GA-A29408
ORNL/LTR-2020/1668

ACCELERATED FUEL QUALIFICATION (AFQ) WORKSHOP II SUMMARY REPORT

Prepared Under
Contract DE-NE0008819
And
Contract DE-NE0008831

Presented January 16, 2020

Complied By
R. Faibish
General Atomics

GENERAL ATOMIC PROJECT 30543
NOVEMBER 2020

GENERAL ATOMICS

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FOREWORD

The files contained in this report are the compilation of all materials pertaining to the second workshop on Accelerated Fuel Qualification (AFQ): AFQ Workshop II. The overall goal of the workshop was to discuss progress since the first workshop in May 2019 in developing the enabling computational and experimental AFQ building blocks, as well as to agree on next steps in advancing the AFQ methodology and its implementation.

1 BRIEF OVERVIEW

The second AFQ workshop, AFQ Workshop II, was held on Thursday, January 16, 2020, in Washington, DC, with 29 participants from industry (General Atomics, Framatome, Lightbridge, TerraPower, Westinghouse), national labs (ANL, INL, LANL, ORNL), DOE-NE, NRC, as well as two aerospace companies who are supporting NASA (Aerospace Corporation and Analytical Mechanics Associates). **The main goal of the workshop was to discuss progress since the first workshop in May 2019 in developing the enabling computational and experimental AFQ building blocks and agree on next steps. A draft of the AFQ Working Group Charter was also reviewed and changes agreed to.** There were 12 presentations given during the workshop, which included overview presentations, information on status of AFQ building computational and experimental building blocks, case studies, and a concluding presentation on NRC perspectives.

2 WORKSHOP AGENDA

Morning Session:

Topic	Presenter	Start	End	Duration
Welcome and Workshop Introduction				
First AFQ Workshop Recap	Ron Faibish (General Atomics)	8:30 am	8:45 am	15 min
Roadmap to Accelerated Fuel Qualification	Mark Adams (General Atomics)	8:45 am	9:20 am	35 min
Fundamental Computational, Experimental, and Theoretical Building Blocks				
High energy heavy ion irradiation for accelerated testing	Abdellatif Yacout (ANL)	9:20 am	9:50 am	30 min
Fission Accelerated Steady-state Testing (FAST) in Nuclear Fuel Development	Matthew Kerr (INL)	9:50 am	10:20 am	30 min
BREAK (10:20 am - 10:45 am)				
Integrating Building Blocks and Bridging Multi-Scale Phenomena				
Overview of a process to develop and identify regulatory	Pete Gaillard (TerraPower)	10:45 am	11:15 am	30 min

Topic	Presenter	Start	End	Duration
requirements and design criteria applicable to metallic fuel				
Nuclear Fuel Applications and Case Studies				
Fuel performance simulations of swelling, fission gas release and creep in U3Si2 informed by atomistic simulations	David Andersson (LANL)	11:15 am	11:45 am	30 min
TCR fuel design and development towards qualification	Kurt Terrani (ORNL)	11:45 am	12:15 pm	30 min
LUNCH (12:15 pm - 1:15 pm)				

Afternoon Session:

Topic	Presenter	Start	End	Duration
Nuclear Fuel Applications and Case Studies (Continued)				
Using statistical uncertainty analyses to determine the importance of irradiation effects on TRISO fuel and materials properties	Madeline Feltus (US DOE-NE)	1:15 pm	1:45 pm	30 min
Case study illustrating how building blocks are applied and the direction TerraPower is moving	James Vollmer (TerraPower)	1:45 pm	2:15 pm	30 min
Energy Multiplier Module (EM^2) accelerated fuel qualification strategy	John Bolin (General Atomics)	2:15 pm	2:45 pm	30 min
Lower Length Scale Modeling Examples	Kallie Metzger (Westinghouse)	2:45 pm	2:55 pm	10 min
BREAK (2:55 pm - 3:10 pm)				
Regulatory Discussion				
NRC input and terminology conversation	Christopher Van Wert (US NRC)	3:10 pm	3:40 pm	30 min
AFQ Technical Working Group Charter Discussion				
Open Discussion	Ron Faibish-Moderator (General Atomics)	3:40 pm	4:30 pm	50 min
Future Actions				
Open Discussion	Ron Faibish - Moderator (General Atomics)	4:30 pm	5:00 pm	30 min
ADJOURN (5:00 pm)				

3 DISCUSSION AND KEY TAKEAWAYS

1. Participants of the AFQ Working Group (WG) agreed that the main premise of the AFQ methodology remains that modeling and experiments should be simultaneously exploited to reduce years of data that would otherwise be required for deployment of new nuclear fuels.
2. Case studies were presented that further demonstrated modeling and experimental tools development to advance and accelerated approach to fuel qualification by coupling the two.
3. The WG agreed that fuel qualification needs to be carried out with a specific reactor design and related safety case in mind.
4. The NRC is seeking input from the team, as part of the public in general, on a key fuel qualification-related congressional requirement in the Nuclear Energy Innovation and Modernization Act (NEIMA) (January 2019) legislation. The specific relevant ask in the bill is as follows:

   "Report required. –Not later than 30 months after the date of enactment of this Act, the Commission shall submit to the appropriate congressional committees a report… for-- (B) ensuring that the Commission has adequate expertise, modeling, and simulation capabilities, or access to those capabilities, to support the evaluation of commercial advanced reactor license applications, including the qualification of advanced nuclear reactor fuel."

The NRC plans to submit the report to Congress by January 2021. The AFQ WG is planning to provide consolidated input to the NRC before their white paper is due to Congress.

4 NEXT STEPS

1. Plan for the third AFQ workshop (AFQ Workshop III) in the late fall 2020 timeframe, with an agenda aimed to follow up on items listed in the takeaways above and any new items as they arise leading to the third workshop.
2. Finalize the AFQ Working Group Charter.
3. Discuss AFQ White Paper outline and drafting assignments.

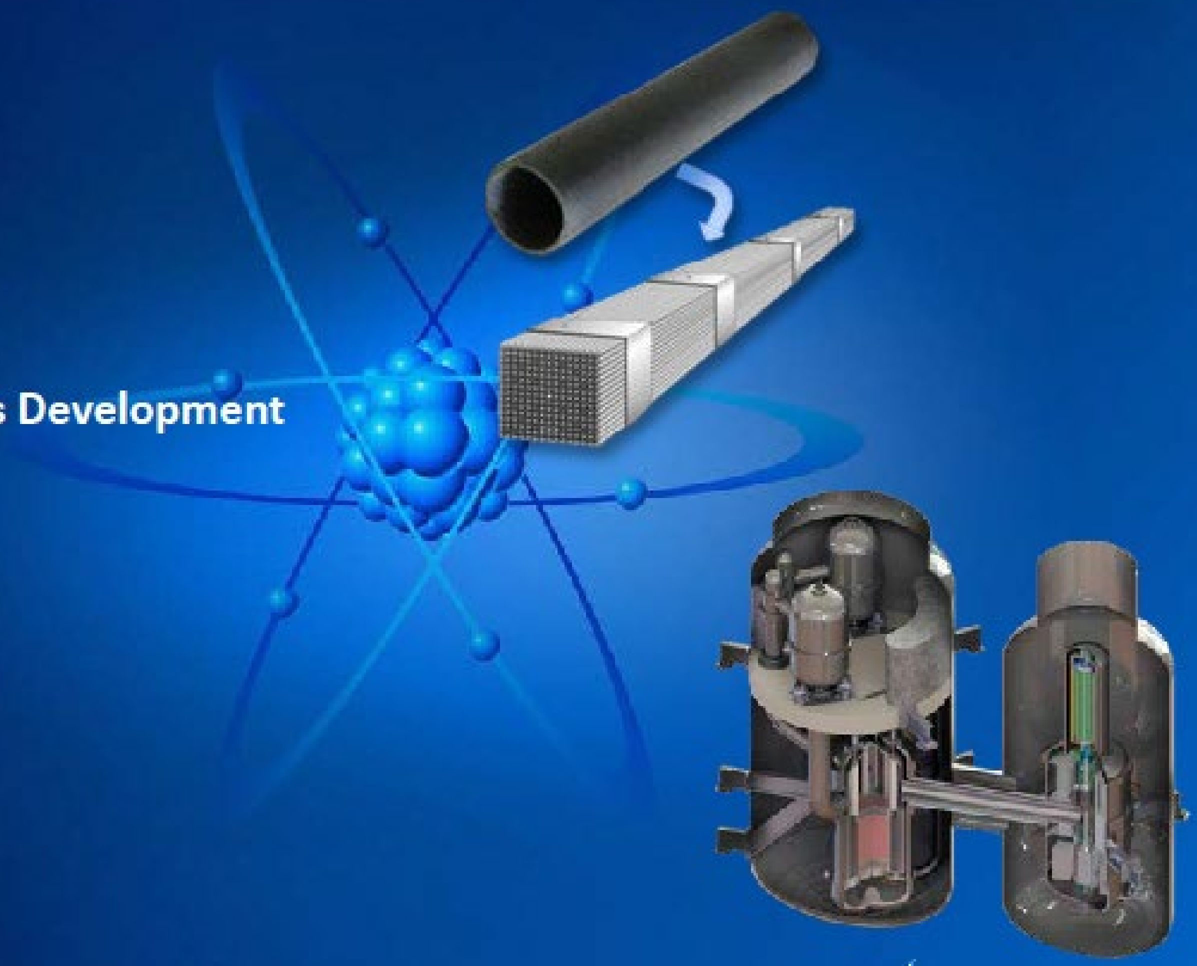
APPENDIX A - AFQ – First Workshop Recap

Accelerated Fuel Qualification (AFQ): First Workshop Recap

By
Ron S. Faibish, Ph.D.

