

NMDQi Nuclear Materials Discovery and Qualification Initiative Conference Overview

Robert Allen Roach

March 2020



The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

NMDQi Nuclear Materials Discovery and Qualification Initiative Conference Overview

Robert Allen Roach

March 2020

**Idaho National Laboratory
Idaho Falls, Idaho 83415**

<http://www.inl.gov>

**Prepared for the
U.S. Department of Energy**

**Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517**

NMDQ Nuclear Materials Discovery and Qualification Initiative

R. Allen Roach
Distinguished Staff Scientist
Director of NMDQi
Nuclear Science and Technology Division
Idaho National Laboratory

Email: Robert.Roach@inl.gov



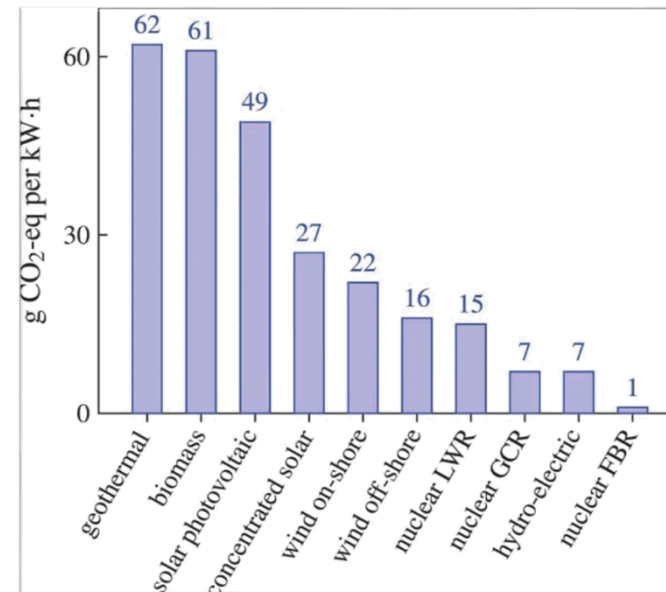
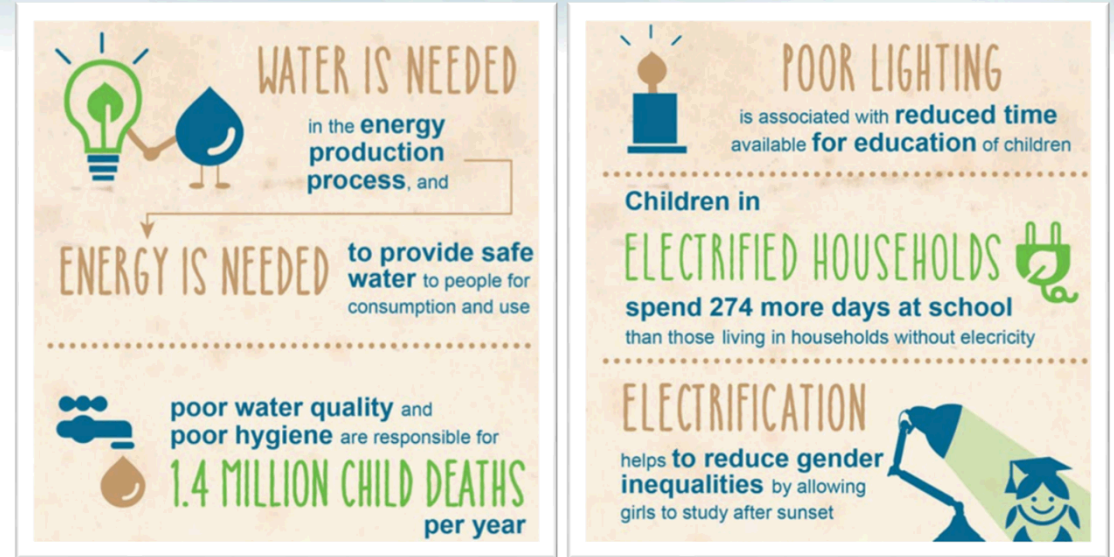
www.inl.gov

NMDQi takes a Grand Challenge approach to accelerate development and qualification of new nuclear materials and fuels for future advanced reactor technologies

