NMDQi Nuclear Materials Discovery and Qualification Initiative

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Apollo Moon Landing


Supersonic X1 Flight


USS Nautilus


EBR-I

“The first step is to establish that something is possible; then probability will occur.”

- Elon Musk

Innovation equates more than the cumulative sum of the individual parts and spurs growth.

Data Analytics

Advanced Manufacturing

Physics Based Modeling

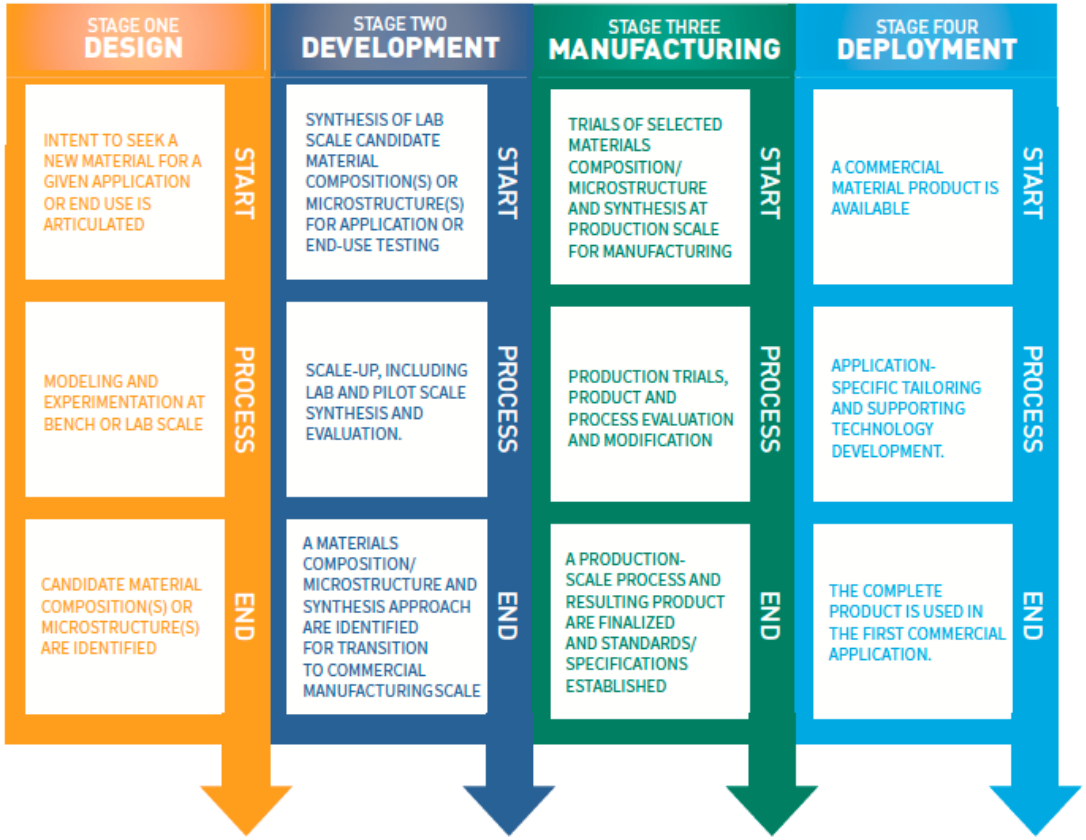
Nuclear Materials and Fuels Irradiation Testing

Computational Nuclear Materials Design

High Throughput Characterization

Where have others been successful?

- **QuesTek Innovations, LLC.** a successful outcome of the **Materials Genome initiative.**
- **Develop and qualify a high strength, lightweight steel** for the hook shank for the T-45 training aircraft where **certification** was **required**.
- **Design to deployment in 8 years** using the materials genome approach.

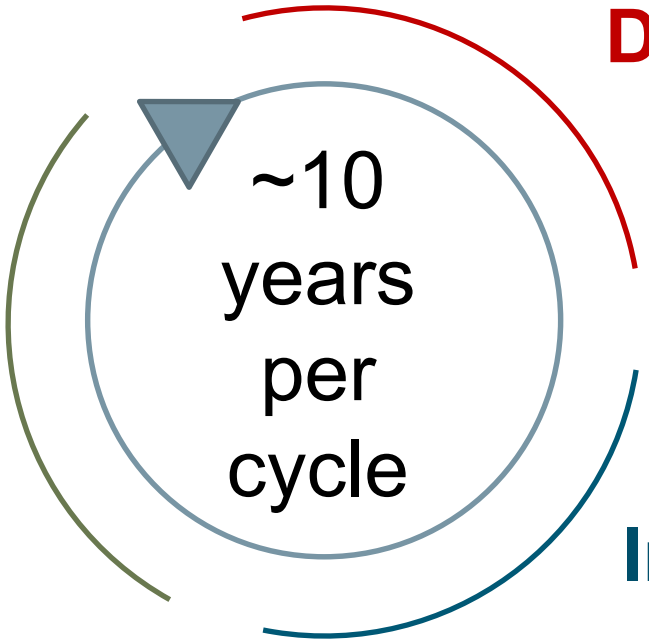


C. J. Kuehmann and G. B. Olson, Material Science and Technology, 2009, **25** (4).

Dave Snyder, Chris Kern, Jeff Grabowski
Aeromat, April 12, 2017, Charleston, South Carolina

