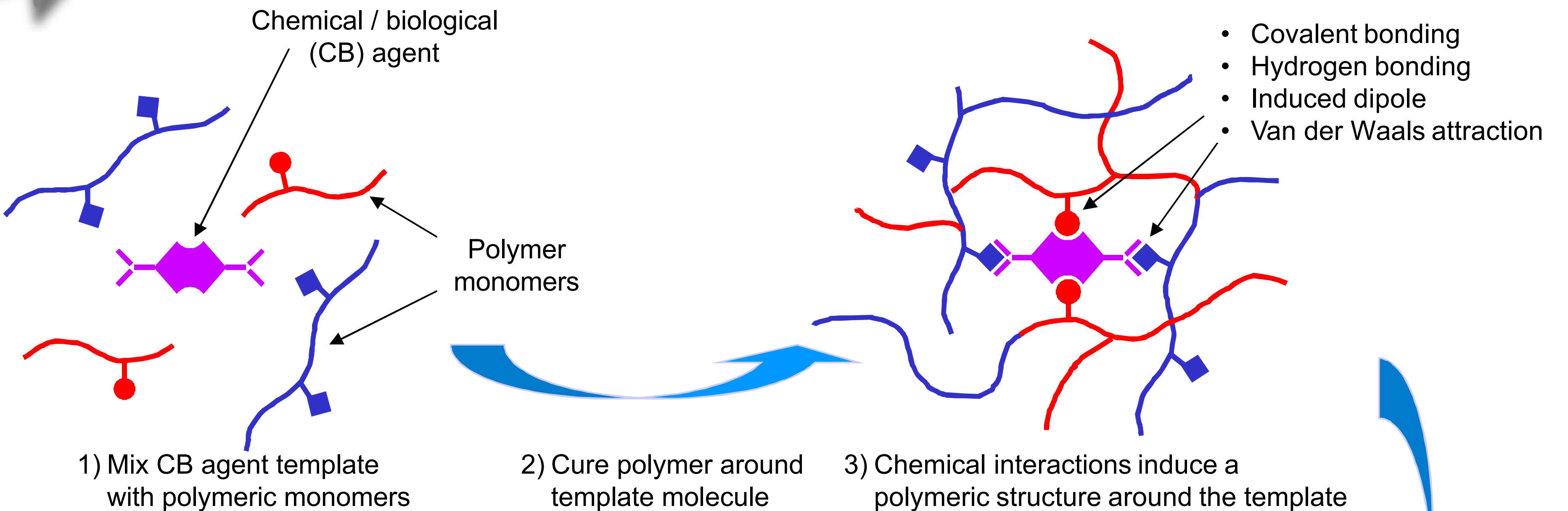
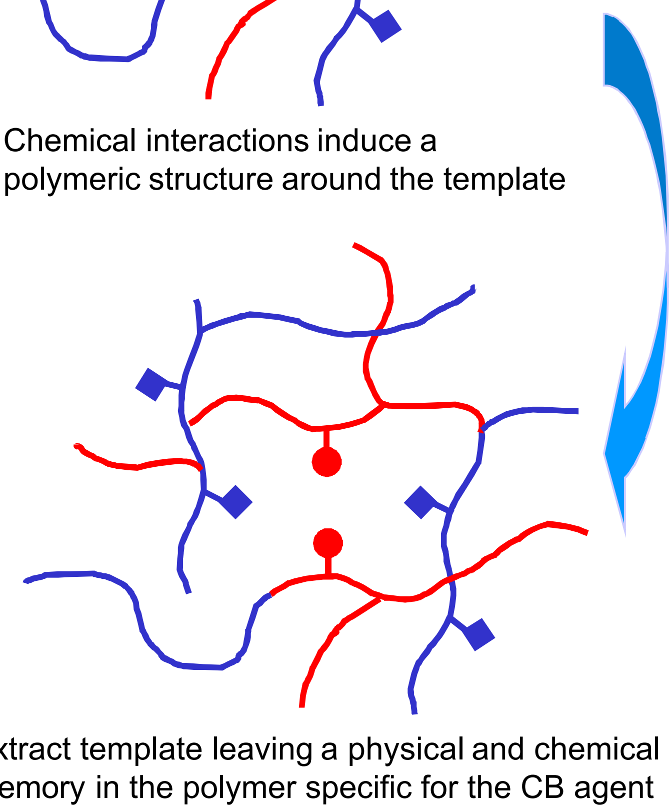
Nano-materials for Chemical and Biological Detection: Molecular Templating





Development of Molecularly Templated Polymers

1. Develop fundamental understanding of imprinting process
2. Identify polymeric factors that influence selectivity and response
    - Functional group density
    - Chain stiffness
    - Cross-link density
    - Thickness / porosity
3. Implement MIP on model templates
4. Demonstrate selectivity in complex chemical environments
5. Develop a library of MIP polymers for classes of CB agents

