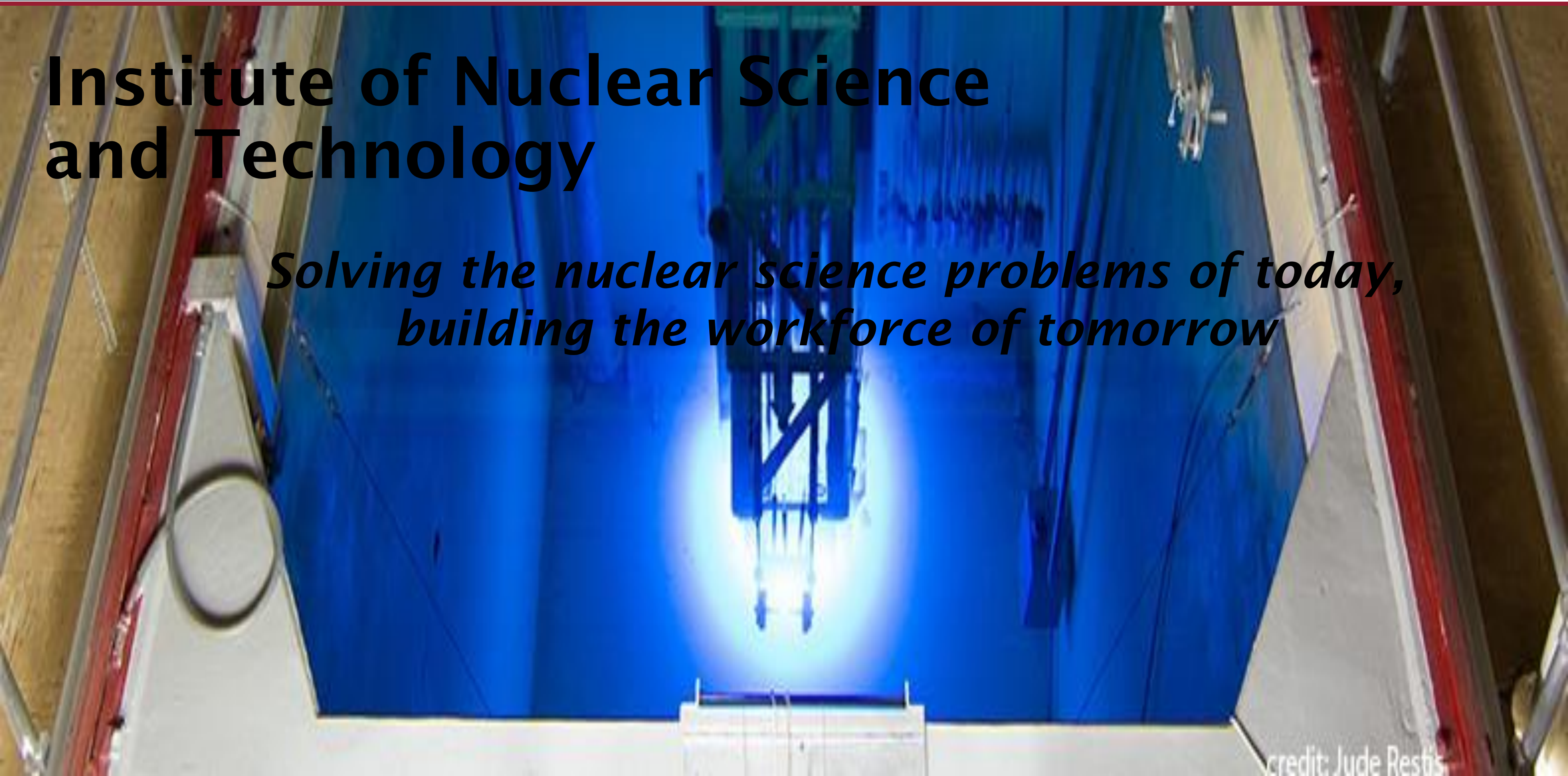
WASHINGTON STATE UNIVERSITY

Institute of Nuclear Science and Technology

Solving the nuclear science problems of today, building the workforce of tomorrow



Overview

- We are 22 faculty from Chemistry, Chemical Engineering, Mechanical and Materials Engineering, Electrical Engineering and Computer Science
- Our mission: A hub for education, multidisciplinary research, and innovation in nuclear science and technology that addresses societal challenges in global security, human health, energy, and the maintenance and restoration of environmental quality.

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Education

- Largest Radiochemistry PhD track in the US
  - Radiochemistry traineeship grant
  - Nuclear Forensics summer schools
- Nuclear materials graduate certificate in Materials Science and Engineering Ph.D program
- Growth of data analytics from undergraduate to graduate certificate in physical sciences (direct application to nuclear)
- Most Ph.D's go on to staff positions at INL, ORNL, PNNL, LANL, Savannah River, etc.
- Many pursue internships or post-graduate fellowships at NNSA –
  - Heather Dion, Steve Lamont, Matt Douglas, Amber Donley, etc.

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Multidisciplinary Research

- Nuclear fuels, waste form development, and waste site management
- Separations (across all scales…from microfluidics to bulk)
- Modeling and Simulation
- Electrochemistry, detection and sensing
- Environmental behavior of radionuclides
- Solution chemistry
- Thermochemistry (kinetics, speciation)
- Radiopharmaceuticals
- Nuclear forensics
- Robotics
- Policy

NSF

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

DEFENSE THREAT REDUCTION AGENCY · UNITED STATES OF AMERICA

TerraPower

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

INL

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

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Nuclear Materials

Security - Safety

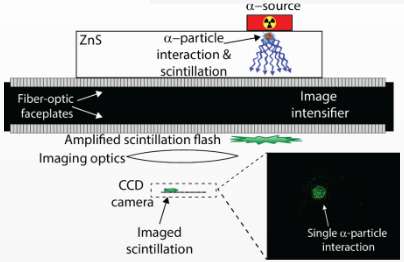
Safeguards By Design

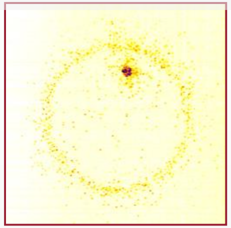
Non-Proliferation

Materials Design - Characterization

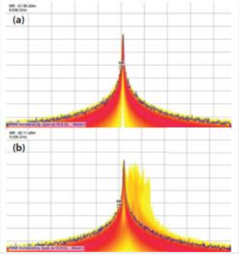
Materials for Sensors

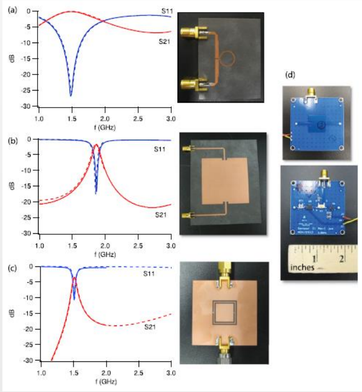
- Nonproliferation
  - Radiation detectors: ZnS scintillators for alpha-particles, x-rays
- Safeguards by design
  - Miniaturized microwave resonators for RFID tags, canister seals, other applications (EMI, vibration, magnetic fields)
- Nuclear navy
  - Magnetic sensors for reactor component degradation monitoring
- Partnerships with PNNL



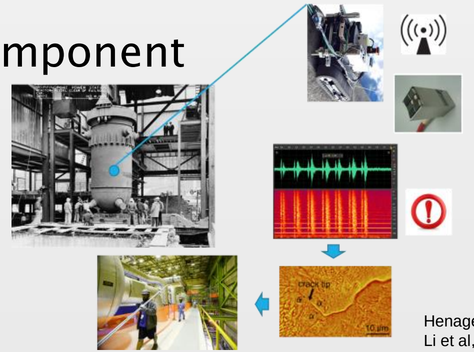


McCloy et al, *J Lumin*, 157, 416 (2015)





Jones et al, *Rev Sci Instr* 84, 084703 (2013)
Jones et al, *Appl Phys Lett* 104, 253507 (2014)



Henager et al, *Acta Mater* 61, 3285 (2013)
Li et al, *J Phys D* 48, 305001 (2015)

Boron-based solid-state neutron detectors

- The ability to detect the thermal neutrons emitted by plutonium is important for nuclear safety and border security
- The conventional gas-filled neutron detectors are large and bulky with a high operating voltage and low detection efficiency
- The performance of a neutron detector strongly depends on the capture cross-section and atomic density of the neutron active material
- Project goal: Develop a boron-based solid-state neutron detector in which the neutron-active region is the semiconducting component of a Schottky transistor