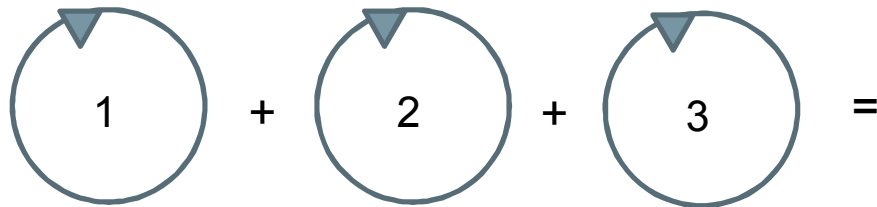
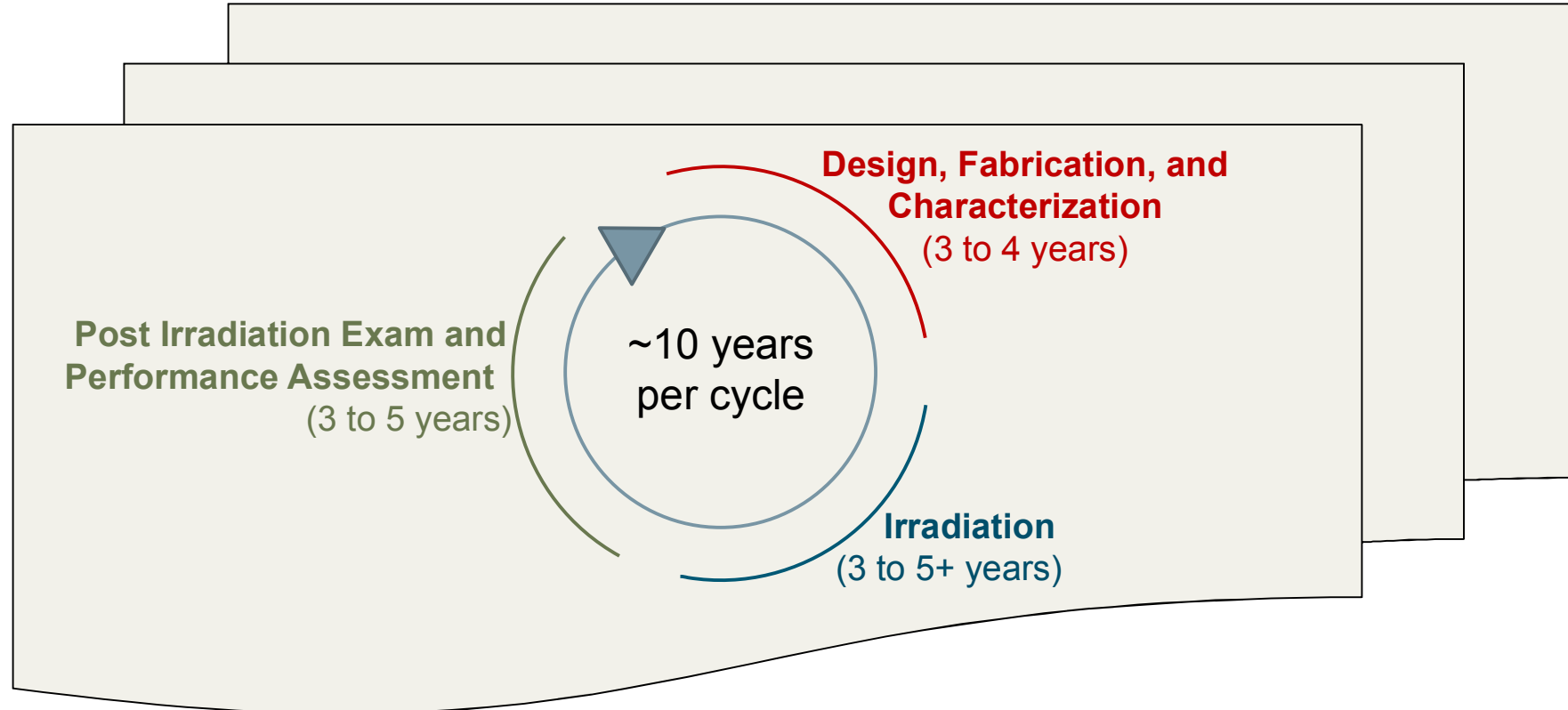
- **NMDQi Mission** is to provide access to cutting-edge tools and knowledge to shorten the time span between concept and material deployment for advanced nuclear reactor design
- Materials Genome Initiative (MGI) for Nuclear materials

First, why nuclear?