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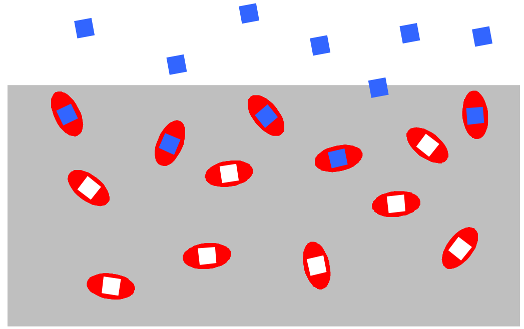
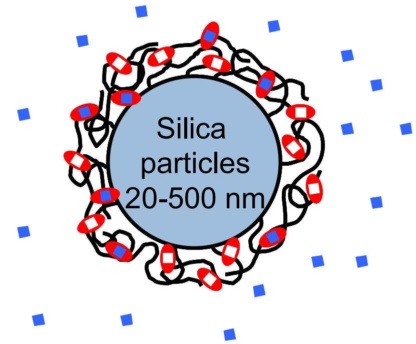
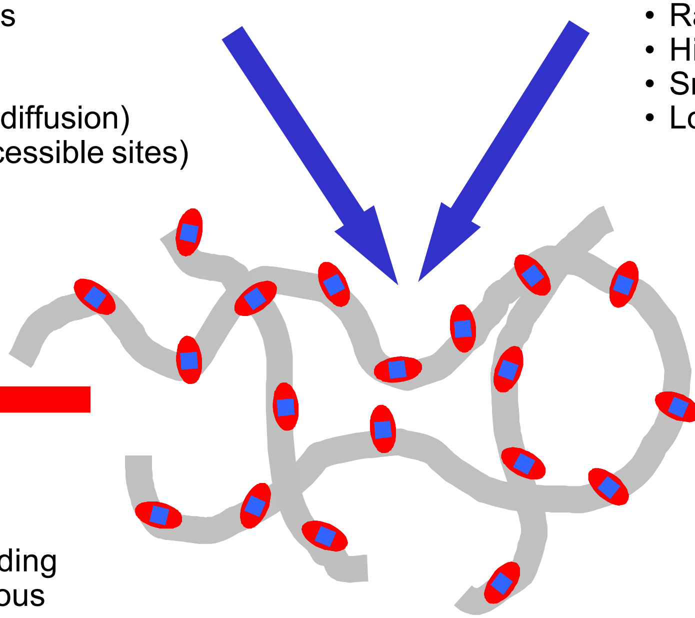
Nano-porosity Polymeric Materials: Scaffolds for High Chemical Adsorption

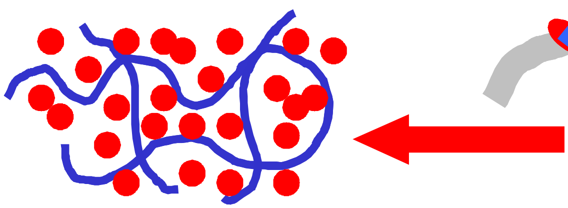


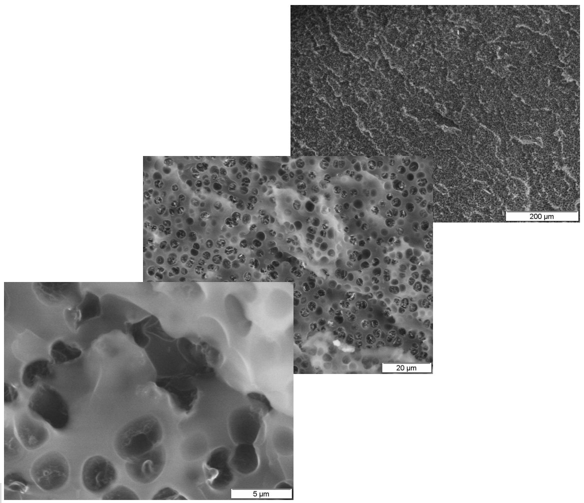


Bulk Sensing Layers
- High number of receptor sites
- High signal
- Buried receptor sites
- Slow sensor response time (diffusion)
- Poor sensor efficiency (inaccessible sites)

Thin Sensing Layers
- Rapid sensor response time
- High sensor efficiency (sites accessible)
- Small number of receptor sites
- Low signal







Solvent Swelling
- Cure polymer with high solvent loading
- Remove solvent leaving highly porous micro-structure
- Micro-structure controlled by
    - polymer-solvent interactions
    - solvent loading

High Porosity Polymeric Scaffolds
- Rapid sensor response time
- High sensor efficiency (sites accessible)
- High number of receptor sites
- High signal

Sandia National Laboratories

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Nano-Composite Targeted Applications

1. Radiation Shielding (X-rays, Gamma Rays, Electrons, Protons)
2. Electrical Conductivity (3-D Packaging of integrated Circuitry, EMI / RFI Shielding, Energy Storage Devices)
3. Thermal Conductivity (Thermal Management in extreme heat environments, Packaging of increasingly dense and powerful integrated circuitry)
4. Micro-nano devices / Flexible Electronics / 3-D Printing and Processing

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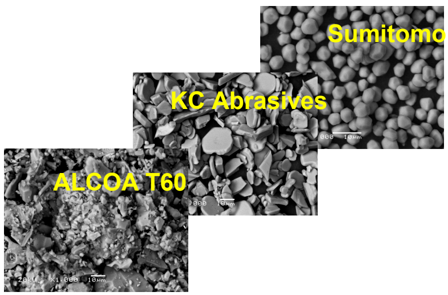
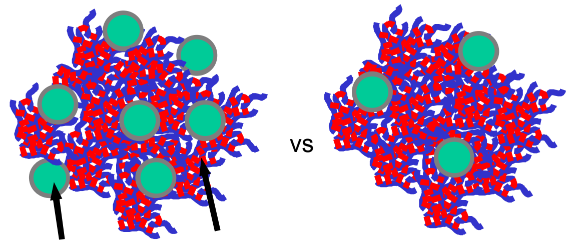
Extensive History with Composites