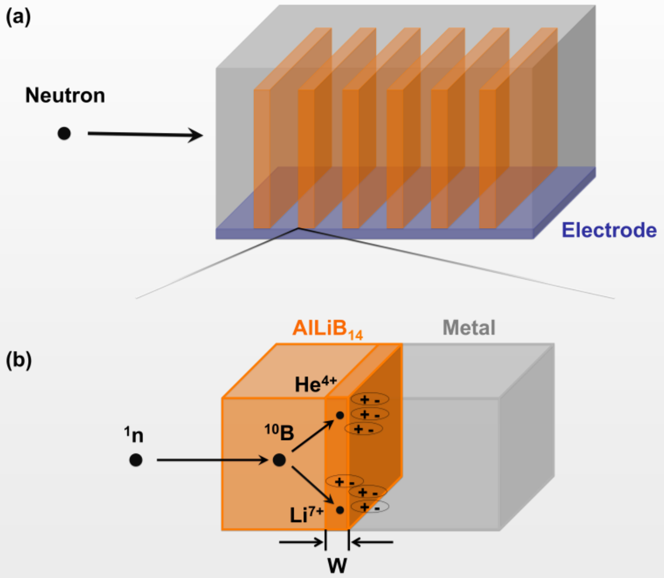
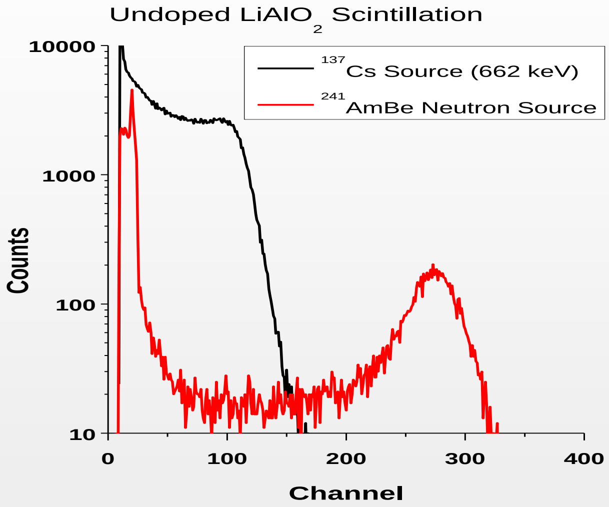
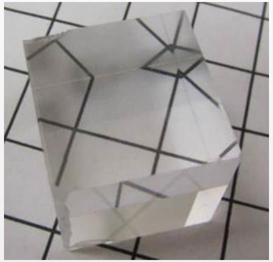


Fig. 5 A schematic view of a layered Schottky heterostructure. (a) A macroscopic view of the neutron active region. The orange denotes the $AlLiB_{14}$ compound that is layered between metal sheets. (b) Neutron reaction in a slab of $AlLiB_{14}$. The ionized species from the reaction are detected at the Schottky interface.

Neutron detection with $LiAlO_2$

- New neutron detectors needed for national security and imaging applications
- High lithium content of $LiAlO_2$ yields excellent intrinsic neutron capture efficiency
- Undoped $LiAlO_2$ single crystals already grown in bulk and demonstrated by Lynn's group to have good neutron detection capabilities
- Optimization of Li-6 content can lead to smaller samples allowing for better gamma to neutron discrimination based on pulse height alone
- Project goal: Optimize activator doping and Li-6 content





Left: Pulse height spectra of undoped $LiAlO_2$ sample produced by Lynn's group demonstrating neutron detection capabilities.

Right: Polished $LiAlO_2$ cube on 1 cm graph paper demonstrating excellent optical quality and clarity.

Security - Safety

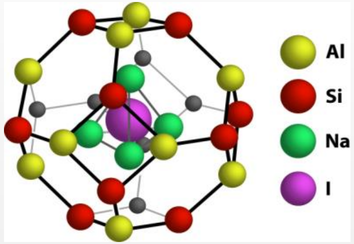
Radiation Response

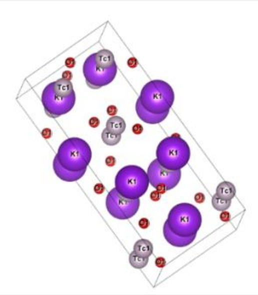
Materials Design - Characterization

Characterizing and Optimizing Radiation Damage

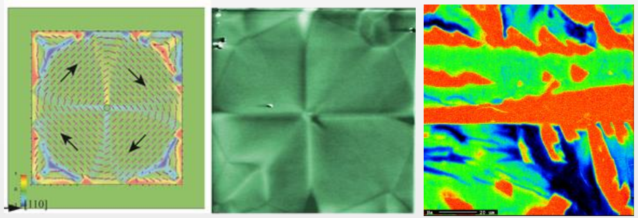
- Materials Science: Ceramics and Metals
  - **Degradation** mechanisms
  - Effect of **disorder** on properties
  - **Glass** composition/structure/property models
  - **Functional** properties: electric, optic, magnetic
  - Advanced **characterization** techniques
- Applications
  - **Nuclear** waste forms (^{99}Tc, ^{129}I, UNF)
  - **Sensors**

Structure





Characterization



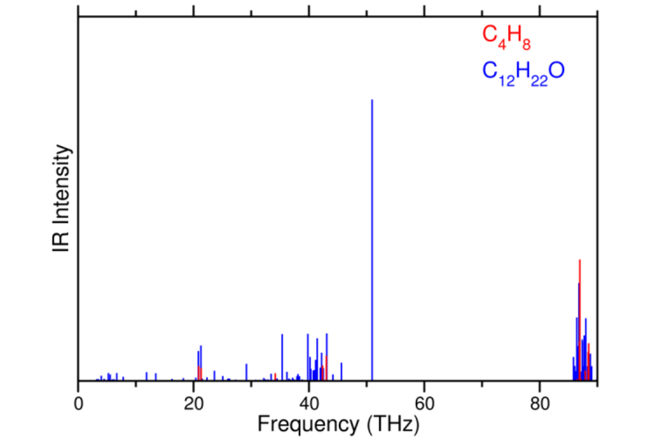
Applications

NOME Materials Laboratory
nuclear optical magnetic electronic

http://labs.wsu.edu/mccloy/

Radiation damage to insulation around nuclear power plant cabling

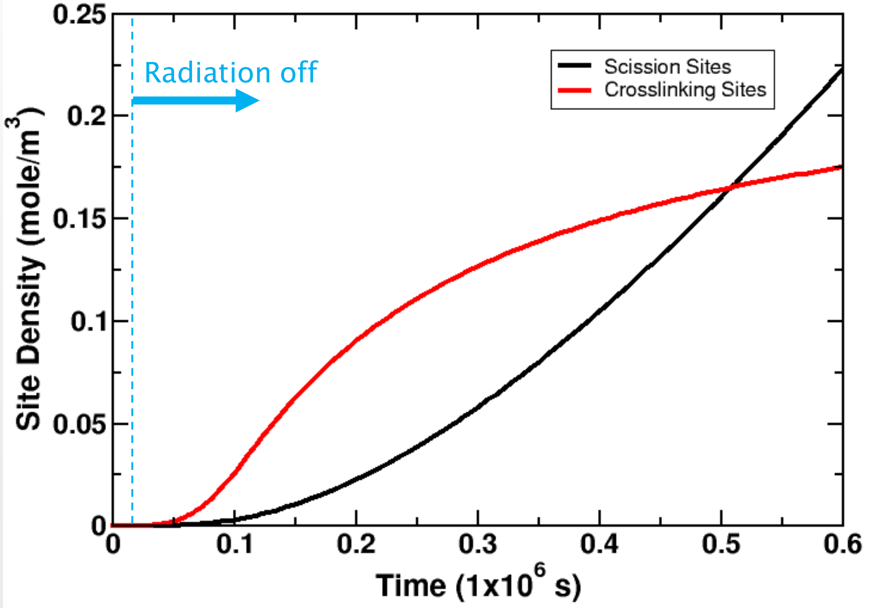
- The recertification of nuclear power plants is a significant issue for the continued production of low-cost, clean, safe electric energy
- There is over 1000 km of electrical cabling in these power plants that that have been exposed to thermal, radiation, and environmental damage and need to be evaluated
- Elongation at break is the ASTM characterization standard for irradiated insulation
- Project goal: Develop alternative characterization methods based on Infrared and Raman spectra or dielectric measurements



The calculated infrared spectra of crystalline polyethylene. The red lines represent the calculated spectral peaks for a supercell containing C_4H_8 and the blue oxidized polyethylene with a carbonyl having a unit cell $C_{12}H_{22}O$.

Kinetic rate theory of radiation damage insulation

- Damage in polymers due to long-term, low-dose radiation cannot be directly determined through accelerated aging studies
- Chain scission and crosslinking due is due to to radical chemistry
- Reaction kinetics are controlled by reagent concentrations, reaction cross-sections, diffusion, and environmental factors
- Project goal: Develop reaction simulation to connect accelerated aging studies to *in situ* exposure



Beckman Group 2016

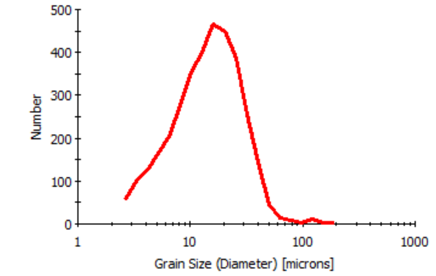
Security - Safety

Non-Proliferation

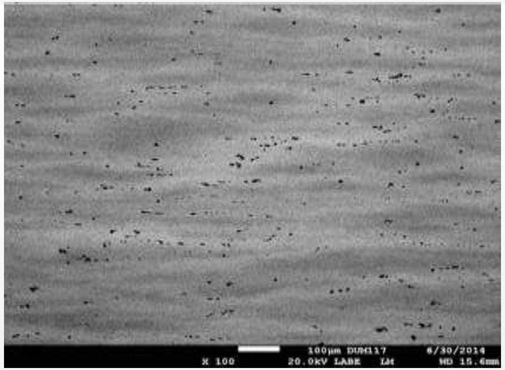
Materials Design - Characterization

Microstructure of U10Mo Fuels

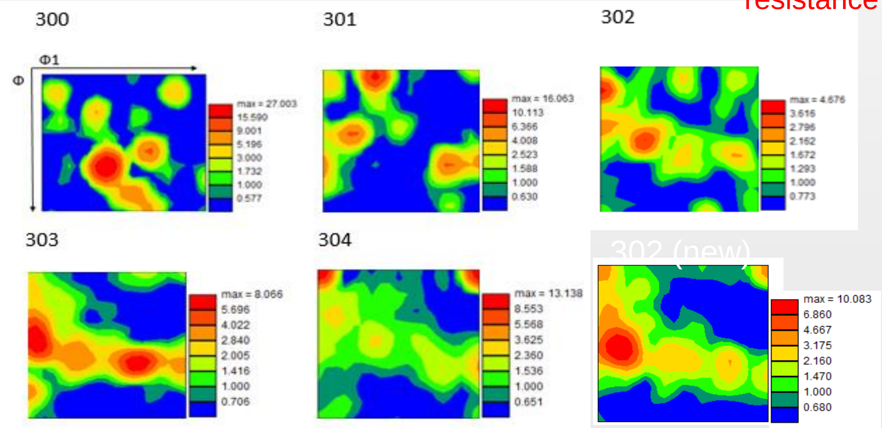
For non-proliferation considerations, high enriched uranium fuel can be replaced with low enriched uranium (LEU) fuel for high performance research reactors. To achieve the requisite high fuel density, uranium alloyed with 10 wt% molybdenum (U-10Mo) shows favorable properties.