- By 2040 the world population is expected to surpass 9 billion people and electricity demand is expected to increase by 93% - UN/UNICEF
- Quality of life is intrinsically linked to power generation
- Education opportunities are directly linked with access to reliable electricity
- Why is nuclear important compared to other energy sources?
- Congress has mandated demonstrations of advanced reactor technology by 2030

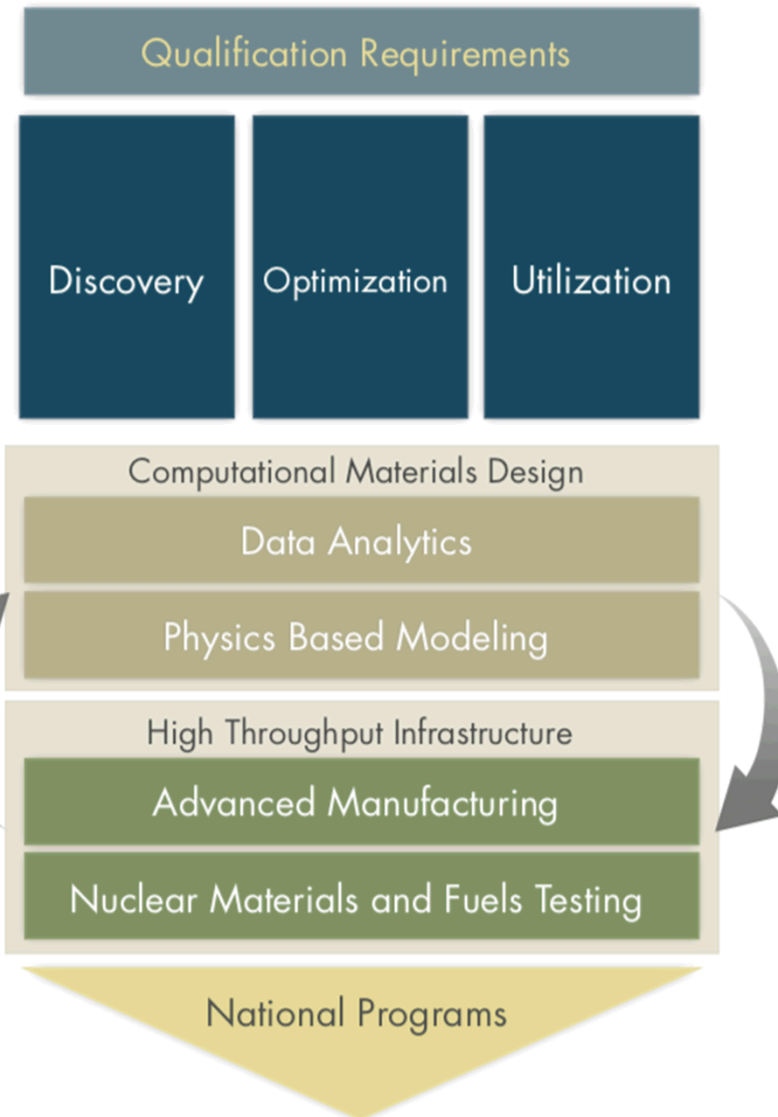


Current Nuclear Materials (e.g. alloys) Development Cycle



Currently a 20-30 year development cycle
Examples: TRISO, HPRR, Metal fuel, advanced claddings, ...