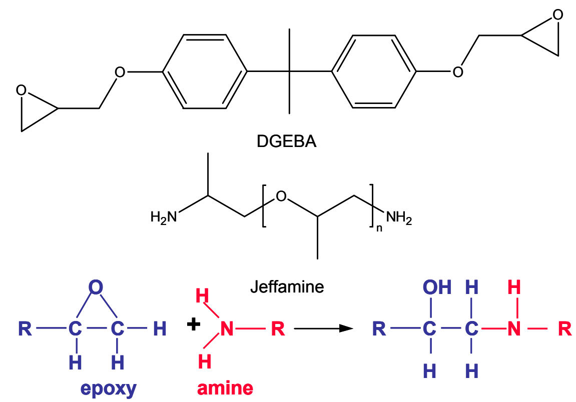
Critical Variables?



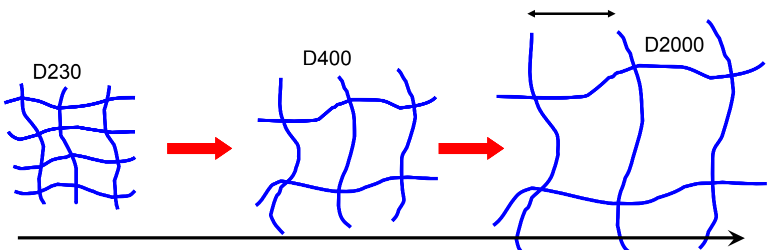
1) Particle shape, size, and size distribution



2) Filler loading

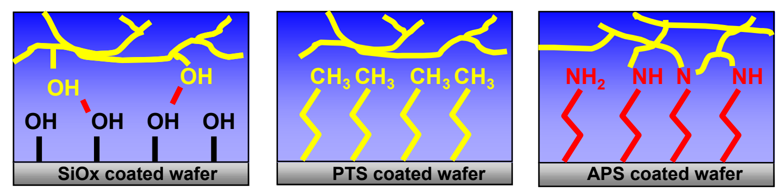


3) Resin chemistry and stoichiometry



Tg decreases, rubbery modulus decreases, CTE increases, diffusion constants increase, energy dissipation increases

4) Polymer crosslink density



5) Filler surface chemistry

How do these variables impact:

- Cured properties
- Processability
- How sensitive are these to subtle changes

Implications for device performance

Joseph L. Lenhart; jllenha@sandia.gov; 505-284-9209

Coatings / Underfills for Radiation Shielding, Thermal Management, Electrical Conductivity

Issue

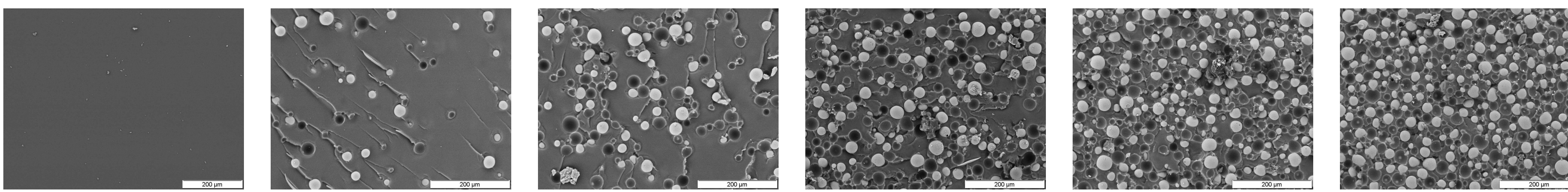
- Drive to reduce mass
- Need for devices to function in various extreme environments

Objective

- Localize material in desired area for maximum benefit
- Disperse high Z, metallic, conductive fillers in polymeric matrix

Advantages

- Reduced mass / volume
- Localized or global benefits
- Simple and flexible processing for wide range of applications
- Complex geometries



0 % 10 % 20 % 30 % 40 % 50 %

Electron Shielding

X-ray, Gamma, Proton Shielding

Performance in a variety of extreme radiation, electrical, thermal environments

EMI Shielding / Electrical and Thermal Conductivity

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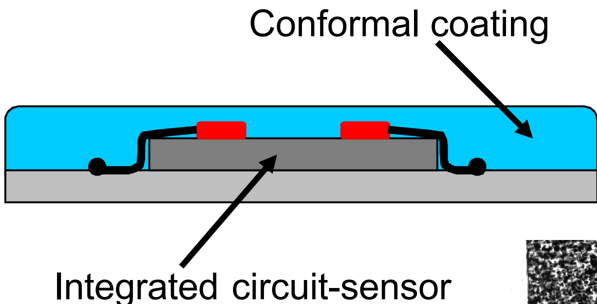
Application Example: Conformal coatings for localized "spot" shielding

Uses for Polymer Composites:
- *Structural composites for global shielding*
- *Conformal coatings for "spot" shielding*