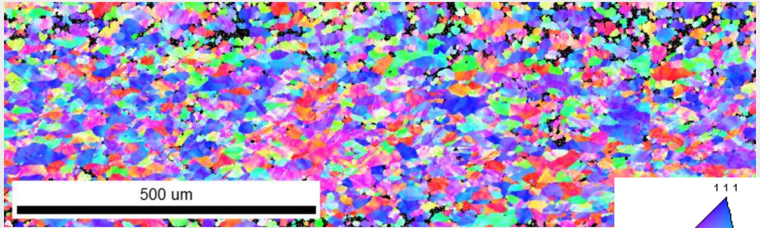


Tests indicate that a large grain size, homogeneous structure, and well-developed gamma fiber have better resistance to swelling for U10Mo.

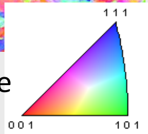


BSE Image showing Mo rich and Mo lean regions. Carbides are somewhat aligned in the rolling direction.



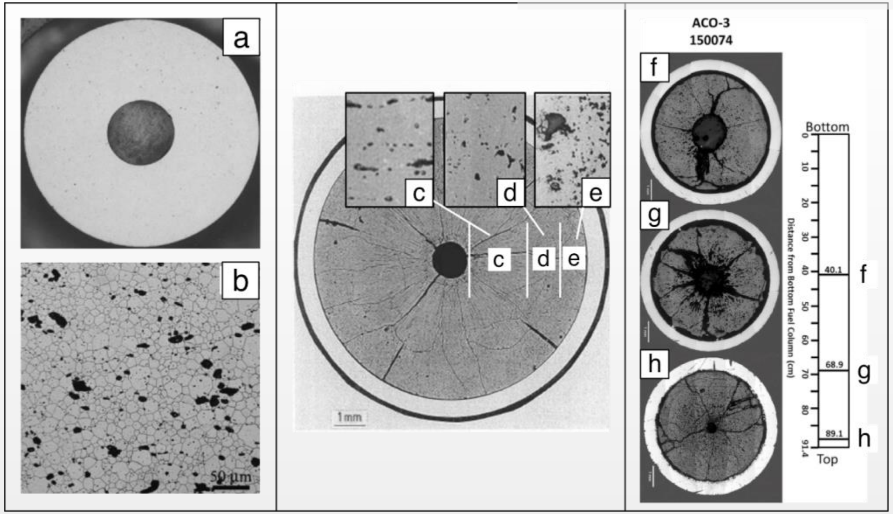


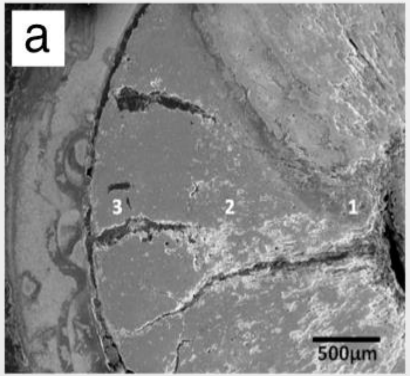
Orientation map of hot-rolled U10Mo structure

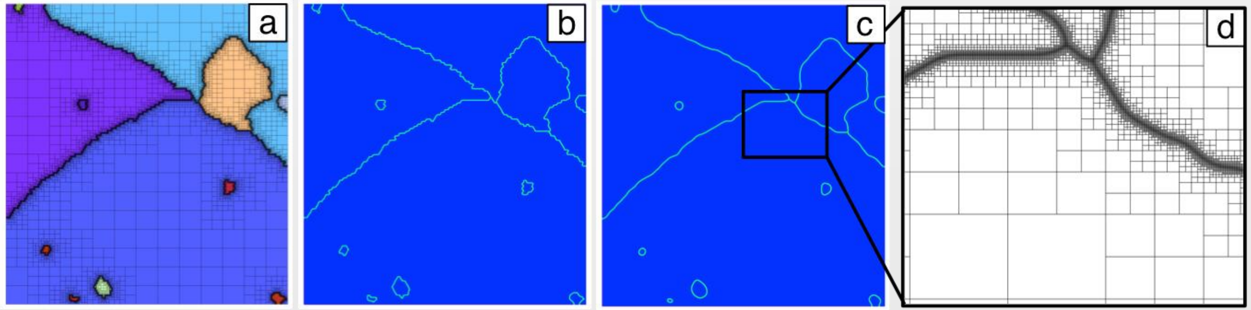


Structure Evolution in UO_2

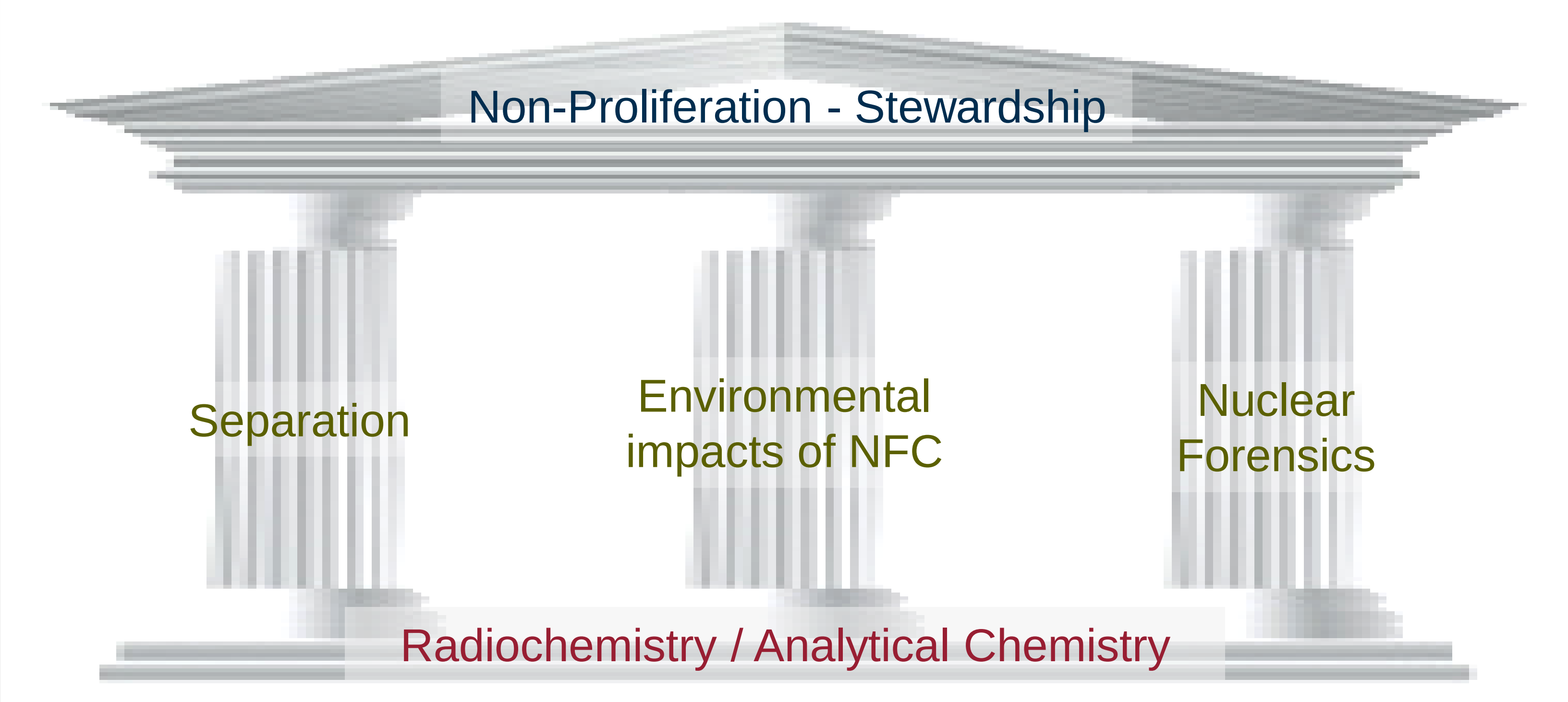
EBSD characterization of structural evolution in UO_2 fuels requires an innovative approach to data interpretation. A phase-field modeling approach is used to ensure that the proper structures are obtained from the low-reliability data.