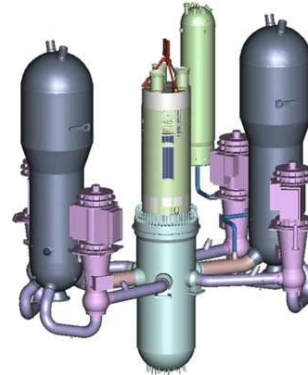
NMDQi Goal = Qualification of New Concepts in a Single Pass



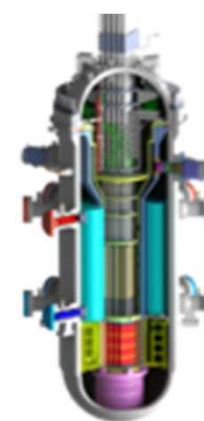
Enabling Technologies and Capabilities:

- **High-throughput material fabrication/characterization** applying advanced manufacturing principles
- **Physics-based M&S** for materials discovery and optimization
- **Data analytics** for machine and deep learning
- **Nuclear material testing** over a wide range of conditions and length scales, including accelerated irradiation testing

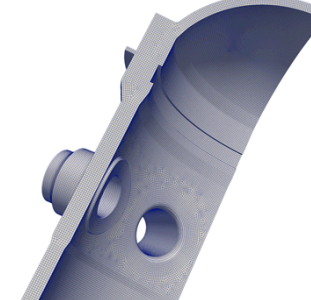
NPP Scale



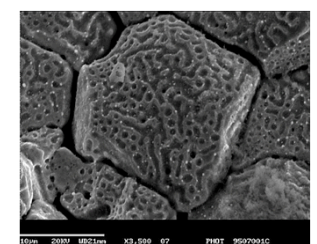