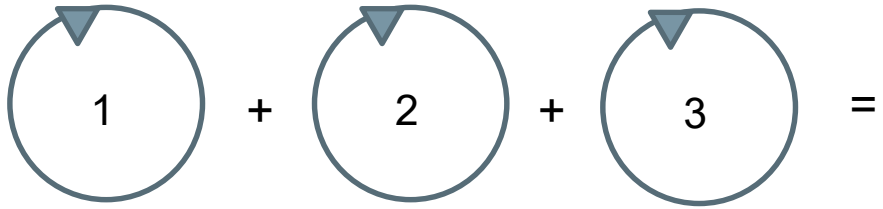
Current nuclear materials (e.g. alloys) development cycle

Post Irradiation Exam and Performance Assessment (3 to 5 years)



Design, Fabrication, and Characterization (3 to 4 years)

Irradiation (3 to 5+ years)



~20 to 30 year development cycle
Example: TRISO, HPRR, Metal fuel, advanced claddings, …

Optimized Approach

Data Analytics & Modeling:
Enabling Materials Discovery and Optimization

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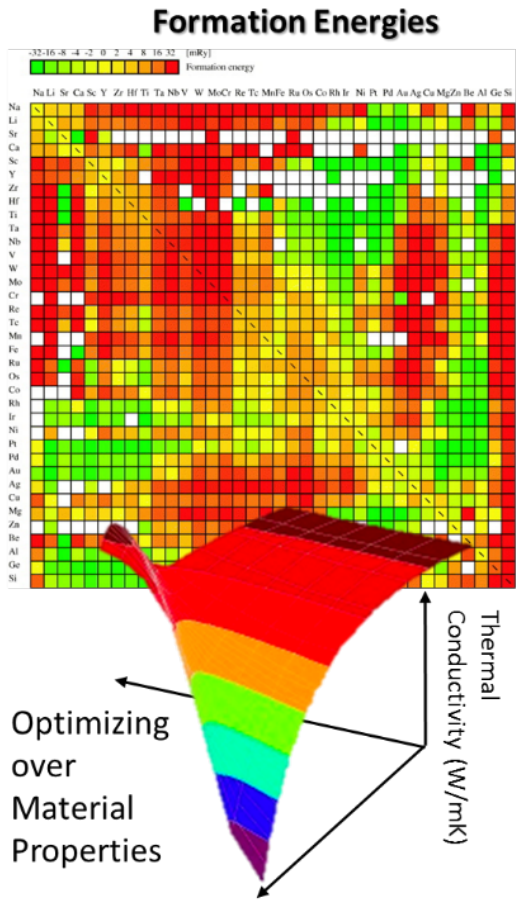
Combinatorial Modeling



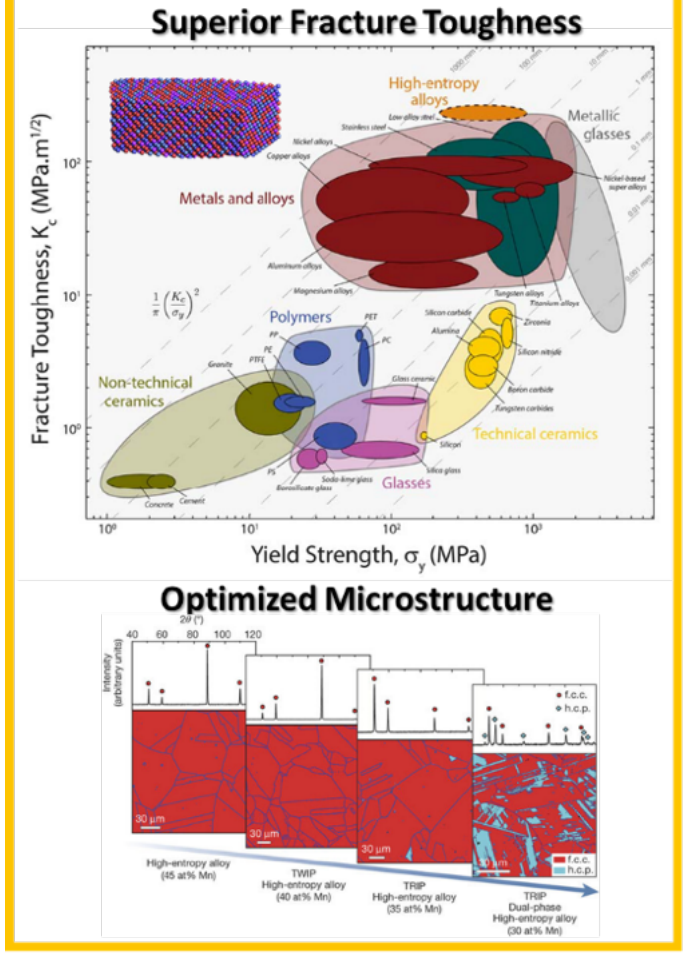
T. R. Munter et. al, Comput. Sci. Discov, 2009, **2**, 015006.