Nuclear Fuel Cycle



Radiochemistry

- Strong education program in radioanalytical and nuclear techniques

- 32 PhD, 6 MS in experimental radiochemistry since 2010
- Facilities:
  - Secured research radiochemistry laboratories in Chemistry Dpt.
  - Nuclear Radiation Center
- Collaborations with multiple National Laboratories to enhance student experiences

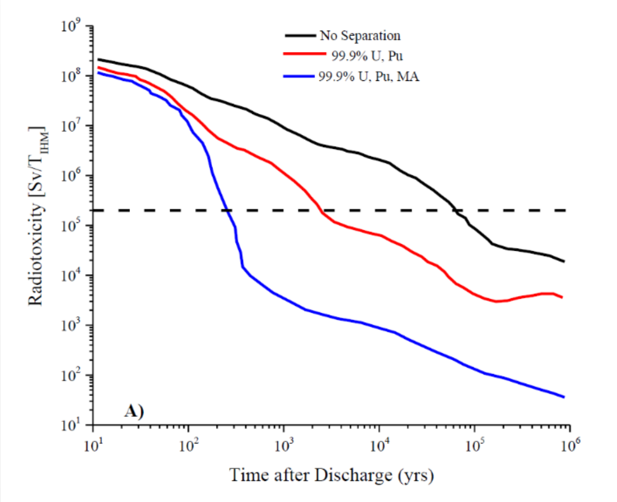
Non-Proliferation - Stewardship

Separation

Radiochem / Analytical Chem

Separation

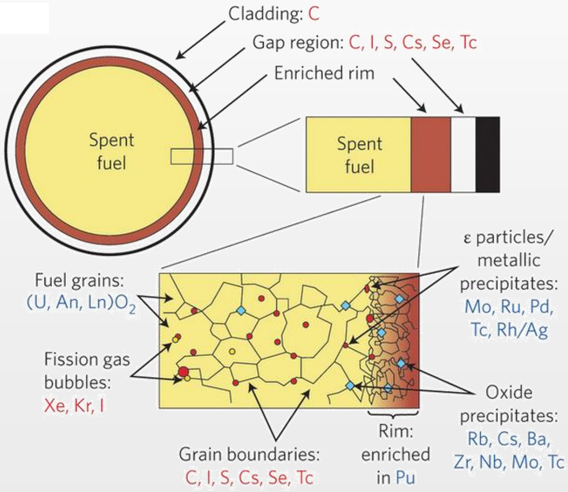
- Fundamental studies to understand the impact of advanced Nuclear Fuel Cycles



- Goals:
  - Basic research to develop safeguards technologies for all Nuclear Fuel Cycles.
  - Developing and understanding of world-wide nuclear materials management.

Environmental Impacts of NFC

- Thermodynamics, Dynamics and Surfaces phenomena

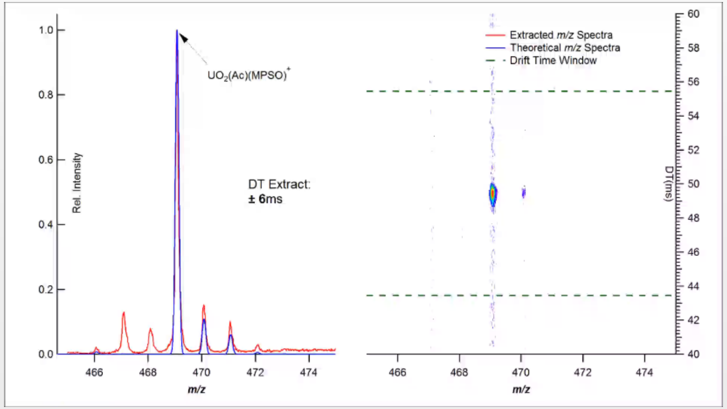


R. C. Ewing, *Nat. Mater.* 2015

- Solid wastes → Structure – thermodynamics relationships
- Aqueous chemistry of actinide materials → Interfacial dynamics and solution chemistry
- Fission gases → Fission gas capture and separation

Nuclear Forensics

- Basic research that provides a technical foundation linking materials characteristics to nuclear events and/or process history
  - <u>Examples of research</u>:
    - *Signatures*: Isotopic, Soluble complexes, Materials
    - *New Fundamental Data for Nuclear Forensics*: Kinetic data driving chemical reactivity, Thermodynamic data describing speciation
    - *Neutrons and Nuclear Forensics*: Materials Irradiations for Treaty Compliance



Rapid Isotopic Determination While Maintaining Chemical Speciation

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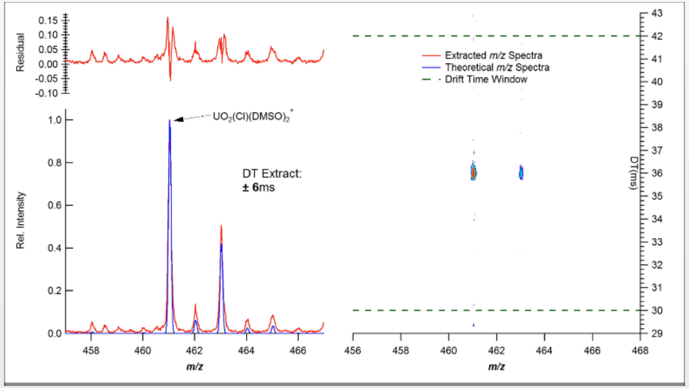

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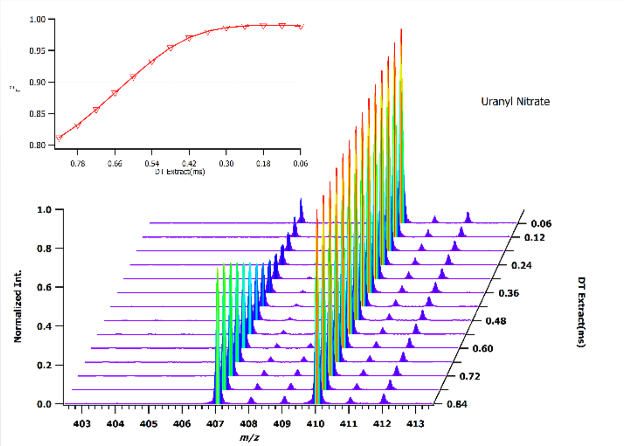
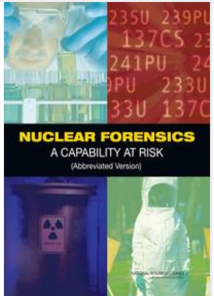


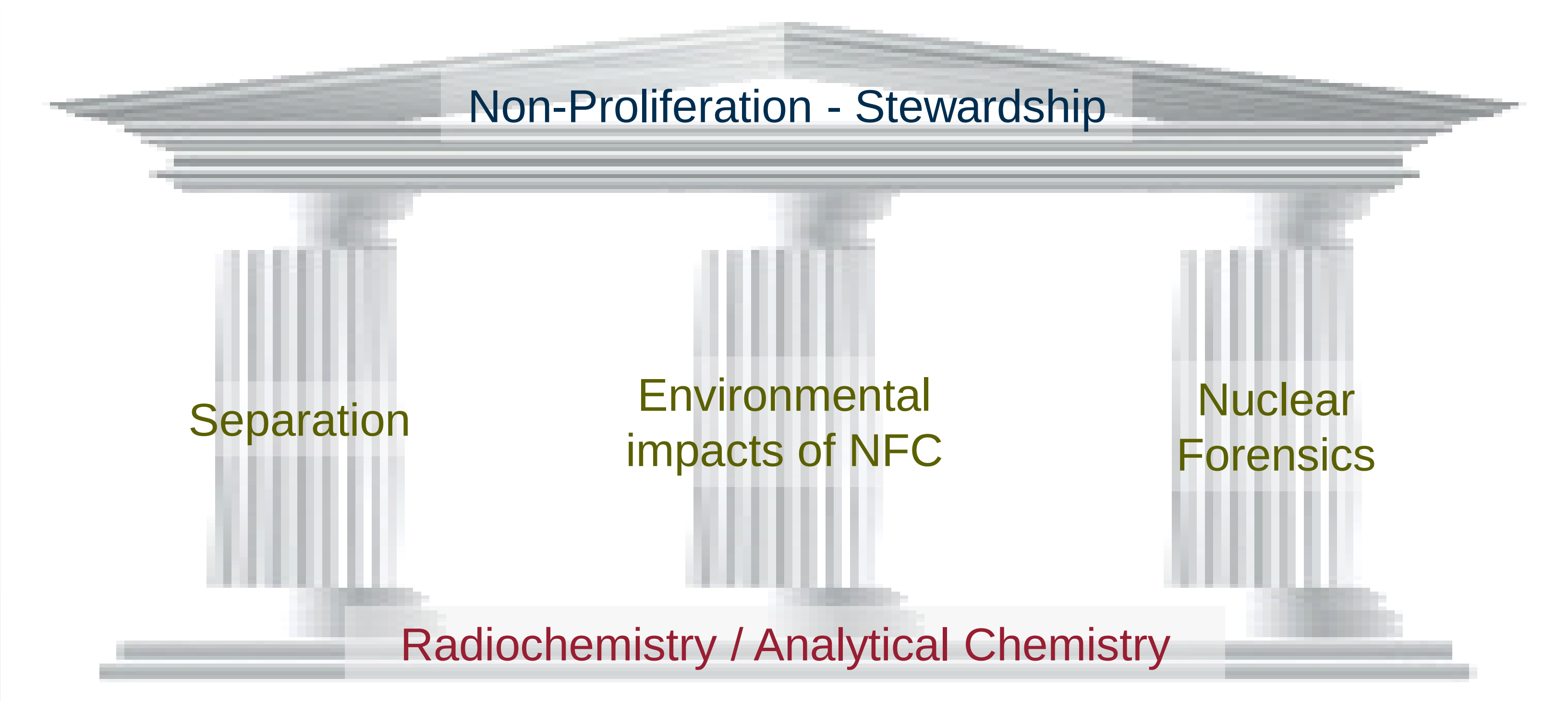
Rapid Isotopic Determination While Maintaining Chemical Speciation