Sr. Director of Business Development
General Atomics

January 16, 2020



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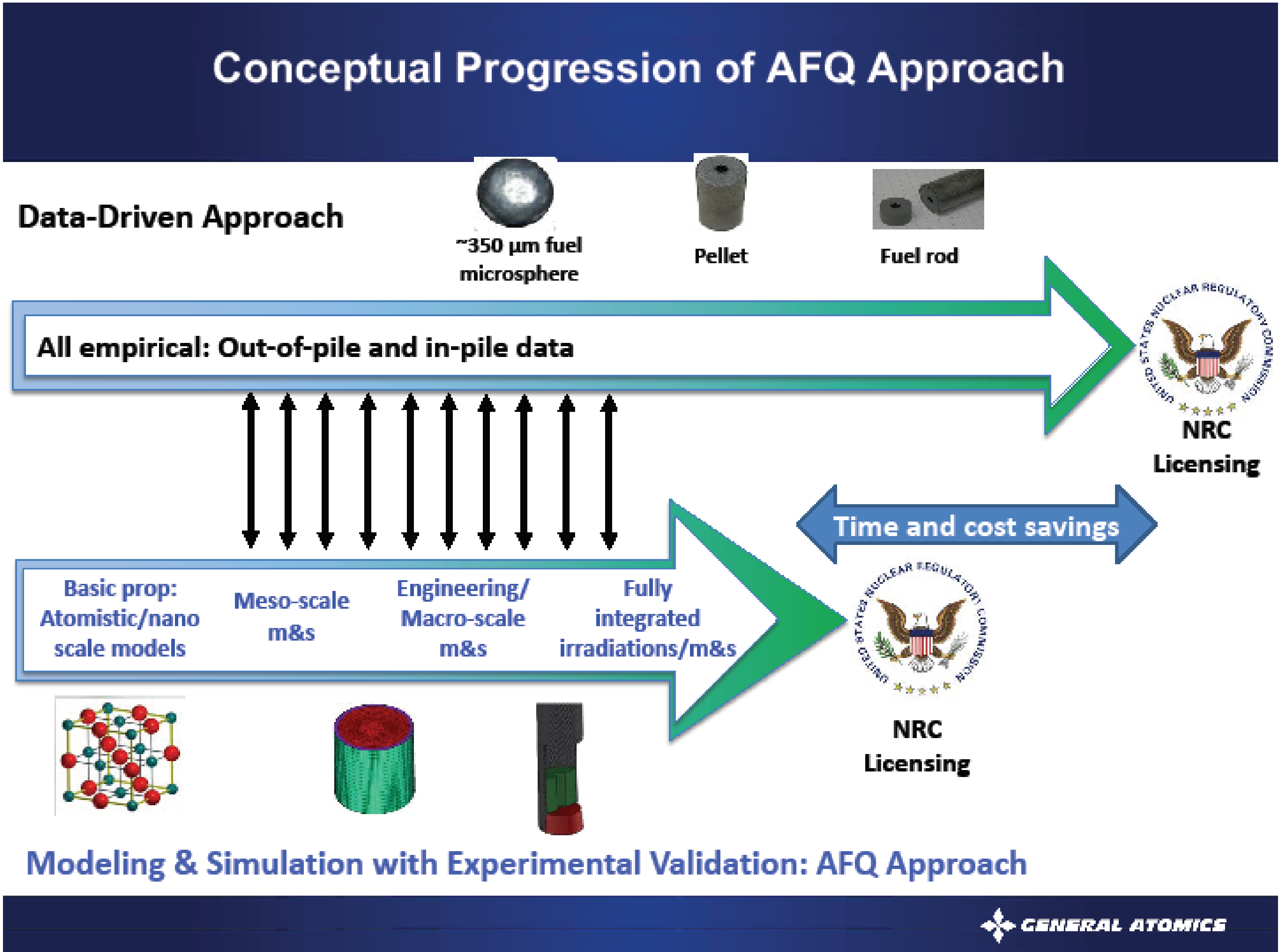
The Proposition

Modeling and experiments must be simultaneously exploited to markedly reduce the years of data that would otherwise be required for deployment of new nuclear fuels.


Conceptual Progression of AFQ Approach
Data-Driven Approach
~350 µm fuel microsphere
Pellet
Fuel rod
All empirical: Out-of-pile and in-pile data
NRC Licensing
Time and cost savings
Basic prop: Atomistic/nano scale models
Meso-scale m&s
Engineering/ Macro-scale m&s
Fully integrated irradiations/m&s
NRC Licensing
Modeling & Simulation with Experimental Validation: AFQ Approach
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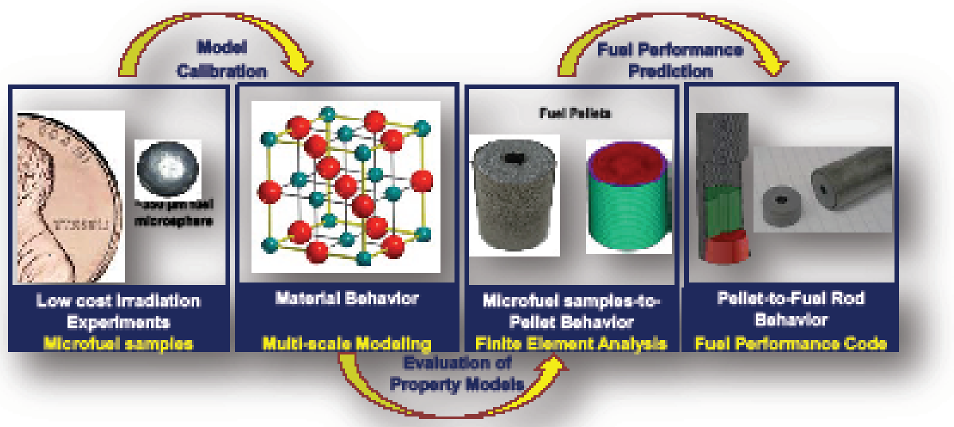
A Key Enabler: Accelerated Fuel Qualification (AFQ)

AFQ Defined:

The combination of microstructurally-informed advanced nuclear fuel performance modeling and simulation (M&S) tools with targeted irradiation and other select experimental data that can significantly reduce the cost and number of irradiation experiments and, ultimately, the cost and time associated with new fuel qualification.