Suggest

Adaptive Engineering

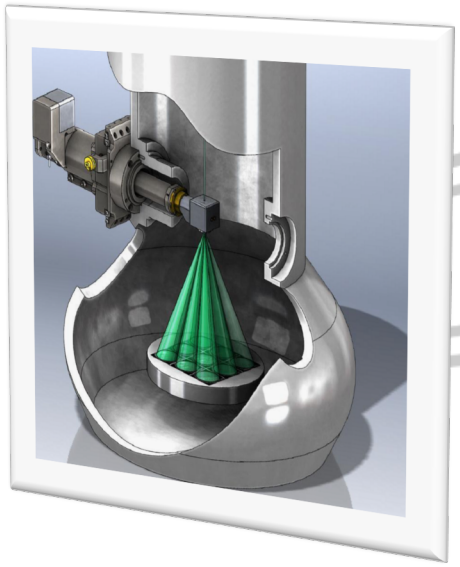
Validate & Augment

Material Properties



Huang, Jen-Chiang, Scanning, 2012, **34**, 325-31.
Z. Li, K. Pradeep, Y. Deng, D. Raabe, and C.C. Nature, 2016, **534**, 227-230.
B. Gludovatz,..., and R. O. Ritchie, Science, 2014, **345**, 1153-1158.

Data Analytics:
Capability for streaming higher throughput materials characterization



INL is advancing the use of deep learning and open materials to characterize and predict crystal structure from datasets in milliseconds.

Aguiar et al. in press, Science Advances, 2019. Funded by INL's LDRD office.

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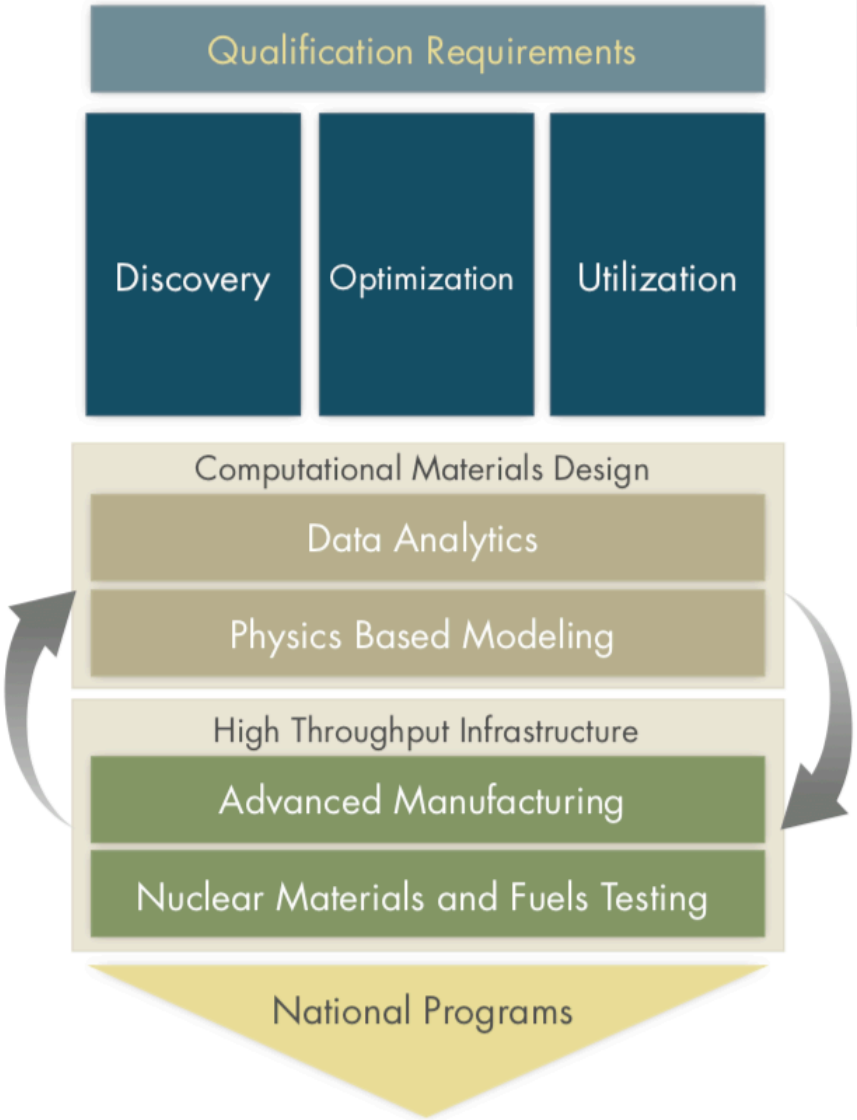


NMDQi takes a Grand Challenge approach to accelerate development and qualification of new nuclear materials and fuels for future advanced reactor technologies.