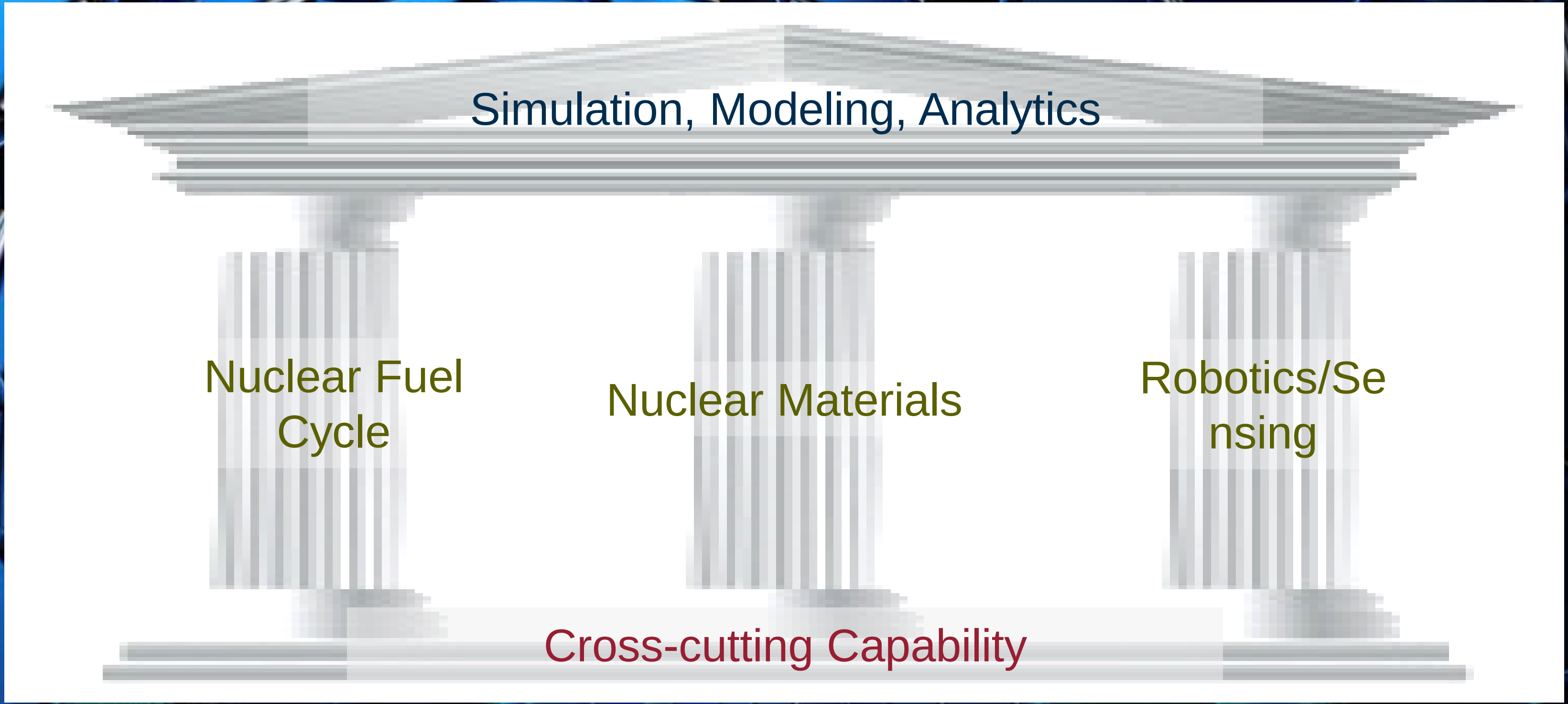
Providing National and International Impact

- Service as Special Government Employees: Governmental advisory boards and committees, US Nuclear Waste Technical Review Board, National Academies reports
- Service to international agencies and organizations, including IAEA and CTBTO
- Cooperative nuclear threat reduction through international engagements and collaboration