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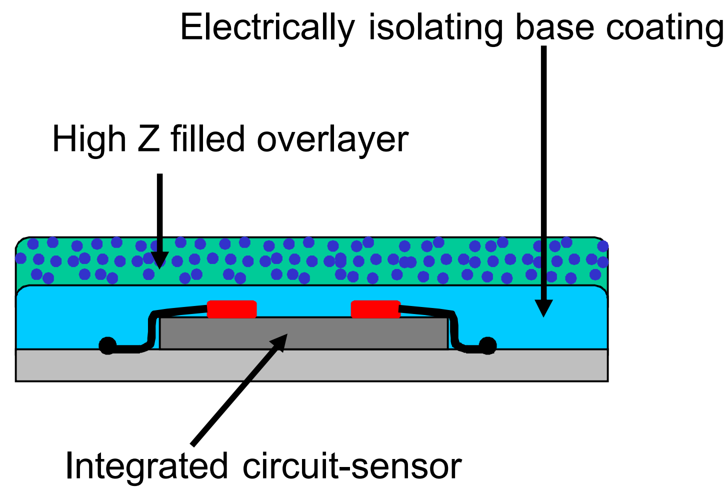

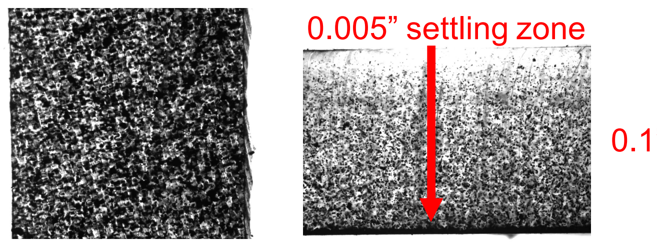

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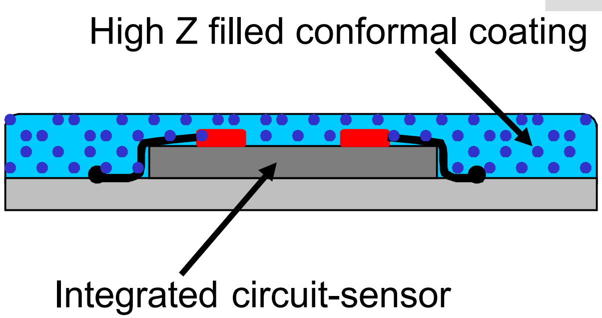


Issues for Spot Shielding
- Settling
- Transparency / Agglomeration

Advantages
- Simple implementation
- Less concerns with particle distribution and layer conductivity

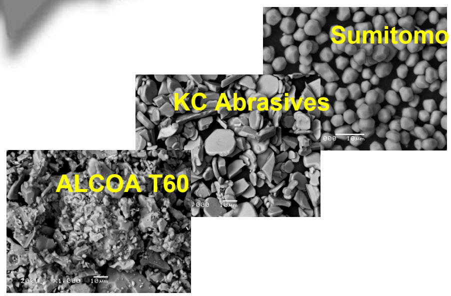
Challenges
- Additional processing step
- Overlayer-base coat compatibility

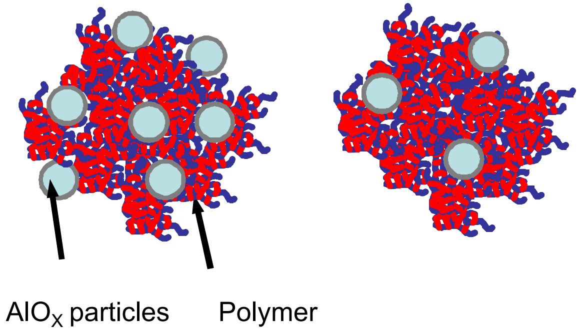
Advantages
- Single step processing
- Integrate with current conformal coatings

Challenges
- Particulate settling
- Conductivity in conformal coating

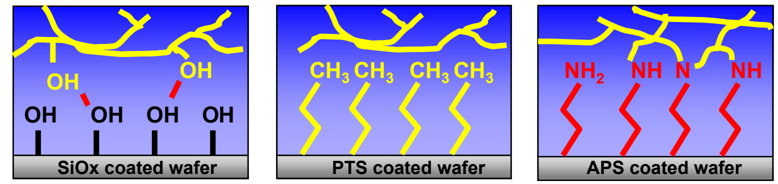
Joseph L. Lenhart; jllenha@sandia.gov; 505-284-9209

Approach: Nano-particulates at High Loadings?





Particulate dispersion and resin processability / viscosity control are key challenges