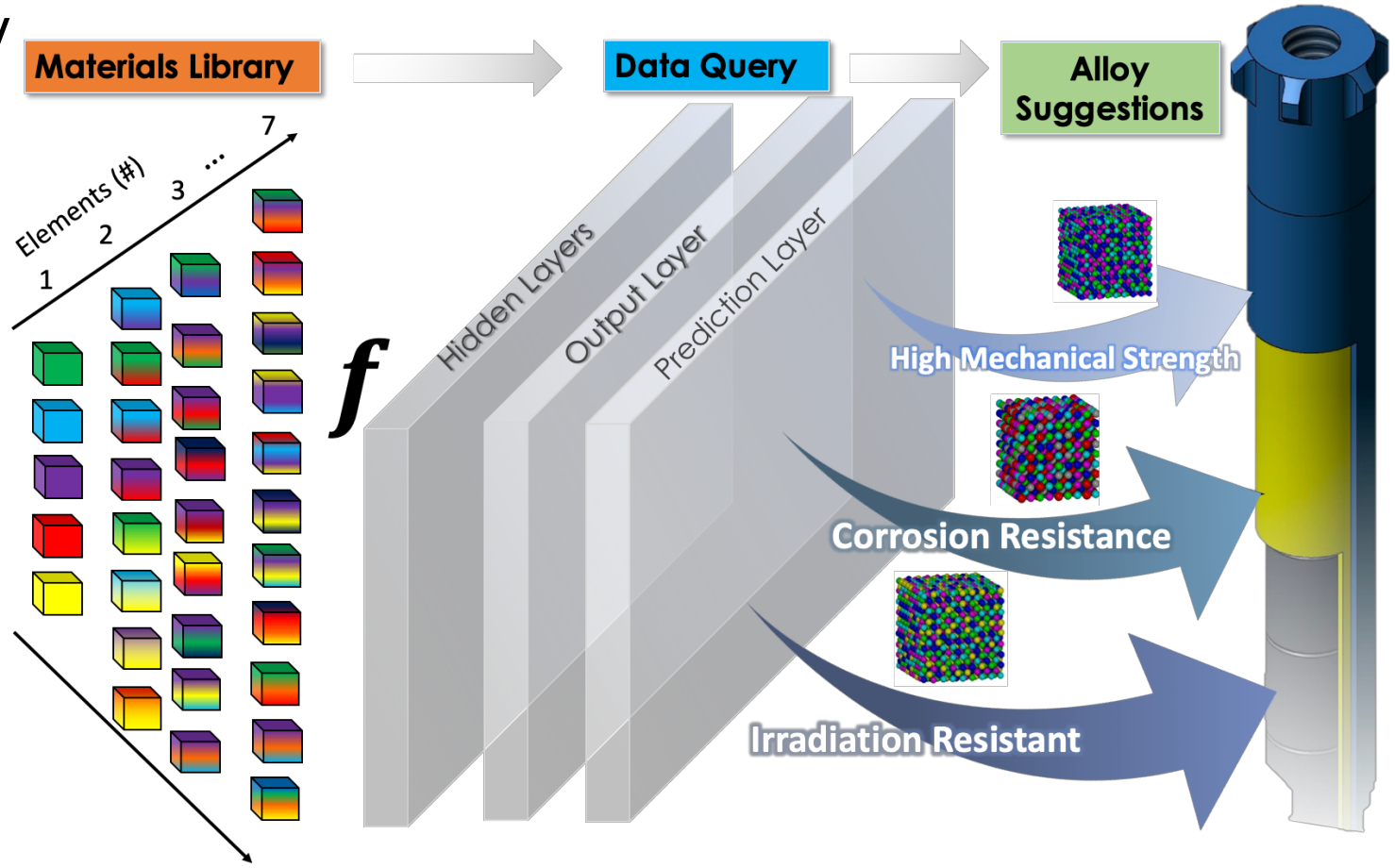
Enabling Technologies and Capabilities:

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

Discovery:

Supports new materials and pipeline development for high-throughput.

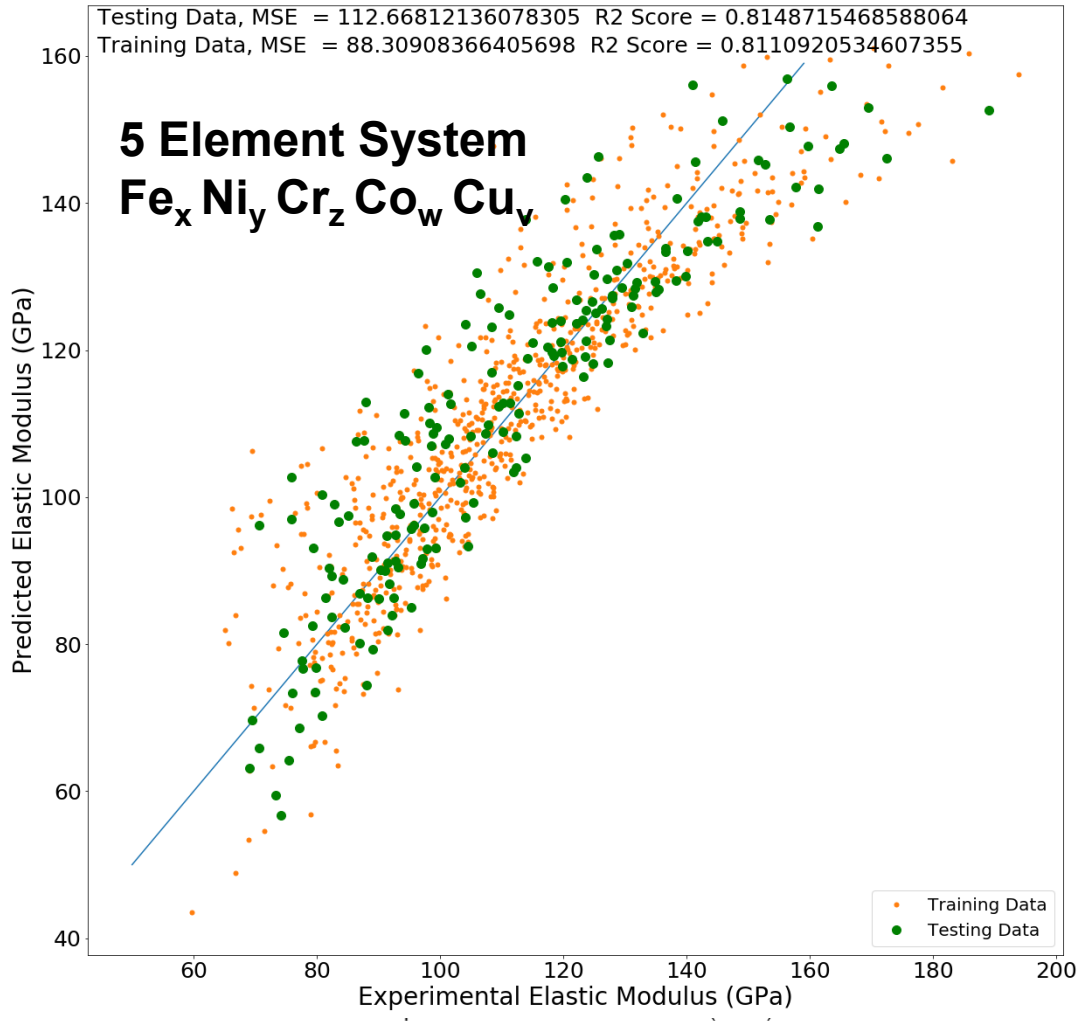
- **Targeting** discovery of new alloy classes that are high strength, low cross section, and stable claddings above 400 °C.
- **Incorporating** modeling and experimental results in the same workflows to enable training, evaluation, and deployment.
- **Establishing** combined modeling and experimental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