Reactor Scale



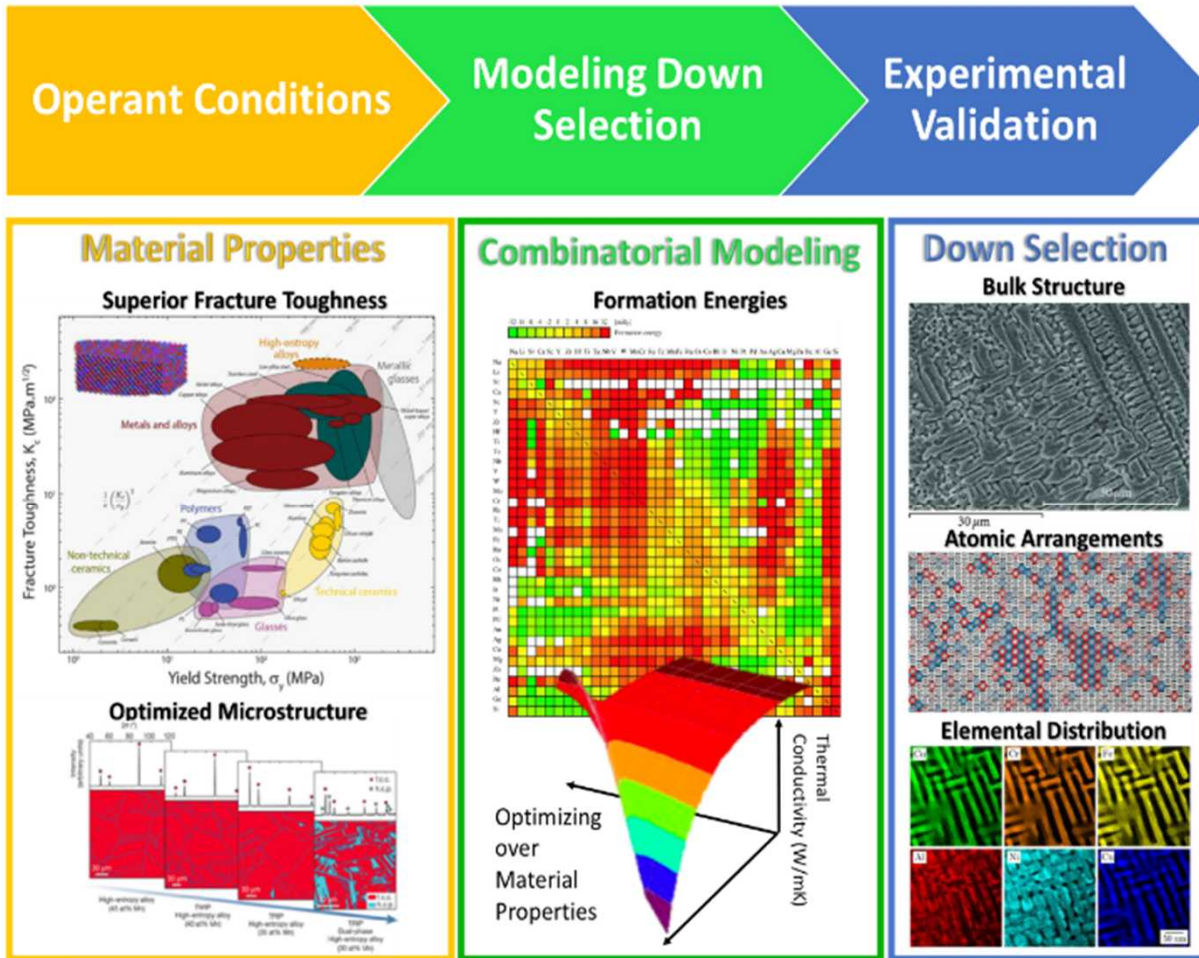
Engineering Materials Scale



Microscale



Supports new materials and pipeline development for high-throughput



- **Targeting** discovery of new alloy classes that are high strength, low cross section, and stable above 400 °C
- **Incorporating** modeling and experimental results in the same workflows to enable training, evaluation, and deployment
- **Establishing** combined modeling and experimental frameworks to shorten the nuclear materials development and research cycle

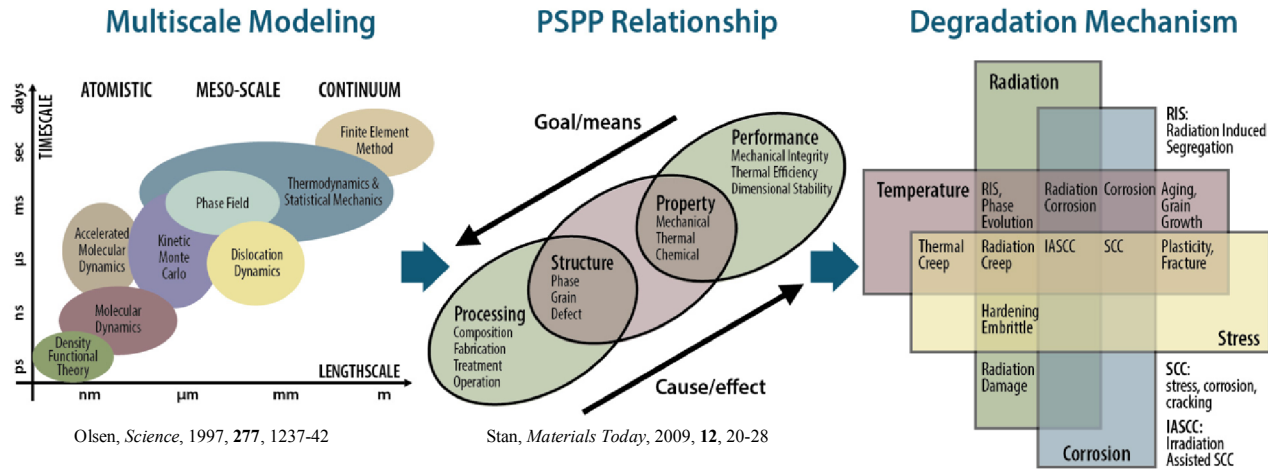
1. Huang, Jen-Ching, *Scanning*, 2012, **34**, 325-31.