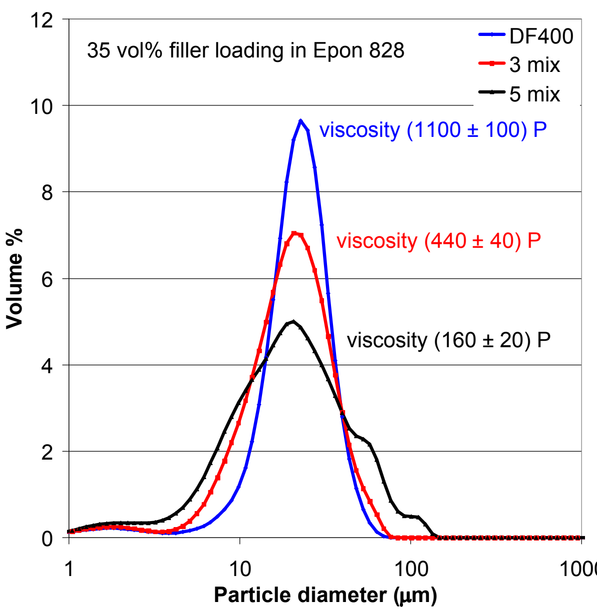


1) Broad particle size distribution to improve packing

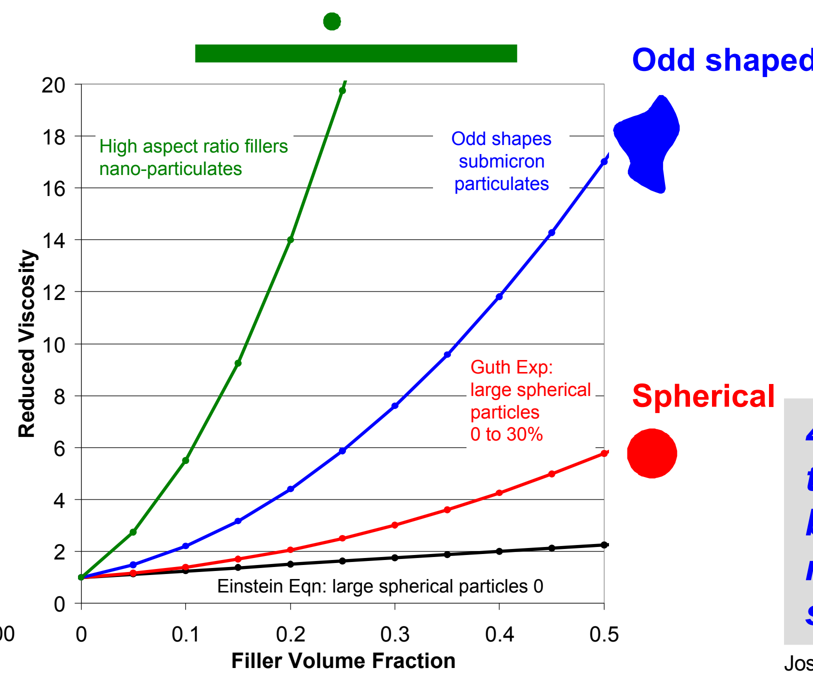
2) Lowest filler loading to obtain desired properties

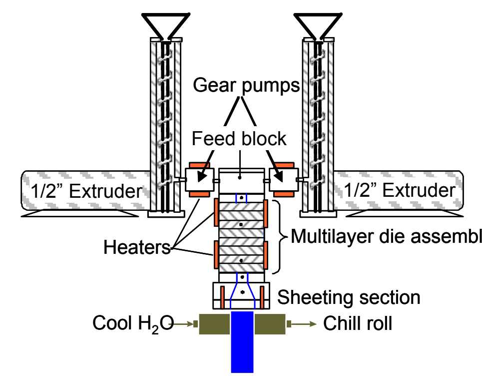
3) Modify filler surface chemistry to screen particle-particle interactions and promote polymer – particle wetting

Broadening particle size distribution leads to decrease in resin viscosity



High aspect ratio and nanoparticles

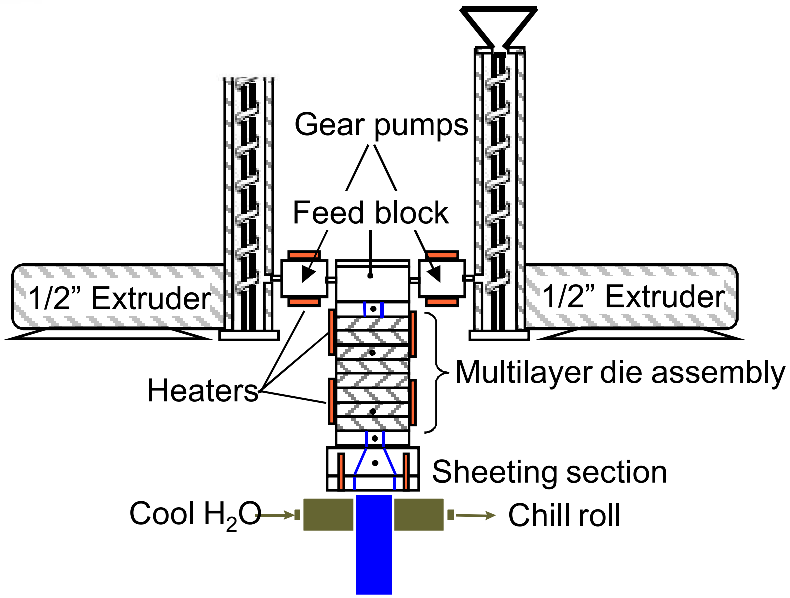




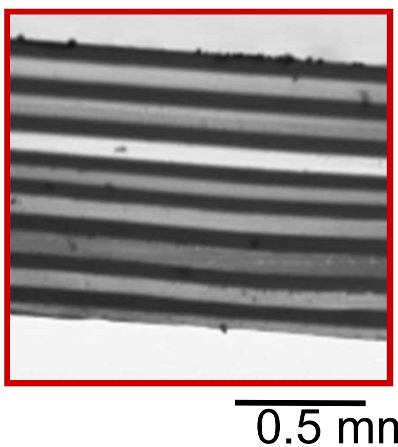
4) Advanced mixing techniques and extrusion based processing to manufacture high viscosity solutions

Joseph L. Lenhart; jllenha@sandia.gov; 505-284-9209

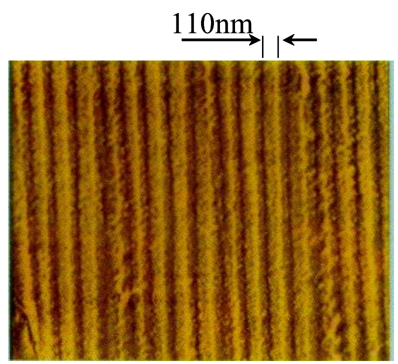
Micro/Nano Layered Structures: Multi-layer Coextrusion



- Single screw extruders with mixing screws (equivalent to twin screw extruder)
- Gear pumps provide precise flow rate control
- Multilayer die assembly increases number of layers within same cross-section
- Sheeting die creates ~1 mm thick tape



$$\delta_{PS} = 23.8 \pm 4.0\,(\mu m)$$
$$\delta_{PP} = 22.9 \pm 5.1\,(\mu m)$$



PC/PMMA multilayer, Dow Chem.