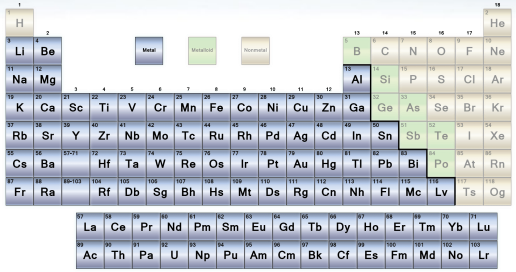
For more information, see poster by Danielle Beatty and Marcus Parry

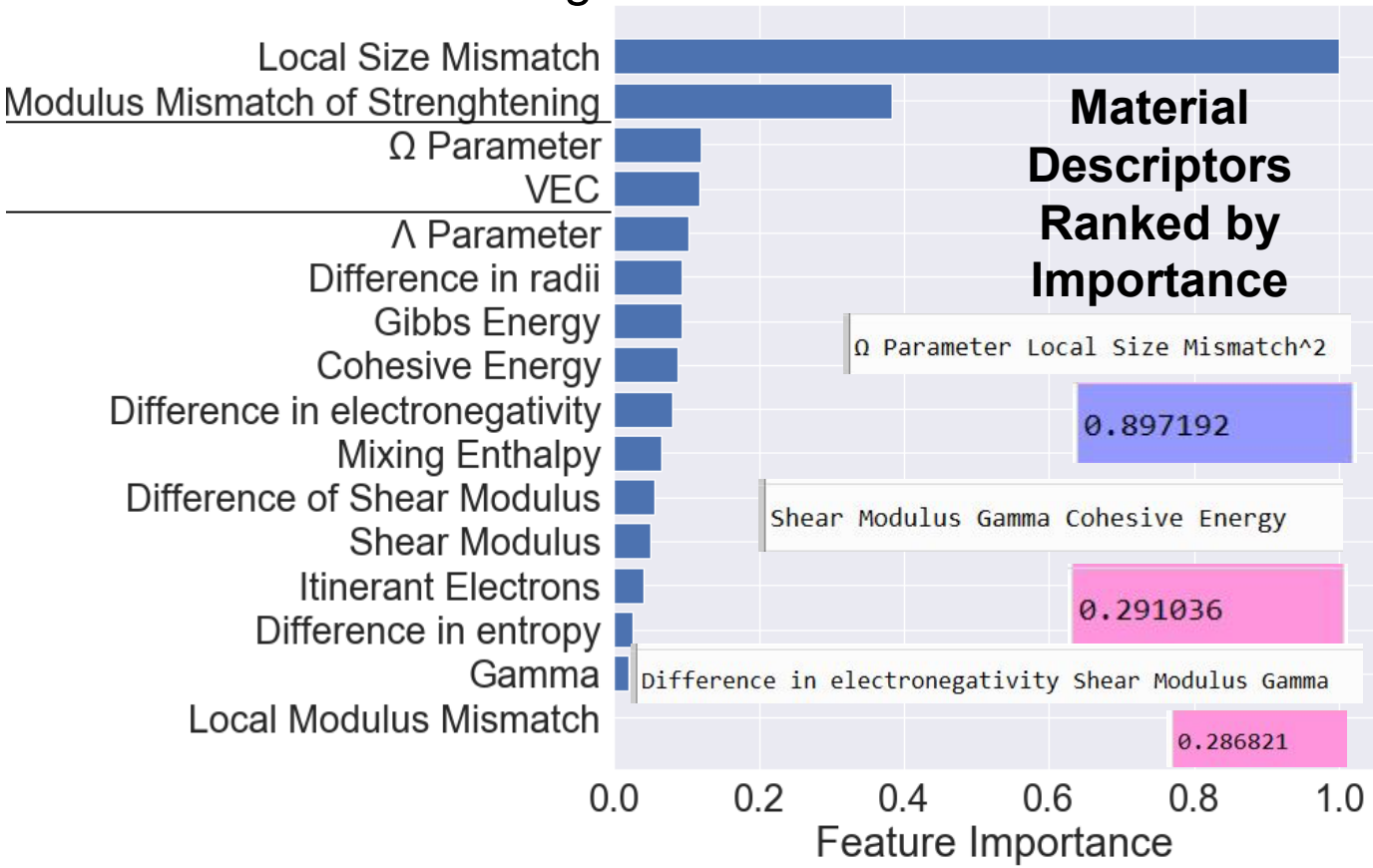
Discovery:
Alloy Composition - Property Relationships