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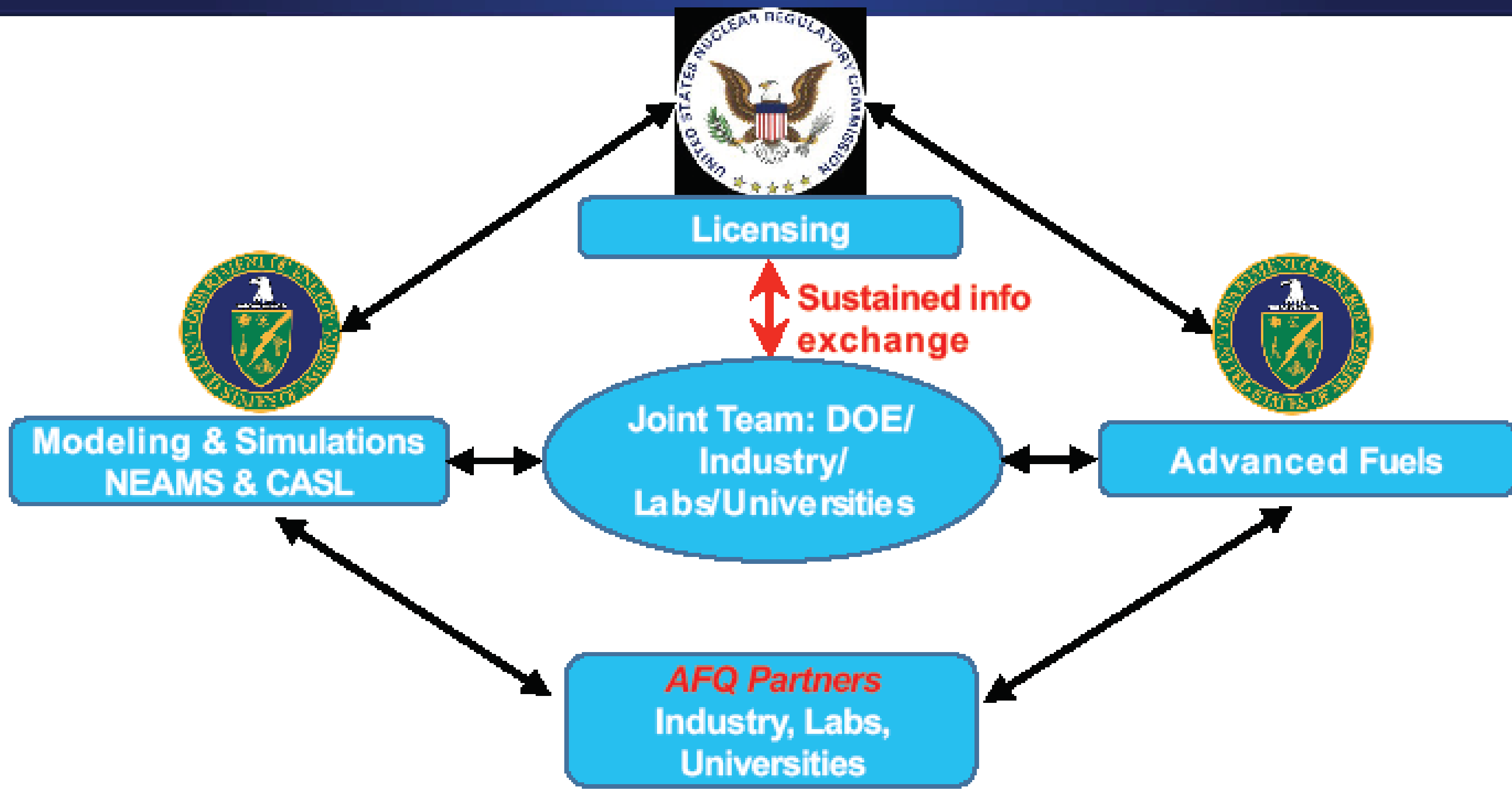
AFQ Working Framework and Key Stakeholders: Making It All Happen



Building a coalition of partners with DOE's overall coordination

Key Take-Aways from First Workshop (I)

- Significant advancements in computational power and tools in the recent years have enabled the increasingly accurate prediction of material properties and behavior from basic principles through complex meso and engineering scale phenomena.

- AFQ methodology has the potential to reduce the high number of new nuclear integral tests that are required to qualify new fuels while maintaining the highest safety standards and requirements.

- All participants strongly agree that the AFQ methodology in no way will substitute the need for integral fuel testing.

Key Take-Aways from First Workshop (II)

- Uncertainties associated with any computational techniques to model or simulate material properties and/or behavior need to be quantified and their implications on validity of m&s results assessed.

- Technical Working Group (TWG) should be established that would be charged with furthering the development and applicability of the AFQ methodology.

- NRC recommended linking any AFQ-related fuel work to safety analysis activities of the reactor system as a whole (i.e., a holistic approach to safety analysis).

Summary and Next Steps

Summary Statement: An agreed-to methodology provides guidance to industry on the path needed to qualify new materials and technologies in an expeditious way that incorporates modeling and simulation with experiments.

Next Steps:

- Plan for a follow up workshop in the fall 2019 timeframe.
- Establish the AFQ Technical Working Group. This could be discussed and agreed upon in the next workshop meeting.

Agenda: Morning Session

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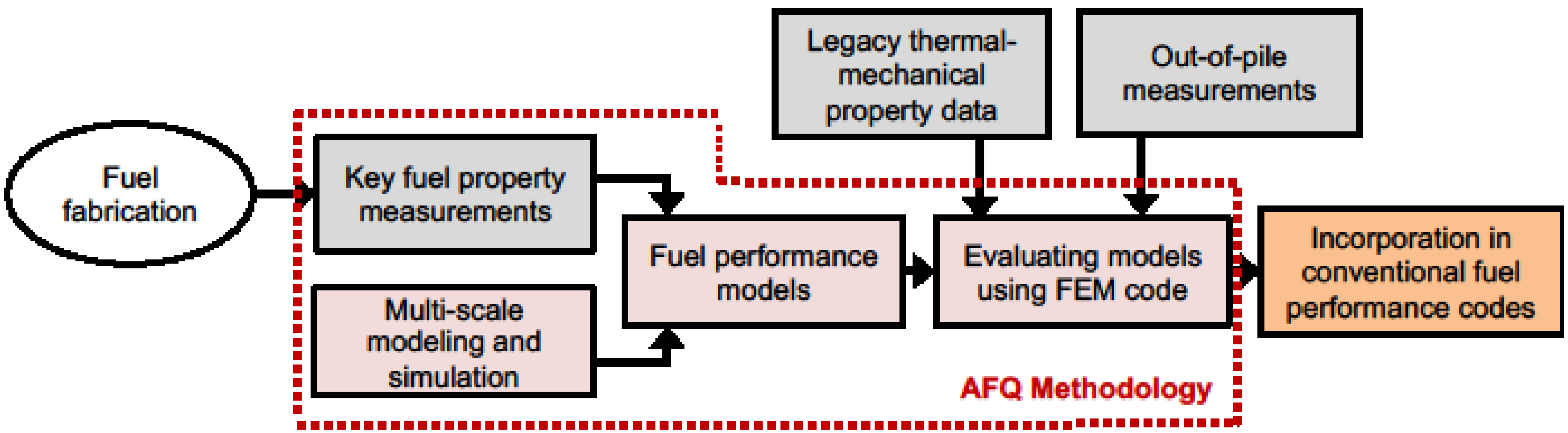
ADJOURN (4:45 pm)				

Transition of Advanced M&S Capabilities into Usable Engineering Tools



APPENDIX B - Roadmap to Accelerated Fuel Qualification

Roadmap to Accelerated Fuel Qualification

By
Mark L. Adams, Ph.D.
Director of Special Programs
General Atomics

Presented at the
Accelerated Fuel Qualification Workshop 2

16 January 2020

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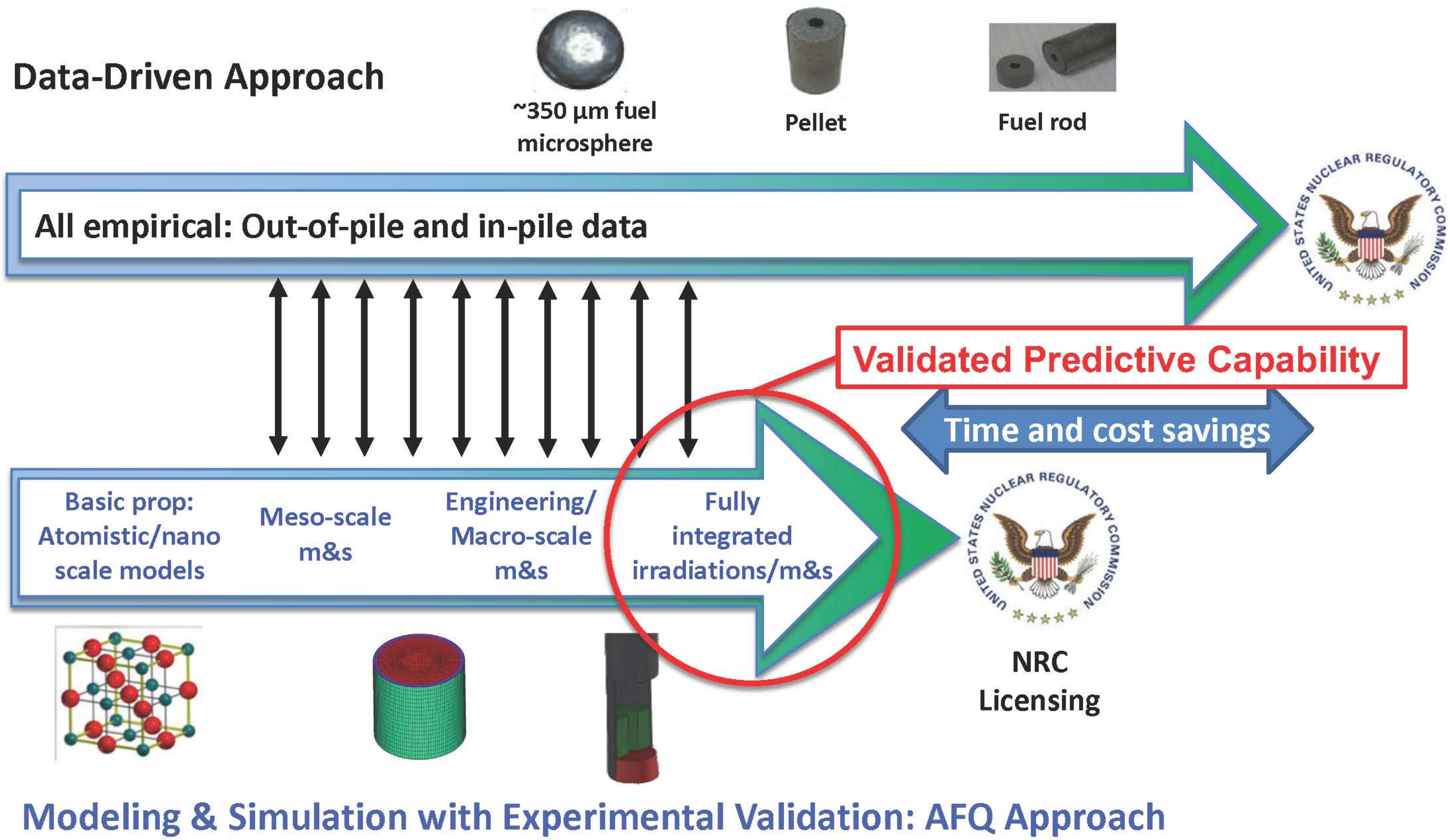
Roadmap to Accelerated Fuel Qualification