- Alternative layering of polymers with different electrical, mechanical, micro-structural, optical properties
- Membranes, sensors, energy storage devices, optical devices, flexible mirrors

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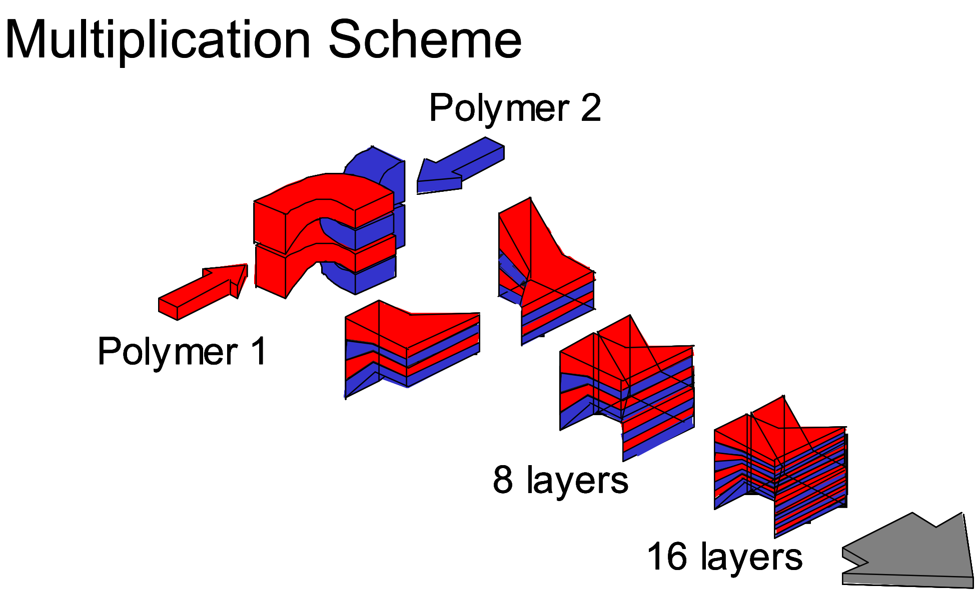
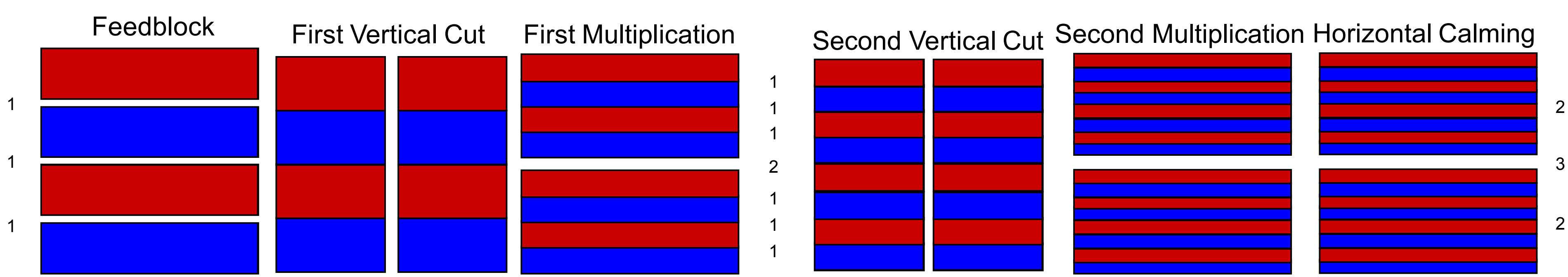
Multiplication Scheme



- **Feedblock produces initial layered structure**
- **Each multiplication element doubles the number of layers**
- **Stacking "n" multiplication dies results in 2^{n+2} layers**
- **Layer stability is largely dependent on uniform laminar flow**
- **Thin layers (submicron) can easily break-up due to instabilities**



•Incorporating "nano-particulates" to control layer properties

Joseph L. Lenhart; jllenha@sandia.gov; 505-284-9209

Year 1: Research / Budget

1. ***Understand / Control particulate dispersion***
2. ***Investigate impact of nano-particle size, shape, loading, on composite properties and processability***

Postdoc 1

Focus:

- Surface modification of nano-particulates (coupling agent deposition, surface intitiated polymerizations, porous coatings)
- Impact of particle size, shape, loading, surface chemistry on flow behavior
- $150K to cover materials, travel, labor for Sandia collaborative staff (does not include postdoc salary)

Postdoc 2

Focus:

- Understanding nano-particle impact in various crosslink density epoxy resins
- Impact of particle size, shape, loading, surface chemistry on cured composite properties (fracture toughness, CTE, Tg, thermal and electrical transport)
- $150K to cover materials, travel, labor for Sandia collaborative staff (does not include postdoc salary)