Regression to Predict Elastic Modulus



- **Training & evaluation dataset: <u>30,000</u>+ alloys** containing varying concentrations
- **Down select to 130 alloys** for fabrication and testing



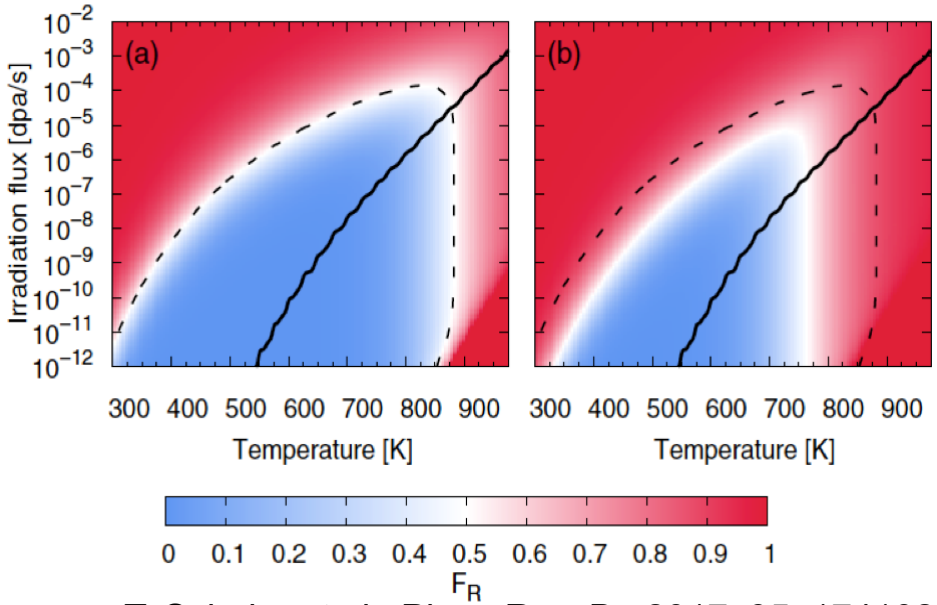


Optimization:
Deploys state of the art design of experiment (DOE) modeling capability to structural materials and fuel development.

Hypothesis: Addition of minor metal additives to 316L stainless steel promotes sluggish diffusion kinetics mitigating irradiation assisted stress corrosion cracking (IASCC).

Model-based Design & Assessment.

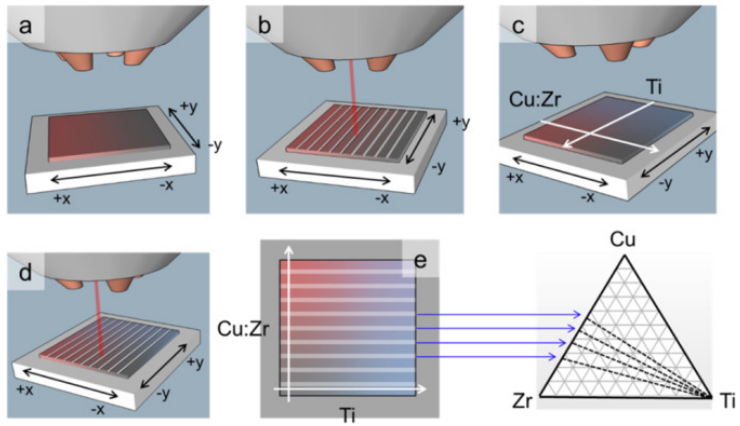
Maximize sluggish diffusion rates over irradiation flux and temperature.



T. Schuler et al., Phys. Rev. B,, 2017, **95**, 174102.

Materials Library Data & Validation.

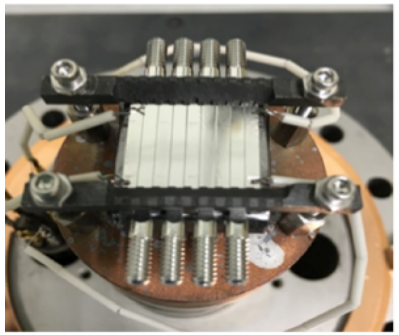
Compositionally-graded samples explore and validate hypothesis.



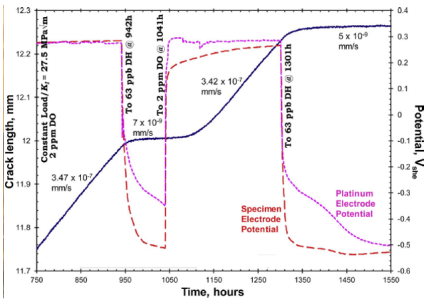
P. Tsai et al. Acta Materialia, 2016, **120**, 426-434.

Testing Assessment.