- **Build on the, "Conceptual Progression of AFQ Approach"**
- **Validated Predictive Capability**
  - Building blocks
  - Coupling multi-physics phenomena
  - Bridging multi-scale phenomena
- **Performance Risk Management**
  - Systems Engineering
  - Risk Analysis
- **AFQ Workshop 2 Opening Comments and Agenda**

Conceptual Progression of AFQ Approach Presented at the First AFQ Workshop



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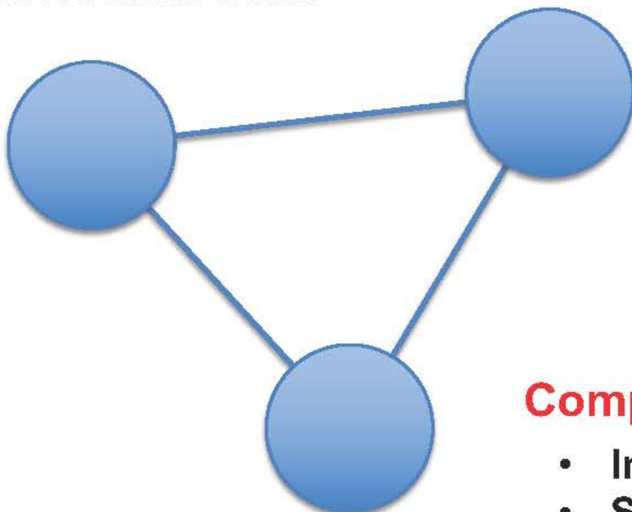
Validated Predictive Capability Building Blocks

Theory

- Explains nuclear fuel performance
- Multi-Physics & Multi-Scale

Experiment

- Validates theory
- Focused & Integral



Computation

- Integrates knowledge
- Solves theoretical models & processes experimental data

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Coupling Multi-Physics Phenomena is a Validated Predictive Capability Challenge

- **Nuclear fuel performance involves multiple coupled physical processes, e.g., hydrodynamic energy equation includes p (pressure from EOS) and Q *(heat generation form fission)*:**

$$\frac{\partial}{\partial t}\left(\rho u + \frac{1}{2}\rho v^2\right) + \nabla \cdot \left[\left(\rho u + \frac{1}{2}\rho v^2\right)\boldsymbol{v} + p\boldsymbol{v}\right] = \rho Q$$

- **Operator splitting can help multi-physics coupling**

$$\frac{du}{dt} = (A+B)u \qquad u(h) = e^{h(A+B)}u(0)$$

$$e^{h(A+B)} \approx e^{hA}e^{hB} \qquad \textbf{First Order}$$

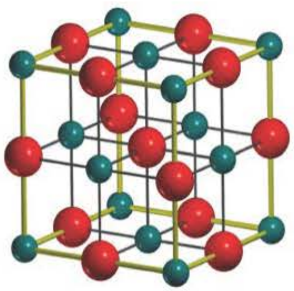
$$e^{h(A+B)} \approx e^{hA/2}e^{hB}e^{hA/2} \qquad \textbf{Second Order}$$

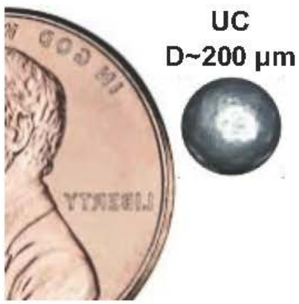
- **Numerical analysis can help quantify uncertainty**
  - **Accuracy** Order of the Approximation
  - **Consistency** Discretized Equation ⇔ Differential Equation
  - **Stability** Numerical Solution ⇔ Exact Solution of Discretized Equation
  - **Convergence** Numerical Solution ⇔ Exact Solution of Differential Equation

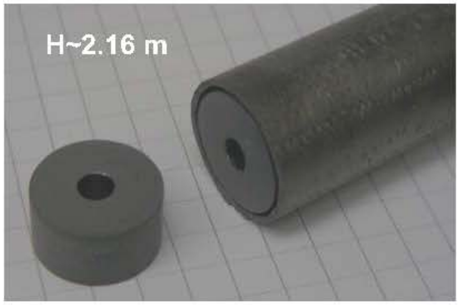
Bridging Multi-Scale Phenomena is a Validated Predictive Capability Challenge

- **Nuclear fuel performance spans an enormous spatial and temporal range**

Atoms [nm] | **Kernel [μm]** | **Pellet [cm]** | **EM² Fuel [m]**







- **Approaches to incorporate multi-scale information:**
  - Tables or empirical formulas
  - Inline model with parameters

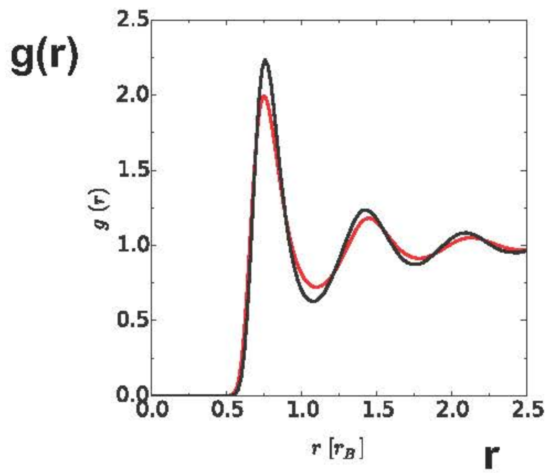
Statistical Mechanics Models can Connect Atomic Properties with Macroscopic Properties

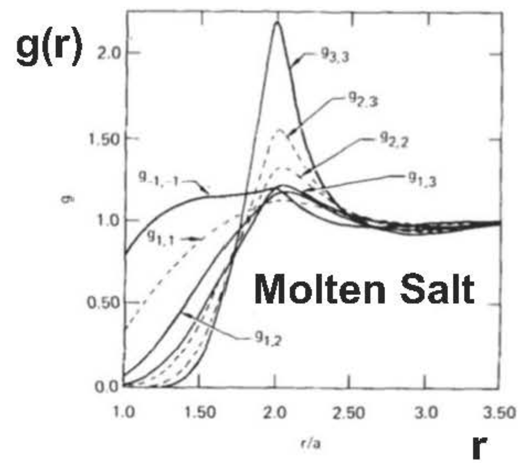
- **Ornstein-Zernike and hypernetted-chain equations connect atomic interaction potential with macroscopic properties**

Atomic Interaction Potential → **Ornstein-Zernike Equation Hypernetted-Chain Equation** → **Thermodynamic Functions**