2. Z. Li, K. Pradeep, Y. Deng, D. Raabe, and C.C., *Nature*, 2016, **534**, 227-230.

Comput. Sci. Discov., 2009, **2**, 015006

<https://www.rutcm.smm.cam.ac.uk/research-themes/high-entropy-alloys>

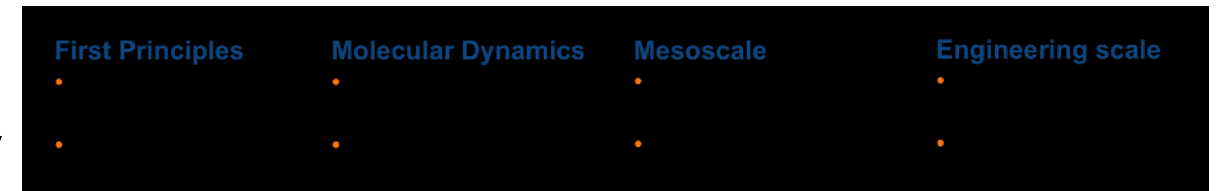
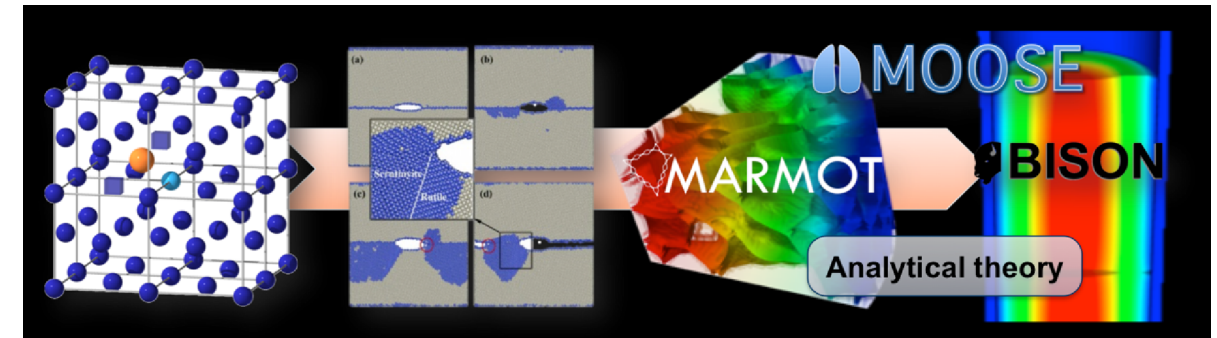
Physics-based Modeling and Simulation



- Understand fundamental behaviors (thermodynamics and kinetics) for predictive capability
- Impact of irradiation (flux) on kinetics – orders of magnitude bridging of length and time scales

Needs:

- Accurate atomistic methods for nuclear materials
- Multiscale, multiphysics modeling
- Efficient scale bridging
- High-throughput modeling for data-driven discovery



Material Testing and Characterization

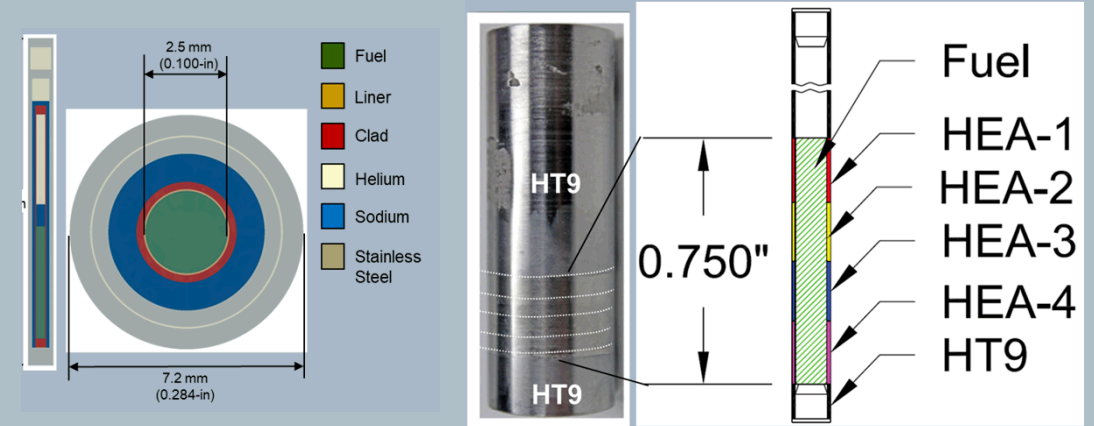
Nuclear facilities capable of supporting high-throughput materials testing:

- HFIR (High Flux Isotope Reactor) (ORNL)
- TREAT (Transient Reactor Test Facility) (INL)
- ATR (Advanced Test Reactor) (INL)

Characterization of nuclear materials not well suited to automated characterization

- Irradiated samples handling requirements
- Specimens can damage sensitive electronic components, precluding loading of multiple specimens
- Heavy shielding and mechanical manipulators makes it slow and difficult to use equipment

Approach to Accelerated Integral Fuel Testing (Fission Accelerated Steady-state Testing)



- Accelerated fuel irradiation test: Up to 10x burnup rate
- Double Encapsulated design facilitates versatile experiment design opportunities
- Improved sensitivities to fabrication eccentricities and variations