Proton irradiation



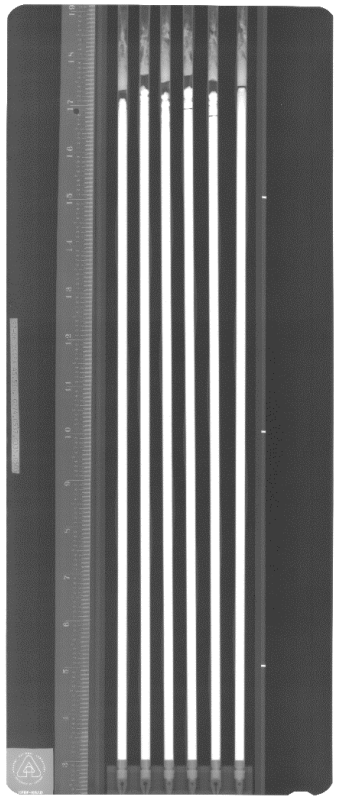
Stress Corrosion Test

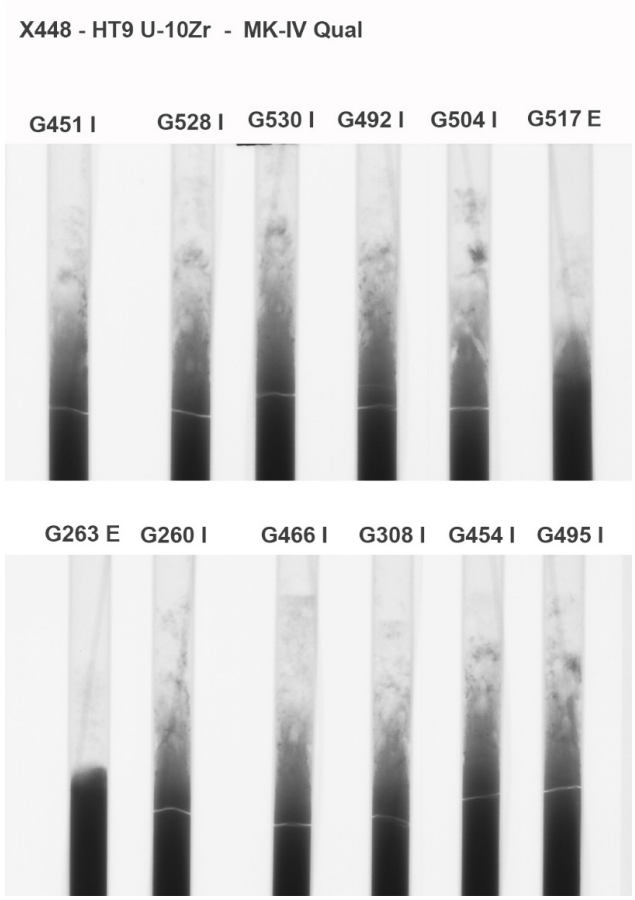


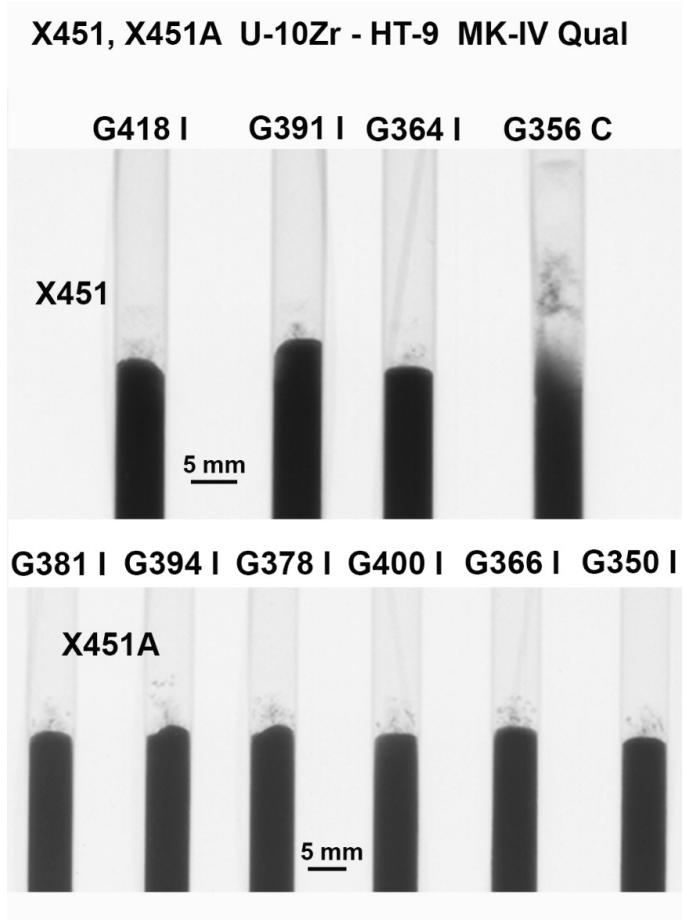
For more information: Daniel.Schwen@inl.gov

Utilization:
Makes use of new and existing sources of data to streamline model development in support of qualification.

For more information:
Doug.Porter@inl.gov







- IFR Materials Information System (IMIS) database **for the legacy** Sodium Fast Reactor (SFR) U-xPu-Zr (0 < x < 28 wgt%), stainless steel cladding.

- **Link to multi-physics modeling and simulation**.