Molecular Dynamics

Density Functional Theory





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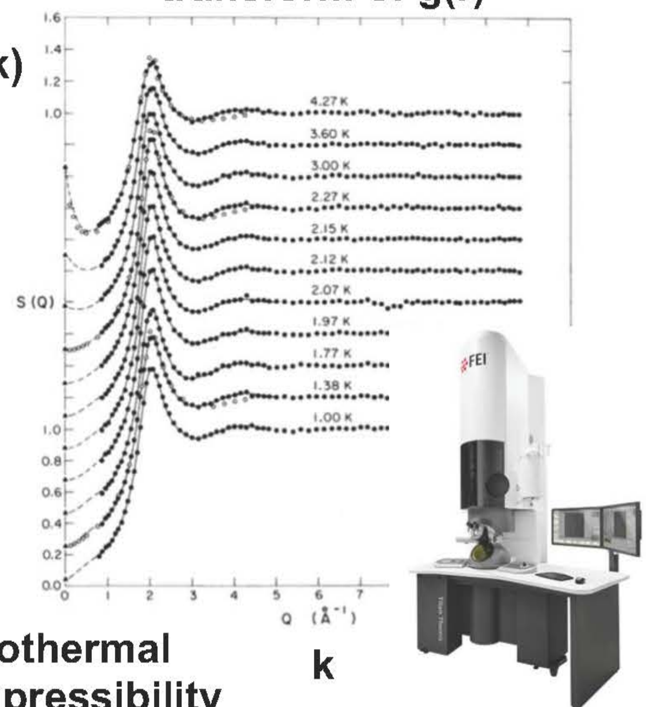
Independent Multi-Scale Experimental Measurements can Reduce Uncertainty

Microscopic Property Measurements

S(k) is related to the Fourier transform of g(r)

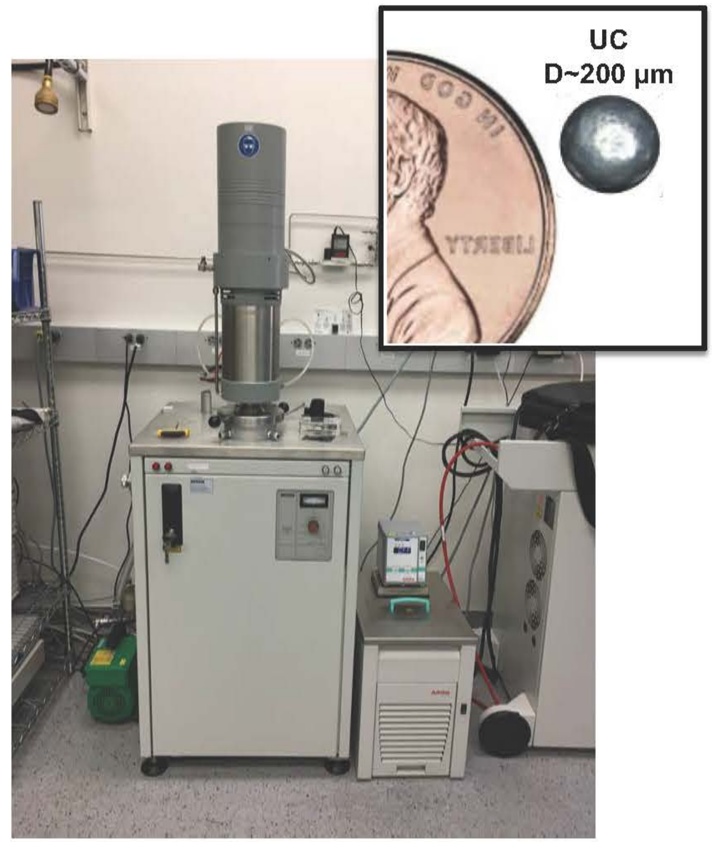
S(k)



Isothermal Compressibility (k→0)

k

Macroscopic Property Measurements



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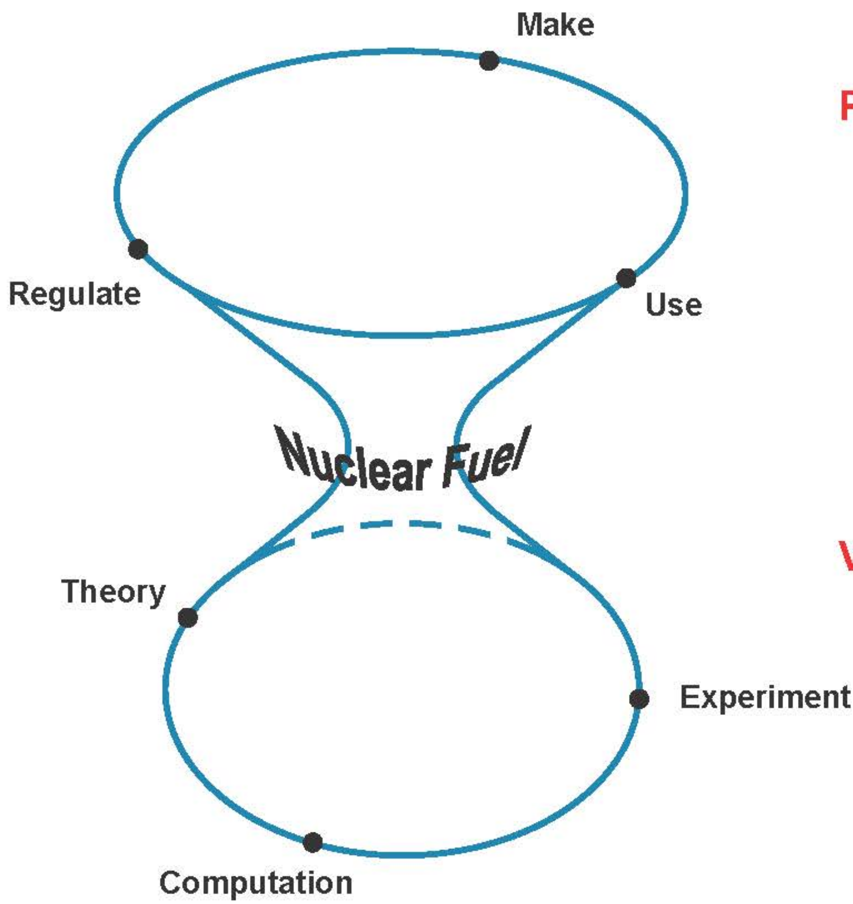
Validated Predictive Capability Enables High-Quality Performance Risk Management

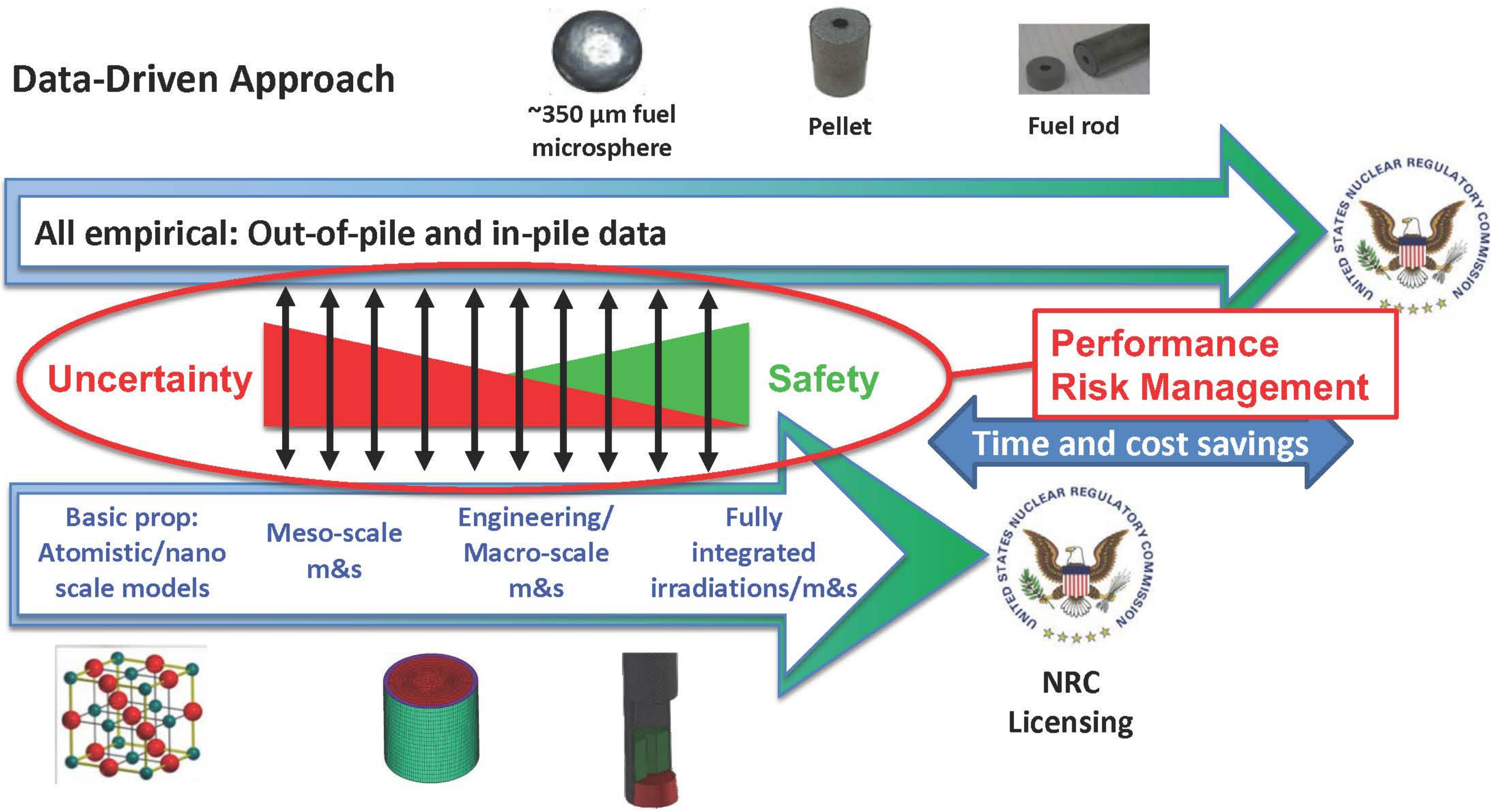


Performance Risk Management

- Systems Engineering
- Margin Assessment, Uncertainty Quantification, and Confidence Factor