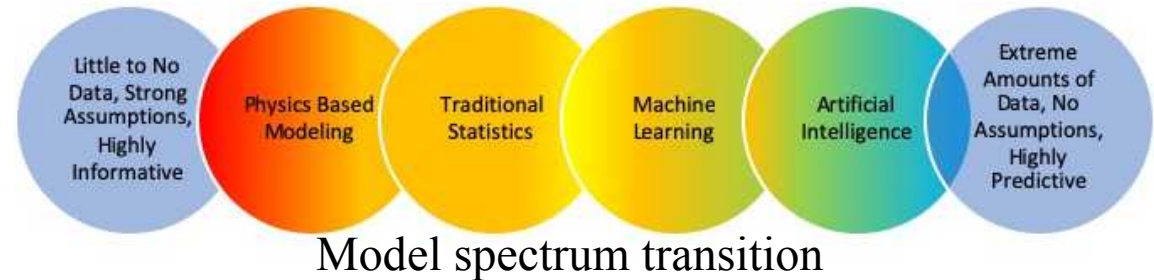
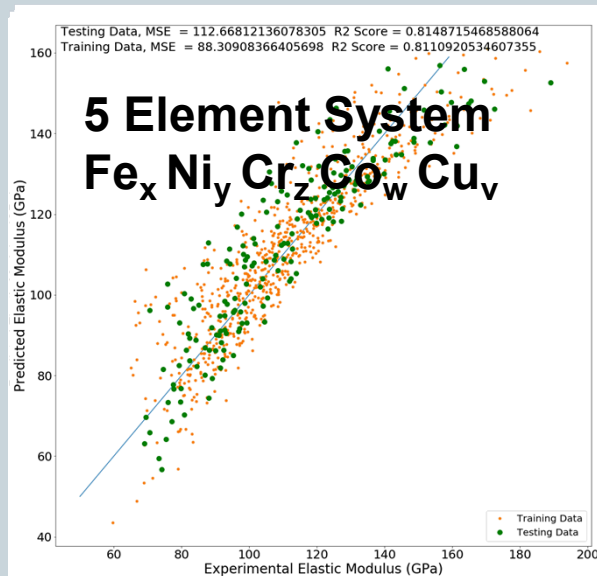
Focus on speed of sample cycling and increasing information from a single sample

Data Analytics for Machine and Deep Learning

- Data analytics efforts will focus on the development and application of a standard database and machine learning techniques to allow predictions of performance
- Must manage the challenge of data scarcity in the process of aiding the discovery and development of new materials
- Integrate with physics-based modeling to drive understanding and prediction with physical meaning
- Define standards for data collection for different techniques to ensure data utility throughout the community and create a common data platform to link data in disparate databases

MPEA Example

Alloy Composition - Property Relationships, Regression to Predict Elastic Modulus

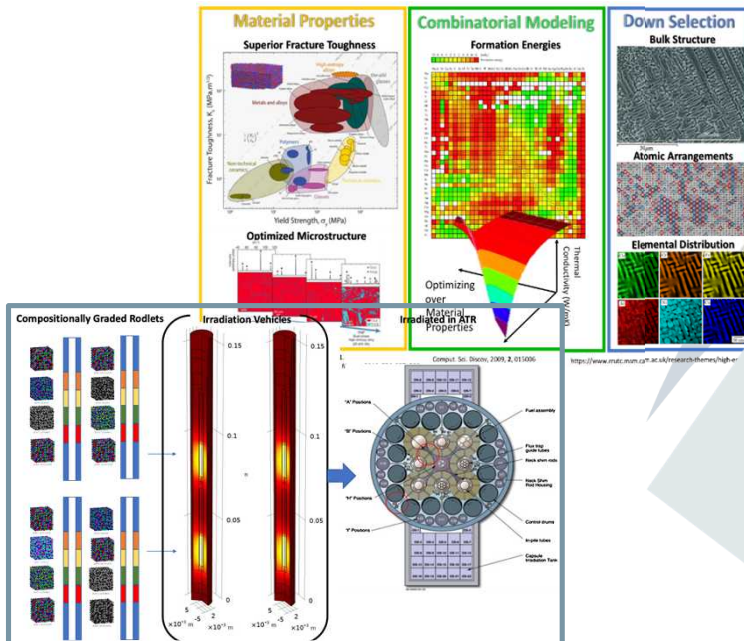


Needs:

- Develop new qualification regime using machine vision / machine learning / physics-based modeling
- Efficient methods of computer vision to classify and quantify microstructures

High-throughput Material Fabrication

- AM is ideal for complex component geometries, prototyping, design flexibility, and rapid turnaround material components
- Effective platform for accessing and assessing alloy compositions, shapes, and potential microstructures to accelerate materials discovery, qualification, and optimization
- Level of process monitoring and control possible with AM is fundamental for quantifying process to enable rapid qualification

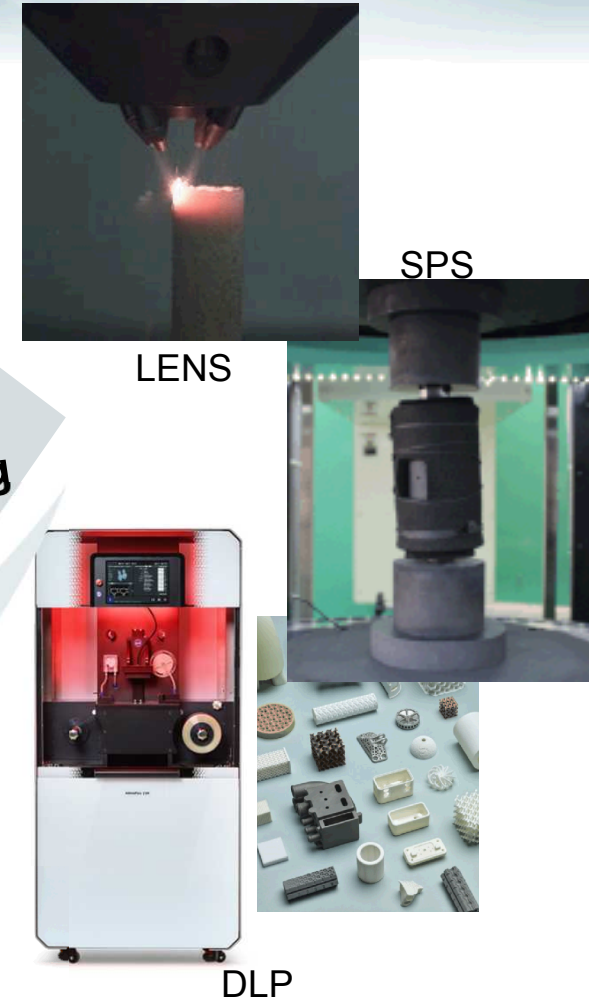


Materials Design

Data Analytics

Advanced Manufacturing

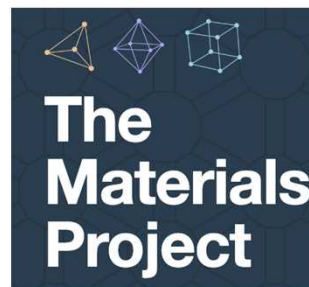
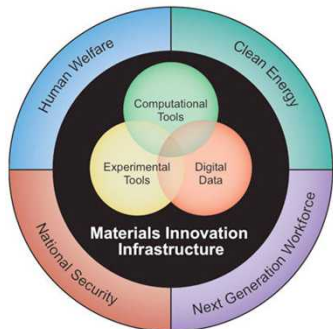
Testing & Characterization



Collaboration is Essential

Internal Working Groups (IWGs)

- Data analytics
- Physics-based modeling
- Advanced manufacturing
- Nuclear Materials and Fuels
Irradiation Testing



CHiMaD

- **Materials Genome Initiative (MGI)-NIST:**
 - **Pioneers** in advancing the agenda on materials informatics for discovery, optimization, and qualification
- **Center for Hierarchical Materials Design (CHiMaD)-Northwestern University:**
 - **Outlining** processing, structure, and properties for nuclear materials
- **Materials Project (MP):** Coordinate on prospective and needs for accessing nuclear materials relevant modeling data
- **University partnerships:** Growing with the NSUF CINR call
- **National Laboratories.**

Thank You!

Further Questions?

Robert.Roach@inl.gov



Idaho National Laboratory