- **Data format must be easily usable by modelers and fuel qualification safety case composers.**

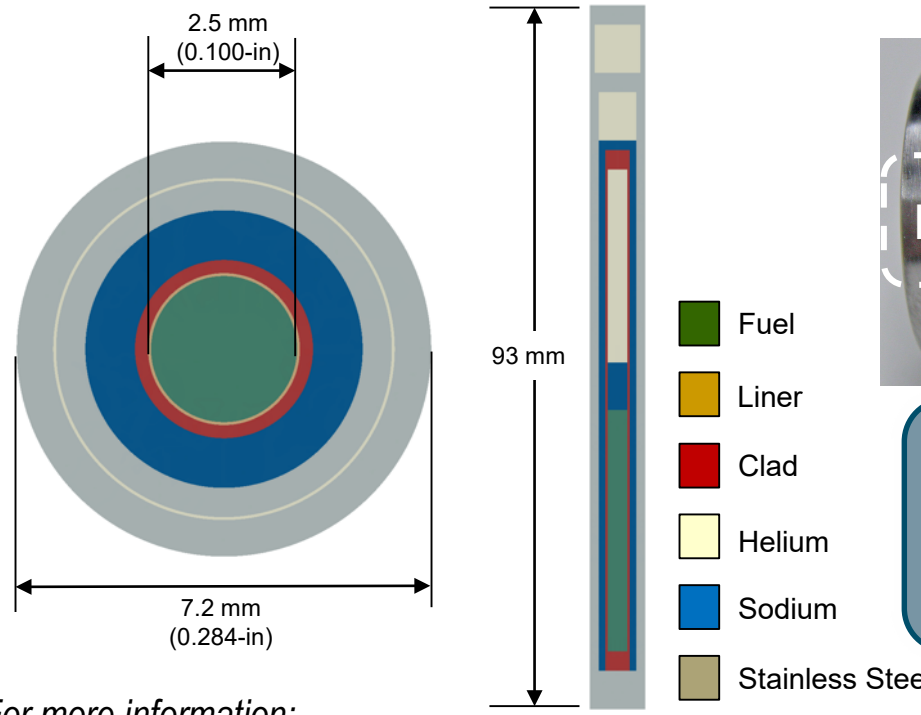
INL is advancing the use of data for model qualification to support accelerated licensing by utilizing unique experimental data from the EBR-II reactor.

Qualification: Accelerated fuel testing platforms
Fission Accelerated Steady-state Testing example

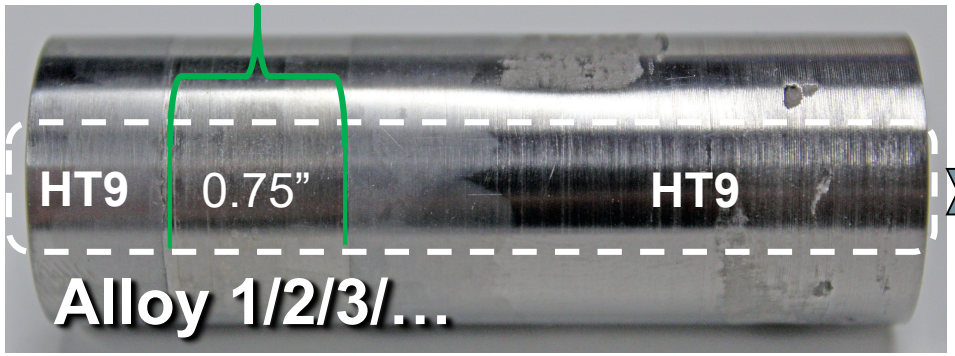
Revised Capsule Design Objectives:

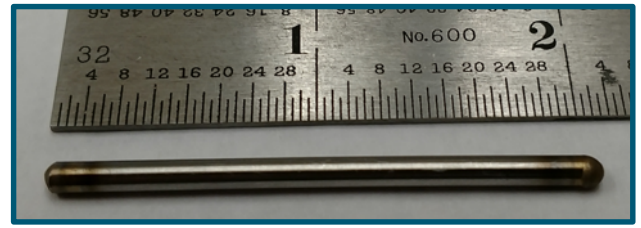
1) Increase power density to reduce time to achieve high burnup
2) Decrease pin diameter to keep peak fuel temperature constant
3) Reduce sensitivity to fabrication tolerances and capsule/pin eccentricity

Fabrication trials for 1/2- and 1/3-scale fuel and rodlets is underway



Semi-integral Irradiation Test Zone





One-third diameter pins could achieve >5% burnup in ATR 55-day cycle and **achieve 30% burnup in less than 2 years.**

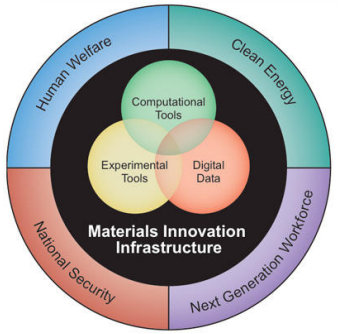
For more information:
Geoffrey.Beausoleil@inl.gov

For more information, see poster by Geoffrey Beausoleil

Collaboration is Essential

Internal Working Groups (IWGs)

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



The Materials Project

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.**

Intersecting Opportunities

Qualification

- ***Requires a frameworks focus*** *on comprehensive approaches to licensing using qualified model development, qualification by performance and/or code qualification for new suggested fabrication and testing methodologies.*

Advanced Reactors

- ***Demonstrate early on new advanced materials and supply chains*** *that expand on U.S nuclear innovation leveraging advances in high-throughput materials and data frameworks.*

Fleet Sustainment

- ***Develop materials and applied technologies*** *that enables sustainment and demonstrate new methods for materials deployment.*

Thank You!

Further Questions?

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