Validated Predictive Capability

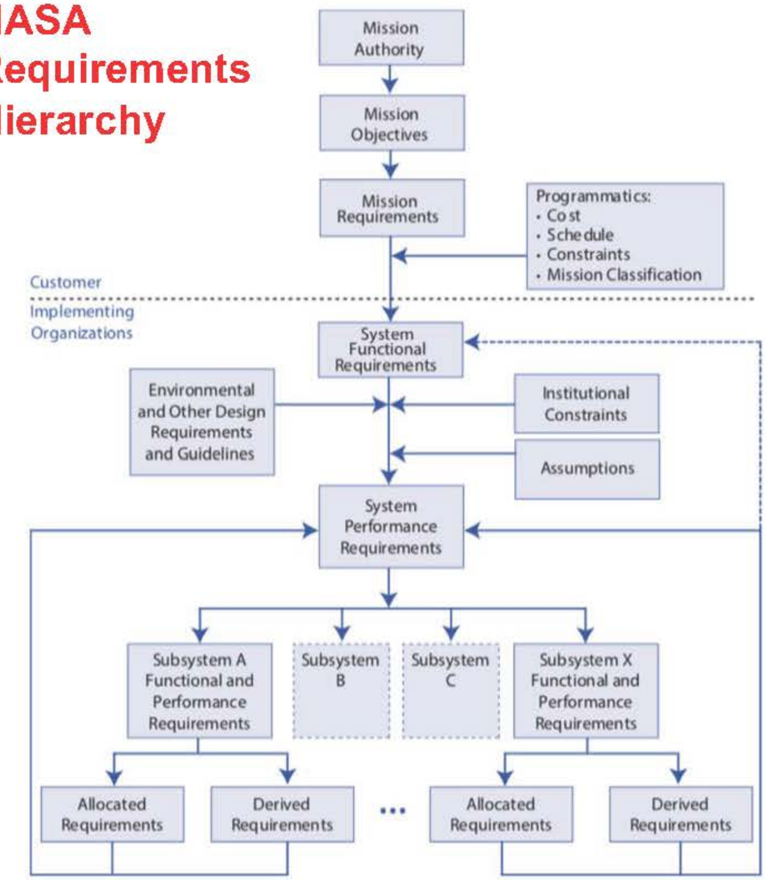
Conceptual Progression of AFQ Approach Presented at the First AFQ Workshop



Modeling & Simulation with Experimental Validation: AFQ Approach

Systems Engineering Approach to Defining Nuclear Fuel Requirements

NASA Requirements Hierarchy



Customer Requirements

System Level Requirements

Subsystem Requirements

Nuclear Fuel Examples:
- Fuel T < Melting T
- Cladding Strain < 1%

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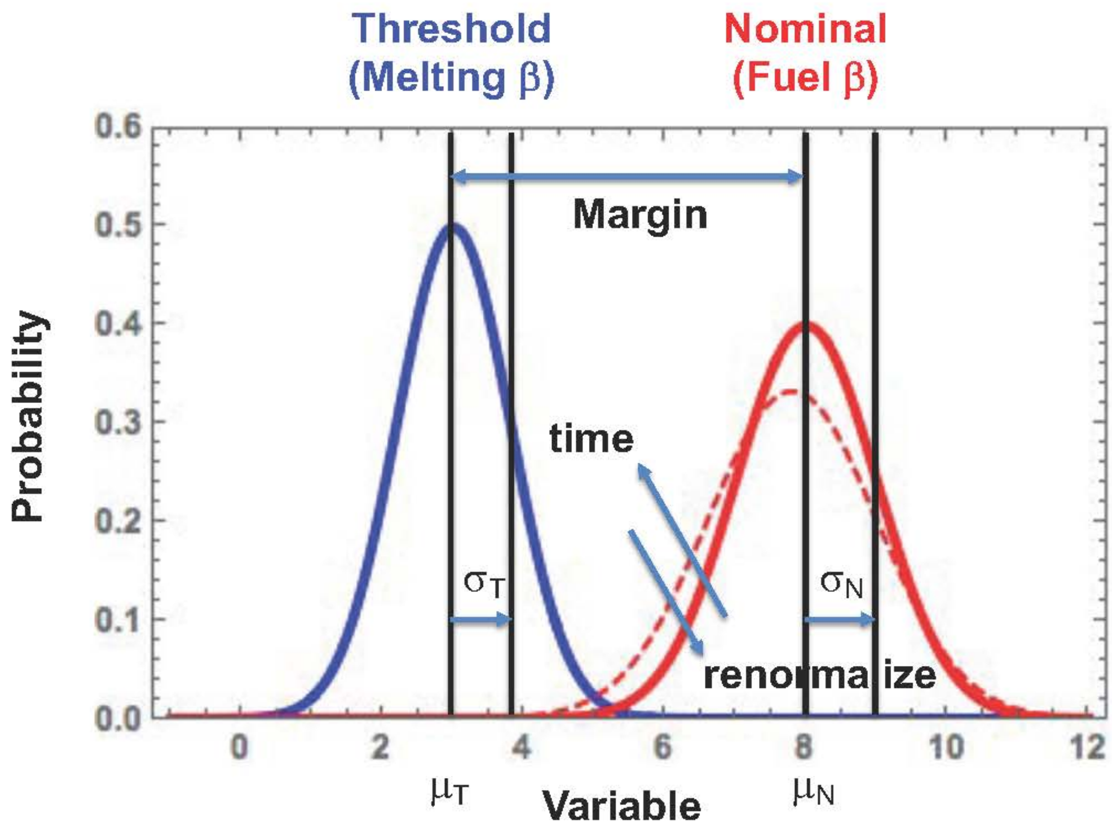
Performance Parameter Uncertainty Quantification & Margin Assessment Improves Safety & Reliability



Margin

$$M = \mu_N - \mu_T$$

Uncertainty

$$U = \sqrt{\sigma_N^2 + \sigma_T^2}$$

Confidence Factor

$$CF = \frac{M}{U}$$

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AFQ Workshop 2 Opening Comments

- **"When successfully demonstrated and applied, the AFQ approach will open a new horizon for exciting new nuclear fuels to strengthen the competitiveness of the US nuclear industry."**

- **This is the second workshop in a series that is intended to move AFQ forward**

- **Two high-level AFQ thrust areas are emerging:**
  - Validated Predictive Capability
  - Performance Risk Management

AFQ Workshop 2 Agenda

- **Welcome and Workshop Introduction (3)**
- **Scienta (Science)**
  - Fundamental Computational, Experimental, and Theoretical Building Blocks (2)
  - Integrating Building Blocks and Bridging Multi-Scale Phenomena (1)
- **Ipsum (Engineering)**
  - Nuclear Fuel Applications and Case Studies (5)
  - Regulatory Discussion
- **AFQ Technical Working Group Charter Discussion**
- **Future Actions**

APPENDIX C - Appendix C: High Energy Heavy Ion Irradiation for Accelerated Testing