Nuclear Fuel Cycle

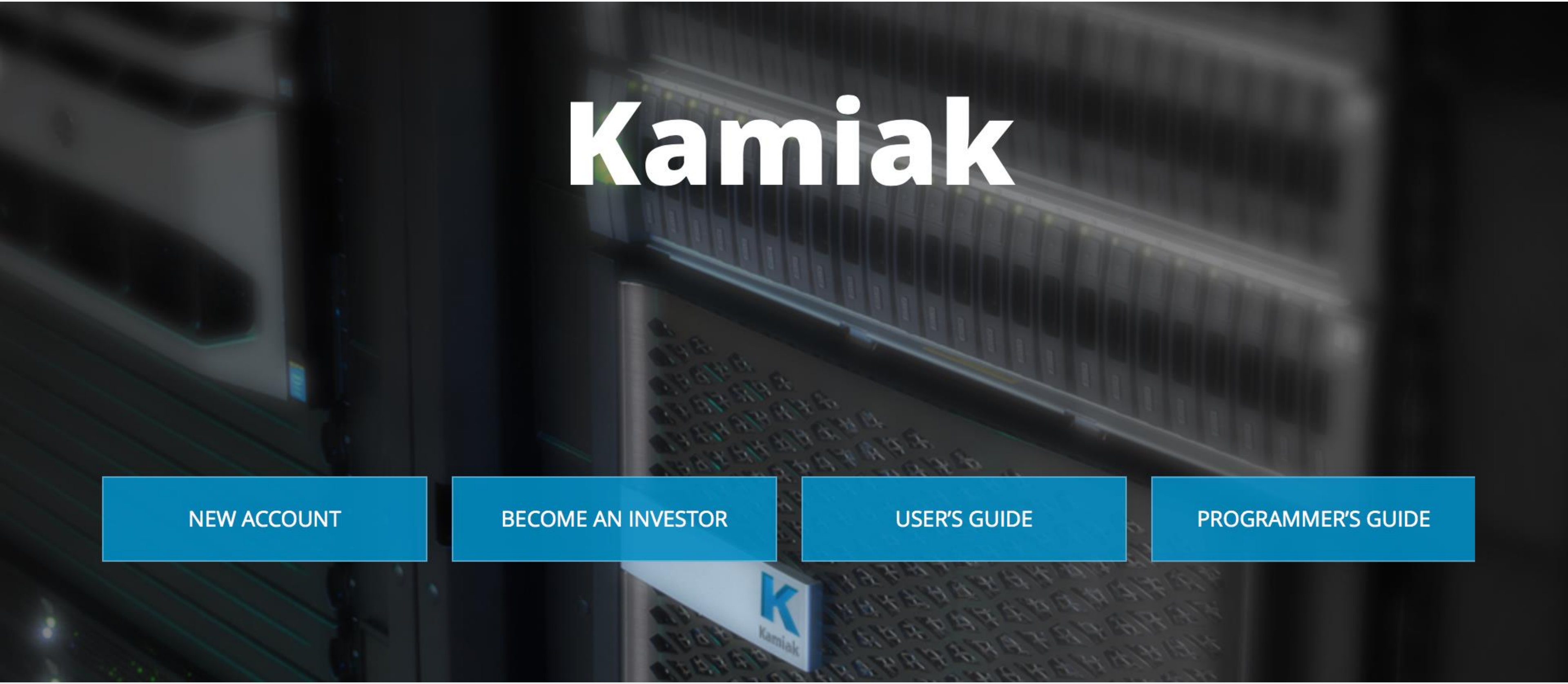


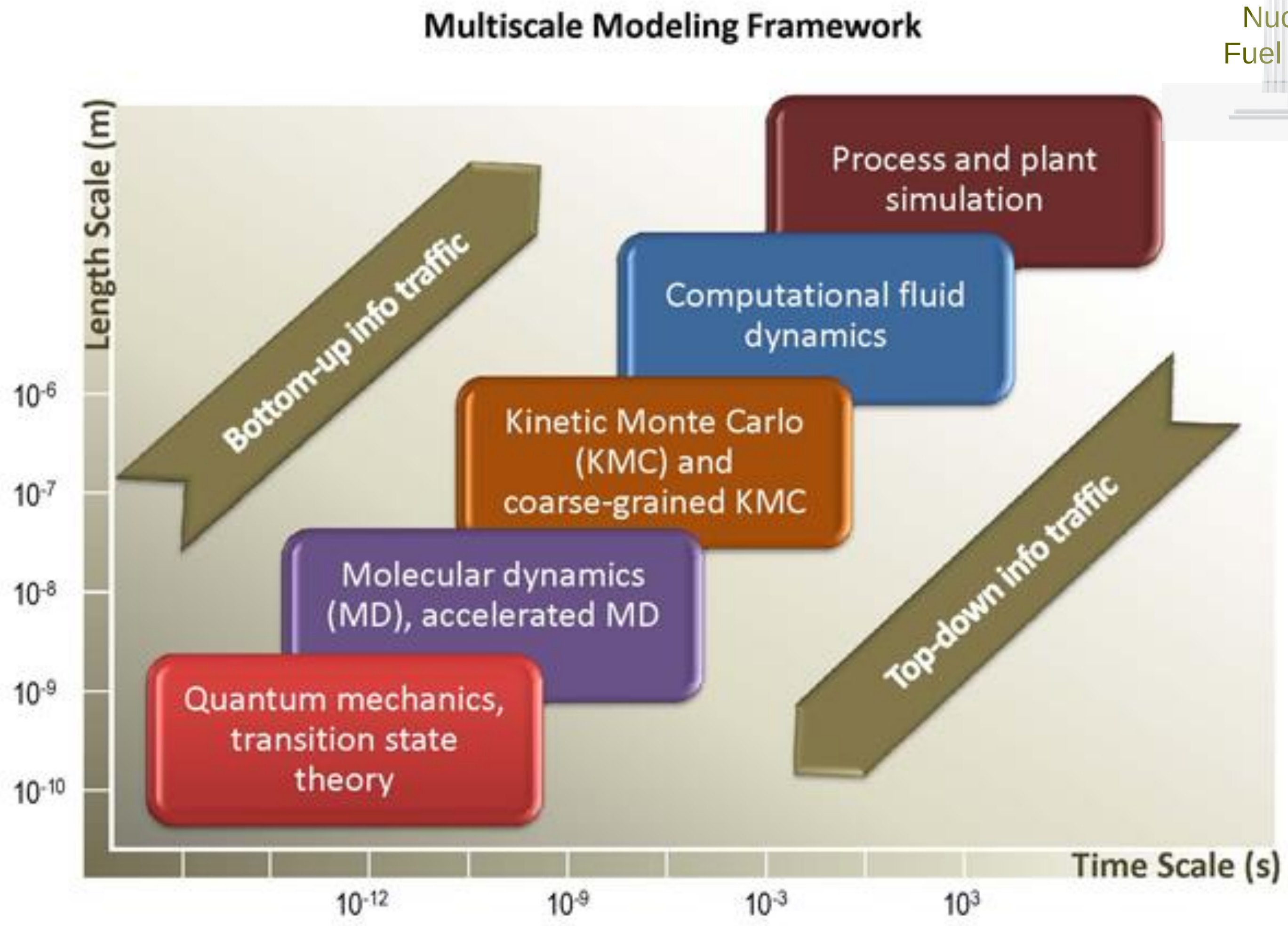

Simulation, Modeling, Analytics
Nuclear Fuel Cycle
Nuclear Materials
Robotics/Sensing
Cross-cutting Capability

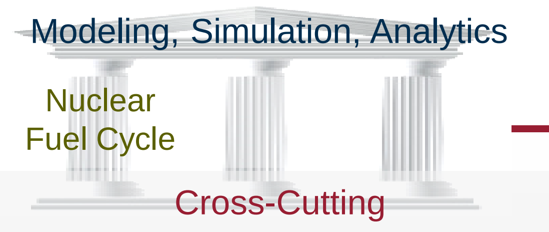
Simulation, Modeling, Analytics

- An essential aspect of the no-testing paradigm for maintaining the integrity of our weapons stockpile
- Permeates other NNSA interests:
  - Sensing and detection for forensics and monitoring
    - How we detect, what we detect, why we think it is there
  - Accurate databases for numerical predictions across length and timescales
  - Component and materials design and performance
- WSU has unique computational expertise that spans length and timescales and is integrated tightly with experimental validation
- Analytics plays an essential role in UQ, signal identification, cross-correlating relationships

Center for Institutional Research Computing



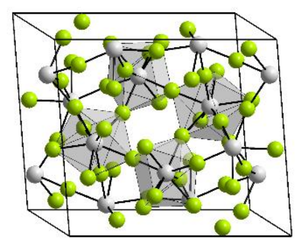

Multiscale Modeling Framework
Length Scale (m)
10-6
10-7
10-8
10-9
10-10
Time Scale (s)
10-12
10-9
10-3
103
Bottom-up info traffic
Top-down info traffic
Process and plant simulation
Computational fluid dynamics
Kinetic Monte Carlo (KMC) and coarse-grained KMC
Molecular dynamics (MD), accelerated MD
Quantum mechanics, transition state theory



Accurate First Principles Calculation of Thermochemical Properties

- Use a highly systematic approach to yield accurate (±3 kcal/mol) predictions of bond and formation enthalpies of actinide-containing molecules
- Current group: 4 graduate students
- Active collaborations with staff scientists at LBL (experiment) and ANL (theory), as well as faculty at Brown, Emory, Utah, Stuttgart, and Tsinghua.
- Our work is being used to populate the Active Thermochemical Network of Rusic at ANL to yield more reliable actinide thermochemistry by combining theory and experiment

Example: Atomization Enthalpies of Thorium Tetrahalides (kcal/mol)



	VQZ-PP	ΔCBS	ΔCV(Th)	ΔCV(X)	ΔDK	ΔSO	ΔZPE	ΔQED	AE(298K)	Expt.
ThF_4	651.6	+3.7	+3.3	+0.6	–7.4	–10.5	–4.0	+0.5	**640.4**	**639±2**
$ThCl_4$	498.3	+5.7	+3.2	+1.1	–5.2	–12.3	–2.5	+0.5	**490.4**	**490±2**
$ThBr_4$	444.2	+5.4	+3.7	+2.9	–4.0	–20.8	–1.3	+0.4	**431.7**	**429±2**
ThI_4	368.2	+4.1	+2.6	+7.3	–4.0	–32.5	–1.0	+0.1	**345.7**	---

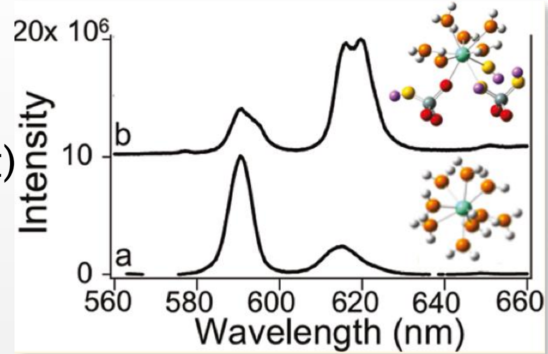
Modeling, Simulation, Analytics

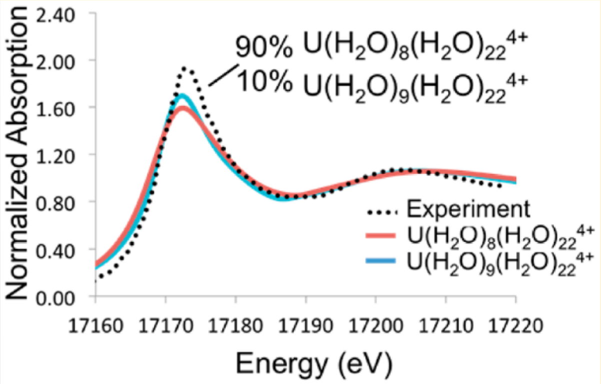
Nuclear Fuel Cycle

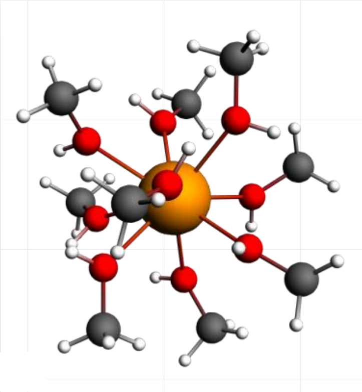
Cross-Cutting

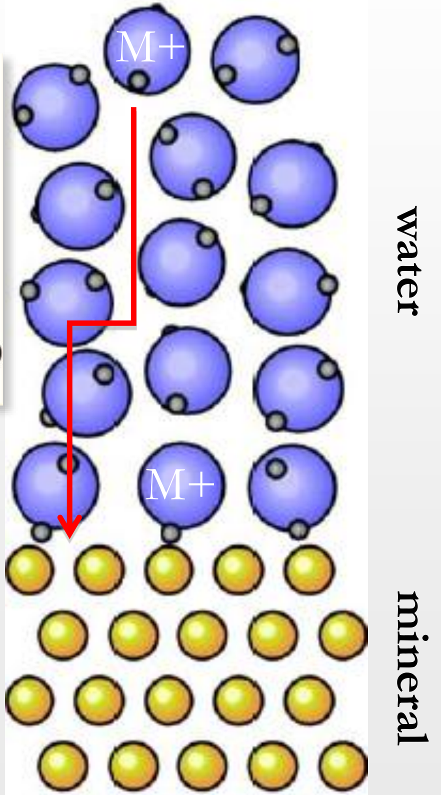
Solution and Interfacial Chemistry of Actinides and Lanthanides

- Speciation
- Separations
- Nuclear Forensics (signatures, transport)