Focus Materials:
Fillers: alumina, nickel, tungsten, carbon nano-tubes
Filler sizes: 40 nm to microns
Polymers: Epoxy resins, silicone elastomers, polystyrene

Year 2: Research / Budget

1. ***Continue fundamental science aspect of year 1***
2. ***Migration to practical aspects of nano-composite application (processing approaches)***
3. ***Advantage of two year collaboration: full leveraging of ongoing Sandia projects***

Postdoc 1

Focus:

- Nano-particulate composite conformal coatings for shielding applications
- $150K to cover materials, travel, labor for Sandia collaborative staff (does not include postdoc salary)

Postdoc 2

Focus:

- Conductive composites processes by multi-layer coextrusion techniques
- $150K to cover materials, travel, labor for Sandia collaborative staff (does not include postdoc salary)

Final Deliverable: Fundamental understanding of factors that control nano-composite properties and processability and processing approaches to exploit nano-composite technology in an array of potential applications

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One year collaboration?

1. ***Understand / Control particulate dispersion***
2. ***Investigate impact of nano-particle size, shape, loading, on composite viscosity***

Postdoc 1

Focus:

- Surface modification of nano-particulates (coupling agent deposition, surface intitiated polymerizations, porous coatings)
- Nano-composite conformal coatings
- $210K to cover materials, travel, labor for Sandia collaborative staff (does not include postdoc salary)

Postdoc 2

Focus:

- Impact of particle size, shape, loading, surface chemistry on flow behavior
- Nano-composite conformal coatings
- $210K to cover materials, travel, labor for Sandia collaborative staff (does not include postdoc salary)

- ***Viscosity / processability / particulate dispersion is the most critical issue for nano-composite implementation and this would be the focus***
- ***Compressing the project to 1 year necessitates the additional funding per postdoc***
- ***Compressing the project to 1 year also does not allow for full investigation of practical implementation aspects that would be a focus of year 2.***
- ***Narrow range of materials investigated ie. Epoxy or silicones but not both***

Group Facilities

Collaboration with External Facilities

- National Synchrotron Light Source (3 beamlines with energy range 180eV to 30KeV, XPS, NEXAFS, EXAFS)
- NIST Center for Neutron Research (neutron scattering and reflectivity)

Spectroscopy / Chemical Analysis

- UV-Vis
- FTIR / Raman
- NMR
- Fluorescence
- Fluorescence microscopy
- GPC

Modeling

- Molecular
- Continuum

Chemical Synthesis

- Polymer chemistry
- Nano-particle synthesis
- Surface chemistry / modification
- Extensive wet chemical laboratories and facilities

Surface Analysis

- XPS / NEXAFS
- AFM
- SEM / TEM
- Contact angle

Mechanical Characterization / Rheology

- Several Instrons
- Stress and strain controlled rheometers

Thermal Analysis

- DMA
- TMA
- DSC
- TGA

Particle Characterization

- Light scattering particle size analyzer
- BET

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Sandia National Laboratories

Materials and Process Sciences Center

Sandia National Laboratories

PETL
Bldg 701

IMRL
Bldg 897

TSRL
Area III

AML
UNM South Campus

The Materials and Process Sciences Center at Sandia National Laboratories provides scientific and engineering materials expertise to support the laboratory's varied missions.

- Programs focus on three theme areas: 1) creation of new materials through the science-based tailoring of composition and microstructure, 2) development of processing methods with an emphasis on process diagnostics, modeling, and control, and 3) materials reliability assessment, and early detection and prediction of materials aging.

- Polymers, ceramics, metals, and advanced analytical techniques, spanning the size range from atoms to macroscopic.

- Approximately 250 people working in 8 departments and includes a robust graduate and post doc research program.

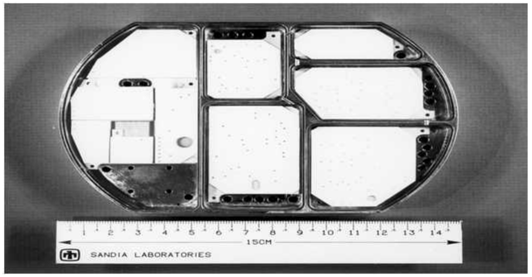
- Core mission of the Center is supporting the U.S. nuclear weapons program in alignment with Sandia's stockpile stewardship responsibilities for DOE Defense Programs.

- Center also supports projects in other DOE program offices, enabling Sandia's role as a multi-program DOE laboratory, and collaborates with many other federal agencies, industrial partners, and academic institutions.

(Rev. 8/31/07)