High Energy Heavy Ion Irradiation for Accelerated Testing

Abdellatif Yacout

Argonne National Laboratory

2nd Accelerated Fuel Qualification Workshop

955 L'Enfant Plaza SW, Washington, DC

January 16th, 2019

U.S. DEPARTMENT OF ENERGY Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

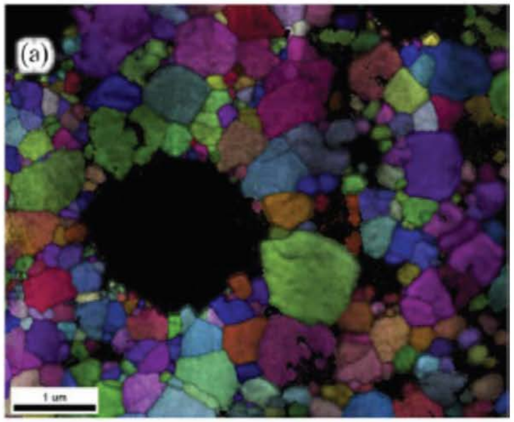
Argonne NATIONAL LABORATORY

CONTENT

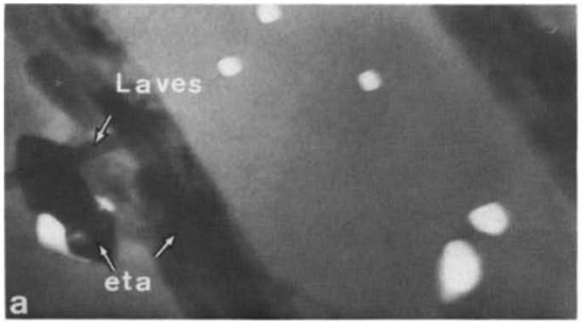
- Radiation Effects in Nuclear Materials
- Advantages of High Energy Heavy Ion Irradiation
- Argonne Tandem Linac Accelerator System (ATLAS)
- Accelerated Testing of Different Fuels with High Energy Heavy Ion Irradiation
- AMIS - ATLAS Materials Irradiation Station
- Summary

RADIATION EFFECTS IN NUCLEAR MATERIALS

- **Radiation Effects in Nuclear Fuels**
  - Major origin: fission fragments with ~100 MeV
  - Energy deposition of fission fragments
    - Point defects accumulation (dislocations, voids, etc.)
    - Amorphization and decomposition
    - Grain subdivision
  - Accumulation of stopped fission fragments
    - Fission gas bubbles
    - Secondary phases and solid solution (solid fission products)



HBS in in-pile irradiated UO2 featuring nanocrystalline grains and micro-pores [1]



Secondary phases and He bubbles in in-pile irradiated SS316 [2]

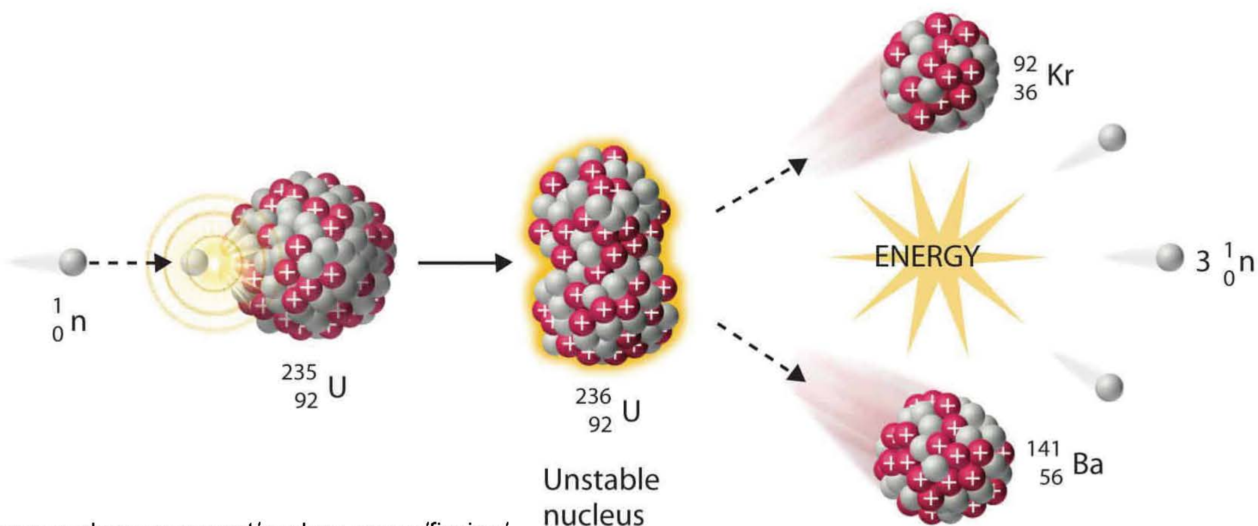
- **Radiation Effects in Structural Materials**
  - Major origin: neutrons
  - Energy deposition of neutrons/secondary ions
    - Point defects accumulation (dislocations, voids, etc.)
    - Amorphization and decomposition
    - Grain subdivision
  - Neutron induced nuclear reactions
    - He bubbles

[1] T.J. Gerczak et al, JNM, 2018 [2] P.J. Maziasz et al, JNM, 1981

ADVANTAGES OF HIGH-ENERGY IONS

▪ Simulate Fission Fragment Damage (Fuels)

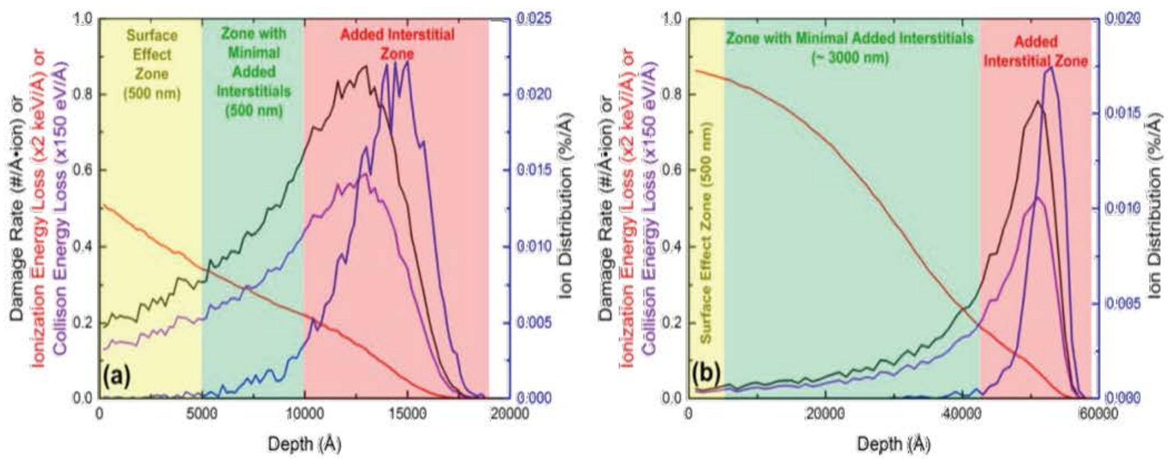
- Each fission reaction produces ~200 MeV energy
  - 2~3 neutron: ~4.8 MeV
  - Prompt gamma: ~7 MeV
  - Delayed energy (decays): ~ 19 MeV
  - 2 Fission fragments: ~169 MeV (major source of radiation effects in fuels)
- **High-energy ions can replicate fission fragments (~100 MeV)**
- Applicable to already neutron-irradiated fuel to achieve higher burnup level
- Implant gaseous/solid fission products