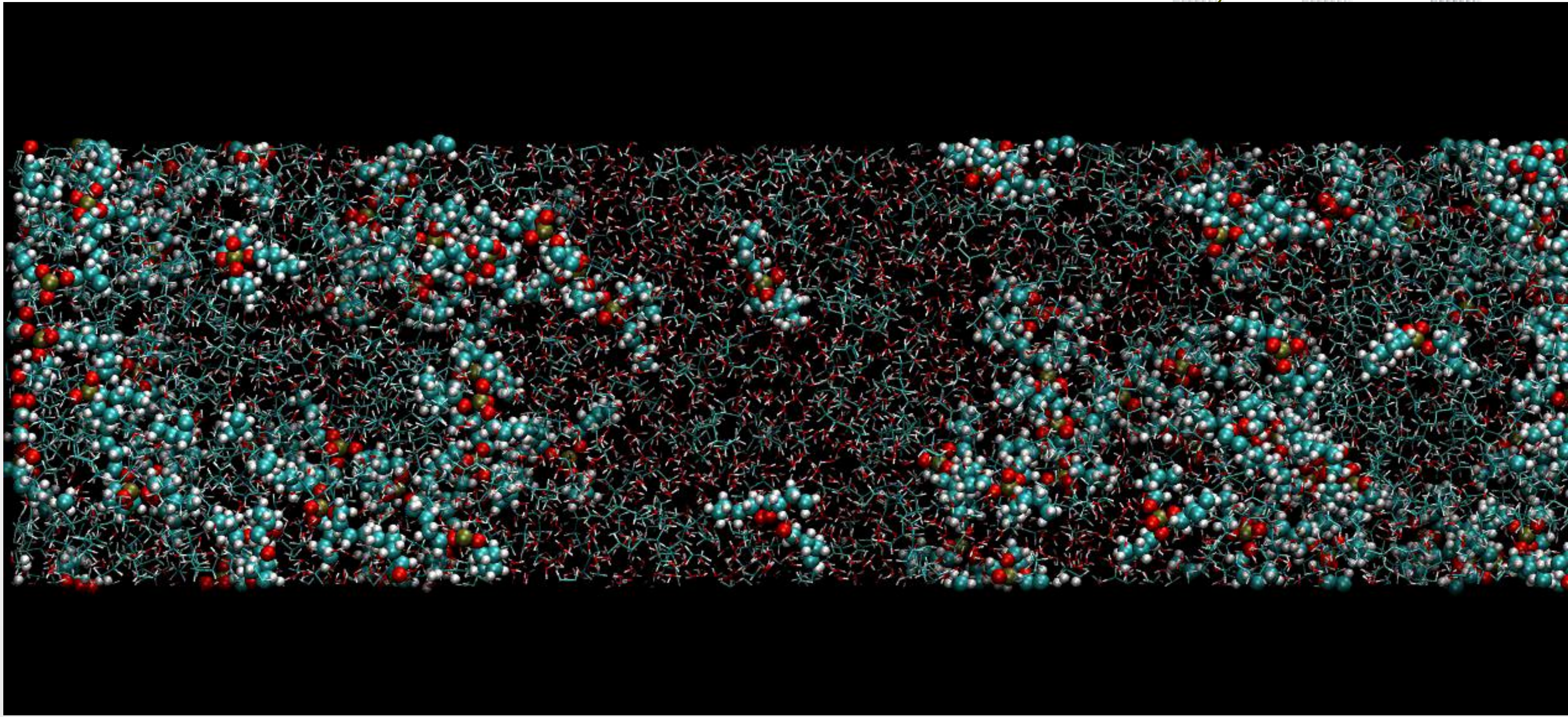






Solution and Interfacial Chemistry of Actinides and Lanthanides

- Understanding mechanisms of oil/water phase segregation to better control actinide/lanthanide separations



Modeling, Simulation, Analytics

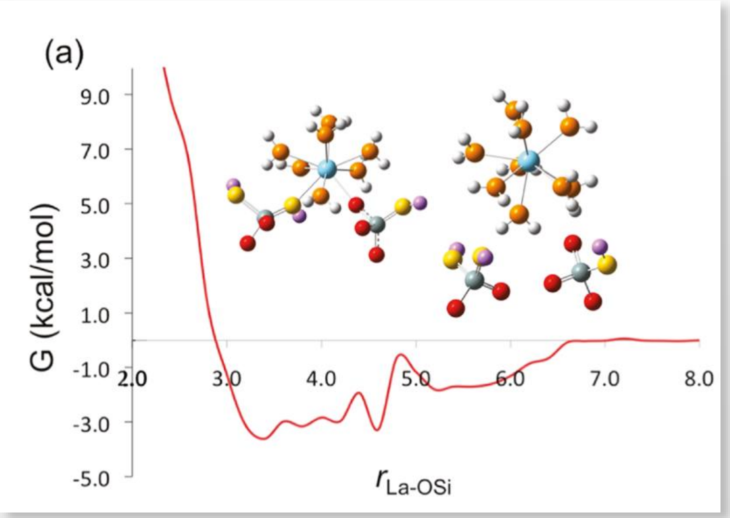
Nuclear Fuel Cycle

Cross-Cutting

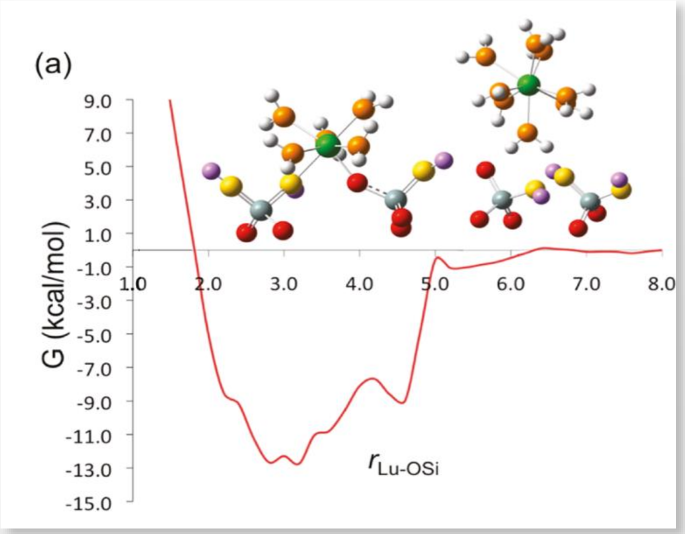
Solution and Interfacial Chemistry of Actinides and Lanthanides

- Mechanisms of sorption of actinides/lanthanides to mineral surfaces

Early lanthanide sorption to quartz



Late lanthanide sorption to quartz

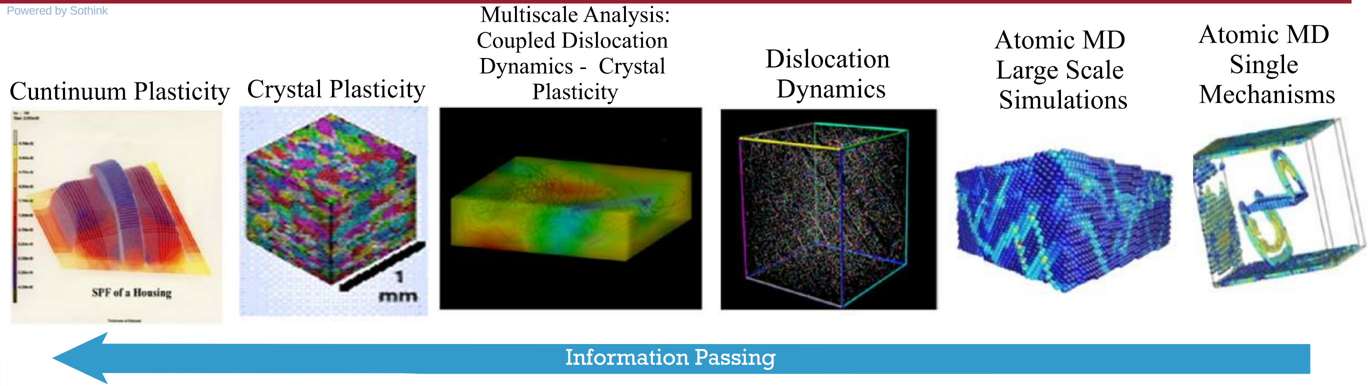


Powered by Sothink

Modeling, Simulation, Analytics

Nuclear Materials

Cross-Cutting



Computational Mechanics and Materials Science (cmms.wsu.edu)

Thermo-mechanical behavior of solids:

Solve engineering and scientific phenomena spanning the length scale and occurring under extreme loading and environmental conditions, with emphasis on deformation, irradiation damage, fracture and material instabilities.

Develop multiscale models that are based on first principle calculations and link scales through information-passing

-**Nanometer to micrometer:** Investigate the mechanical performance of metals and composites with emphasize on nanolaminate metallic/ceramic structures, composites and thin films.

-**Micrometer to macrometer:** Investigate the behavior of metals and geological materials under extreme conditions: radiation, shockwaves, metal forming, high speed machining, superplastic forming, etc.

Modeling, Simulation, Analytics

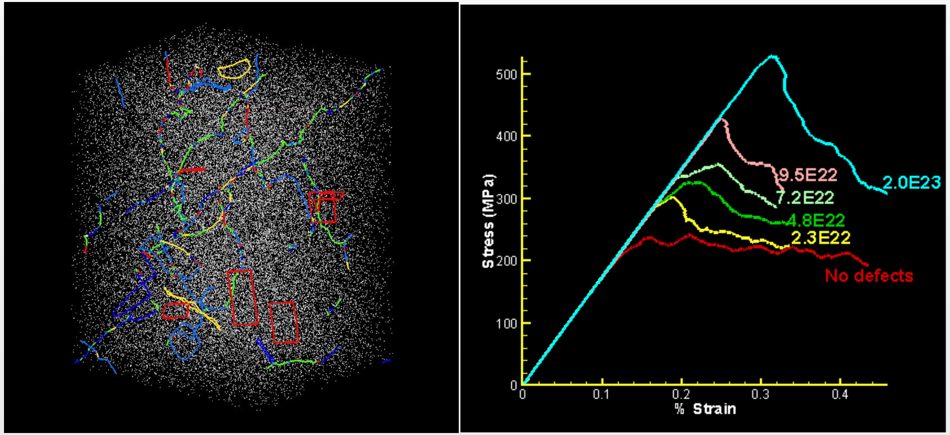
Nuclear Materials

Cross-Cutting

Multiscale Models and Methods for Nuclear Materials

Goal: Develop physically-based capability that predicts aging behavior & performance & in-service lifetime of structural materials used in nuclear reactors with focus on advanced steels.

- Current designs are based on extrapolation of data from short-term tests to predict the lifetime and reliability of structural components. Predictive multiscale modeling and simulations can improve upon this.