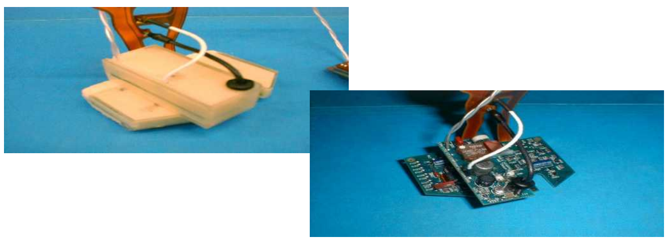
Organic Materials Expertise

Sandia National Laboratories



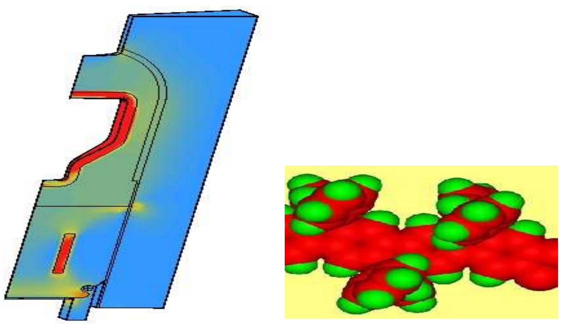
Sticky foam for asset protection

Anthrax decontamination foam

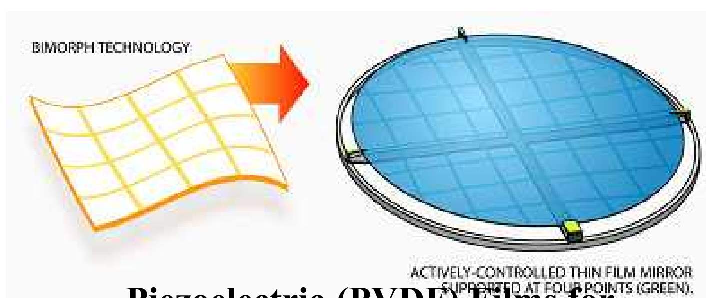


Removable encapsulatnts

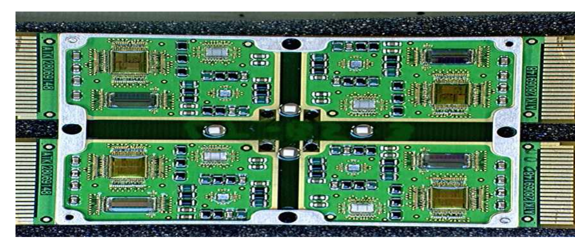
Explosion mitigation



Encapsulation of nuclear weapon components



Piezoelectric (PVDF) Films for Advanced Space Mirror Concepts



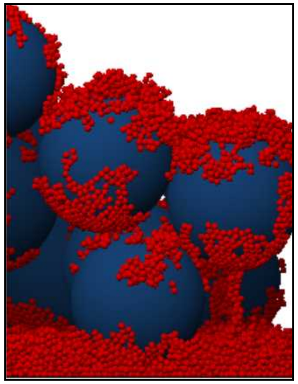
Anti-Tamper technology coatings

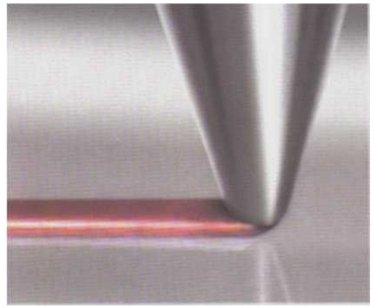
CINT
Center for Integrated Nano-Technologies
A facility jointly owned and operated by SNL and LANL

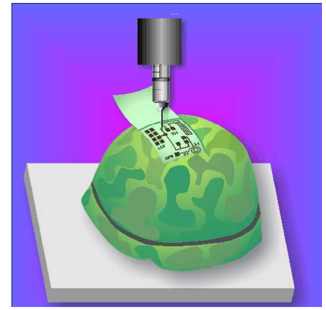
Nanomaterials Expertise

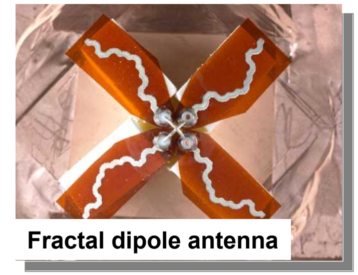
Sandia National Laboratories

DARPA MICE mesoscopic integrated conformal electronics





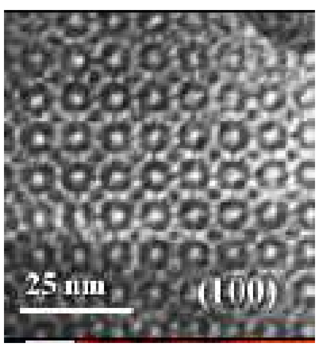


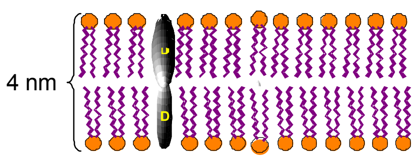


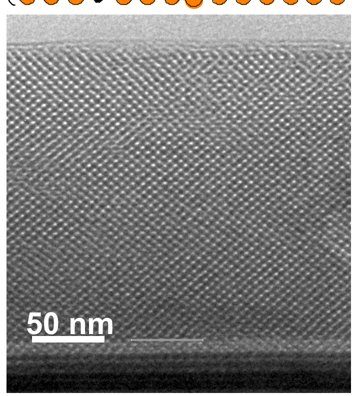
Fractal dipole antenna

Nanostructured inks and conformal direct write electronics

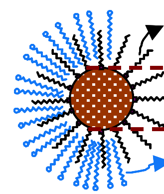
DARPA DSO

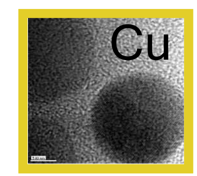




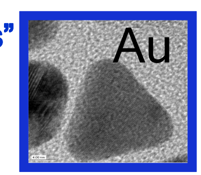


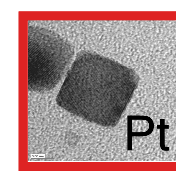
Nanostructured materials as sensors and filters





Nanoparticle "Lucky Charms"
Synthesis of Nanocrystals with Controlled Shapes, Sizes, and Compositions





Nanoparticles as tags for protein expression