Multiscale simulations (*discrete dislocation dynamics coupled with continuum mechanics*) of irradiated metals reveal the mechanisms underlying plastic flow localization and irradiation-induced hardening: dislocation pinning an unpinning by irradiation-induced clusters of defects. *e.g. Mastorakos & Zbib. A multiscale approach to study the effect of chromium and nickel concentration in the hardening of iron alloys. J. Nuclear Mater., 449, 101-110, 2014.*

Multiscale Models a
Materials

Simulation, Analytics

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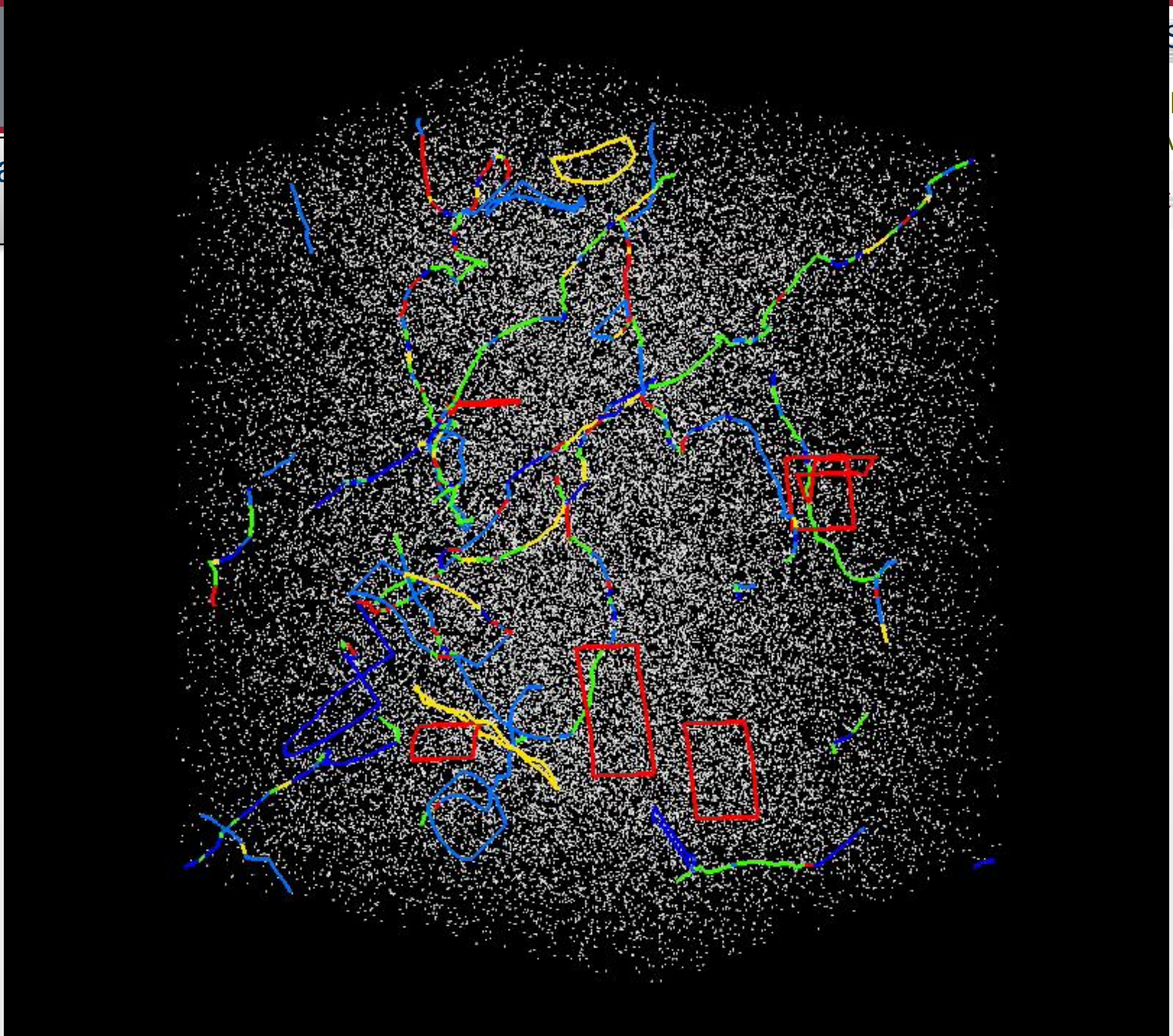


Modeling, Simulation, Analytics

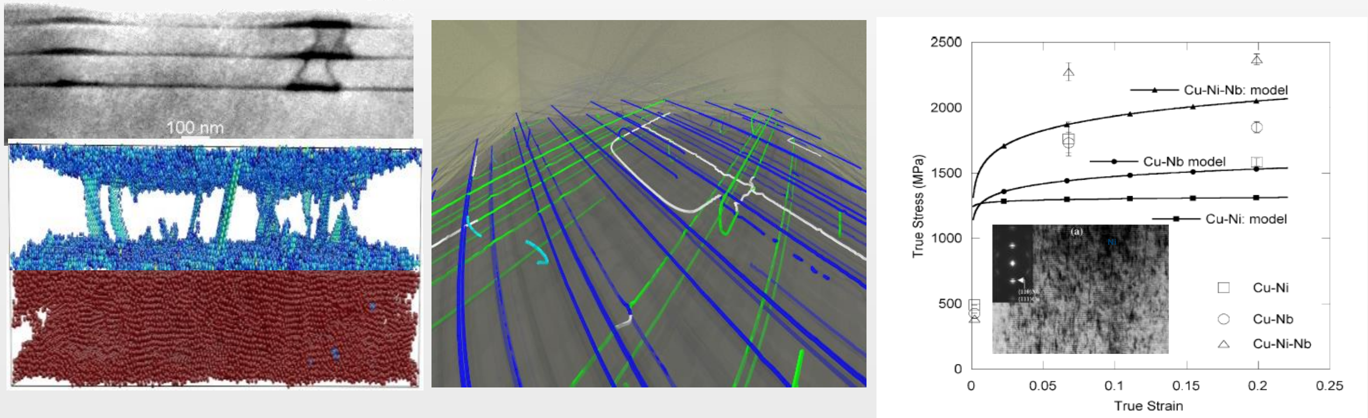
Nuclear Materials

Cross-Cutting

Mulitscale modeling and optimization of advanced interface materials for high energy environments

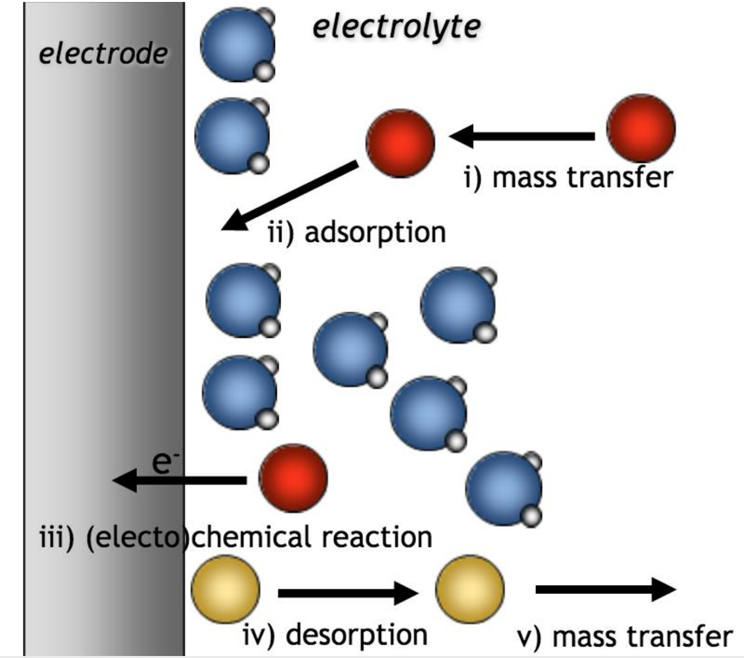
Goal: Design and optimize **N**anolaminate **M**etallic/**M**etallic/**C**eramic (**NMM/C**) structures to enhance the resistance to corrosion, fatigue, and irradiation-induced damage.

Current models are phenomenological, assuming certain deformation mechanisms that are derived from limited empirical data. Multiscale modeling and simulations can reveal the fundamental physics of the deformation mechanisms of NMM/Cs.

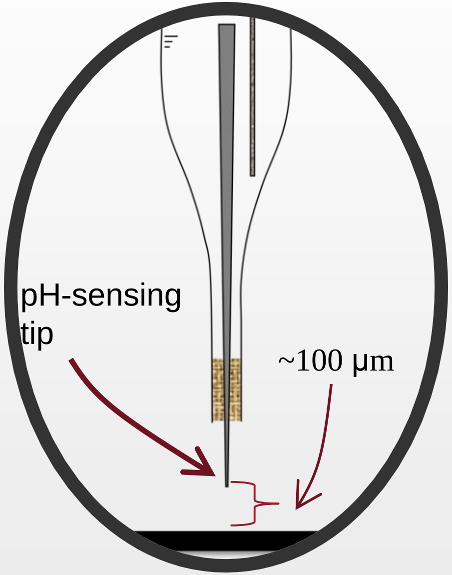


Multiscale simulations (molecular dynamics (left) coupled with large scale discrete dislocation dynamics (middle)) reveal deformation mechanics in NMM's guiding the design of a tri-layer NMM system with improved superior properties (left)). e.g. *Abdolrahim, Zbib & Bahr. Multiscale modeling and simulation of deformation in nanoscale metallic multilayer systems. Int. J. Plasticity, 52, 33-50, 2014.*

Electrochemical reactions for actinide/lanthanide detection



Microelectrodes to monitor processes near surface for modeling



Electrode surface

Transport in electrolyte by Tanja Kallio @ http://slideplayer.com/slide/1625653/