https://www.nuclear-power.net/nuclear-power/fission/

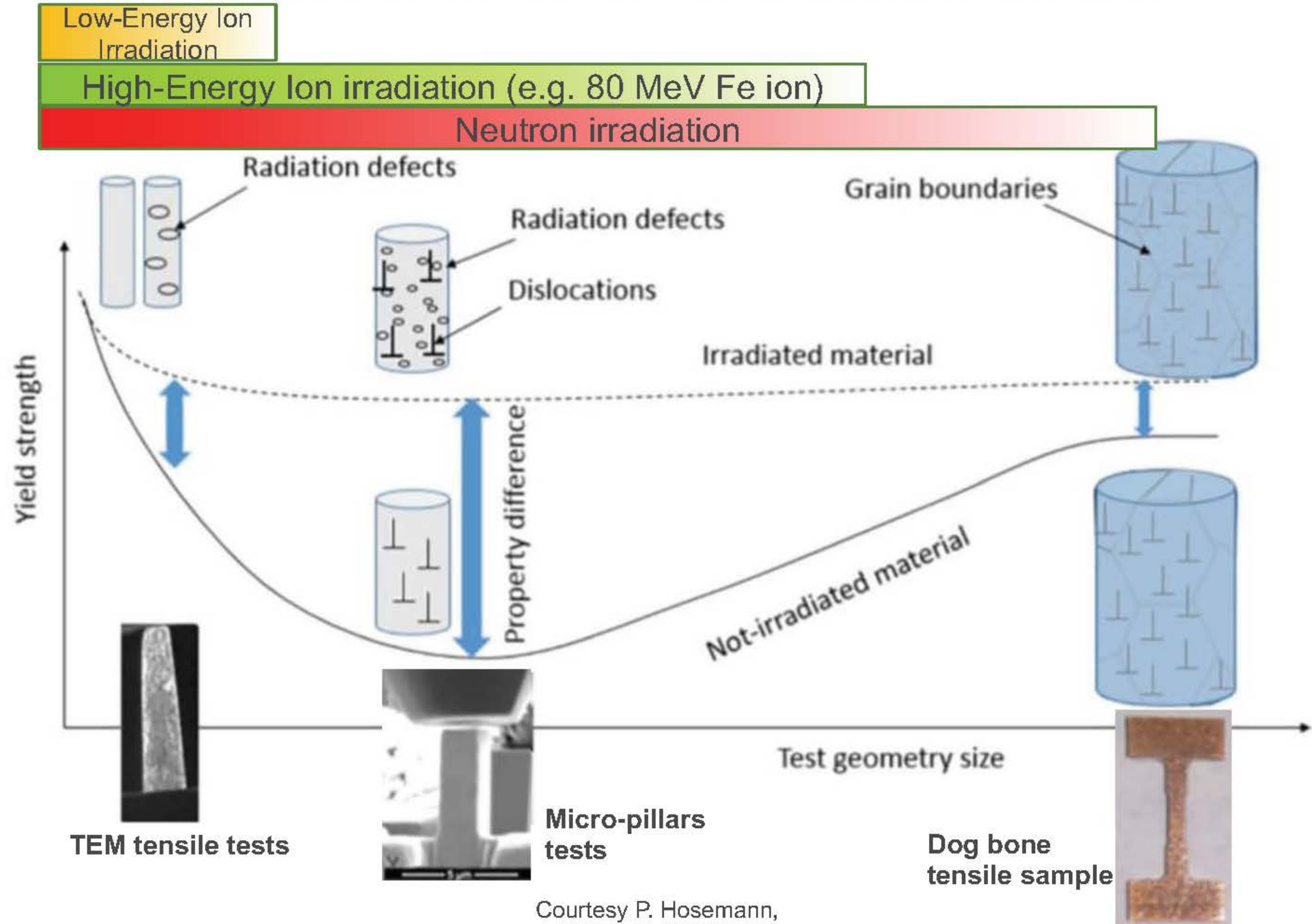
ADVANTAGES OF HIGH ENERGY HEAVY ION IRRADIATION

- ***Motivations:***
  - Fuel development: direct replication of high-energy fission fragments: e.g. 100 MeV Xe
  - Extensive damage range within irradiated materials
- ***Uniqueness:***
  - Ultra high energy: 1 MeV/amu or higher
  - Vast ion diversity (almost entire periodic table coverage)



Damage Profiles Induced by 5 MeV (L) and 54 MeV (R) Fe ions in Steel (SRIM Simulation)

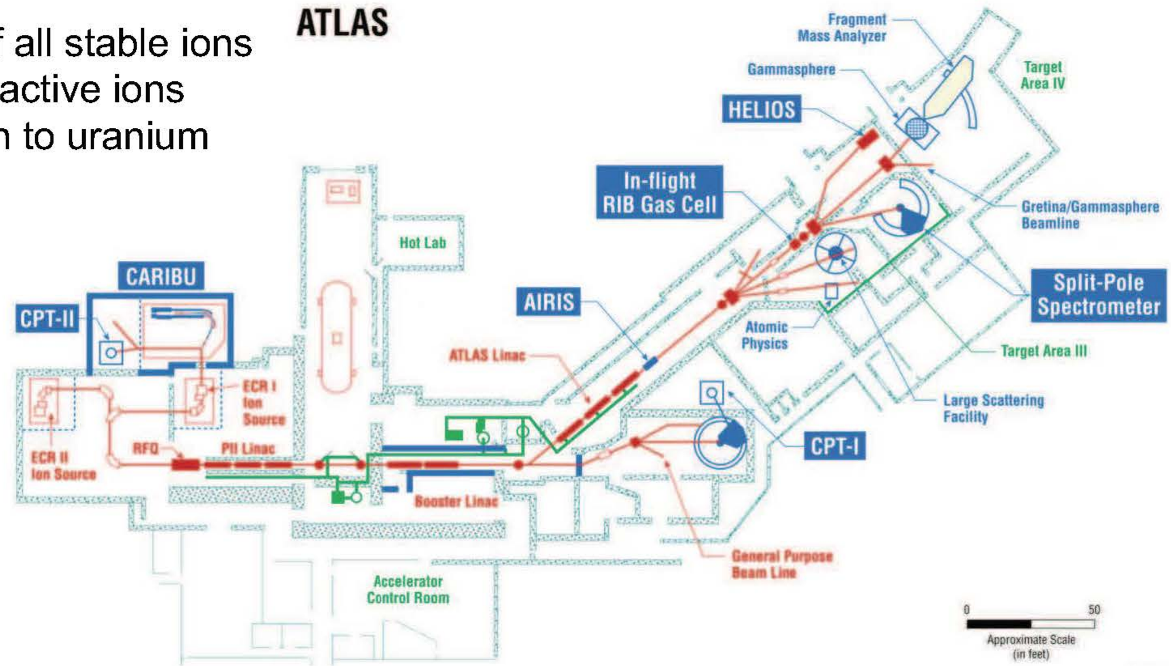
MECHANICAL PROPERTIES AT MULTIPLE SCALES



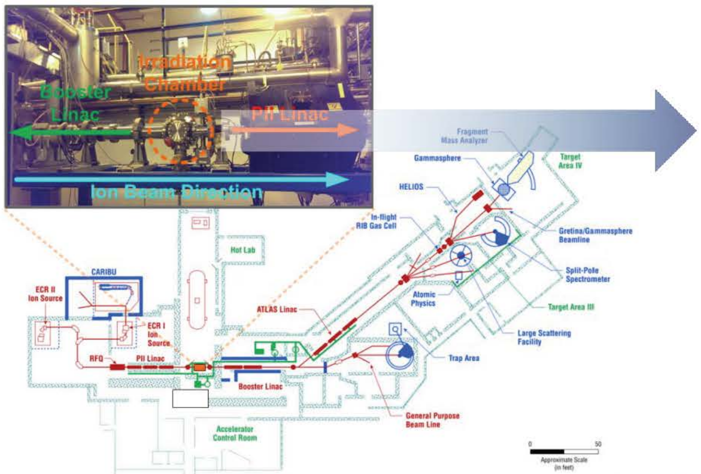
Courtesy P. Hosemann, UC Berekly

ARGONNE TANDEM LINAC ACCELERATOR SYSTEM (ATLAS)

- DOE office of science user facility
- ATLAS Capabilities
  - Nuclear structure research facility
  - Superconducting linear ion accelerator
  - Energy: up to 17 MeV per nucleon capability
  - Available Ions
    - full range of all stable ions
    - Some radioactive ions
    - From proton to uranium

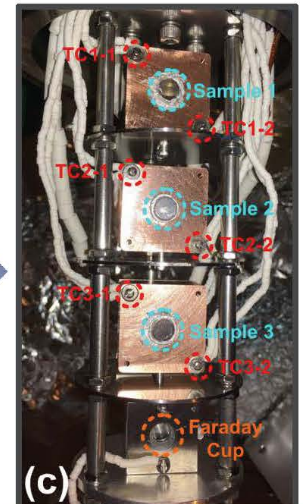


ION IRRADIATION CHAMBER AT ATLAS



Ion Irradiation Chamber Established at ATLAS

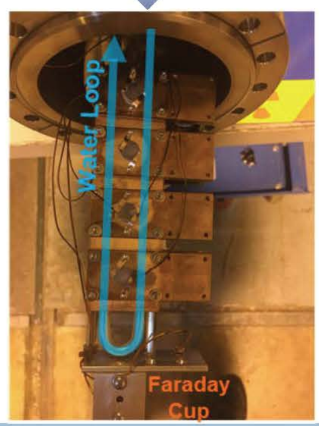
Irradiation Chamber



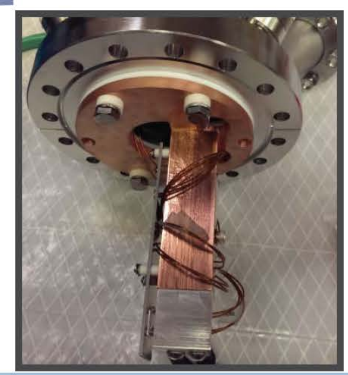
Hi-Temp Sample Stage (>300C)

▪ Features of the Chamber

- Between PII and Booster LINACs
- Up to 1.5 MeV per nucleon
- Ion type: proton to uranium (e.g. 56 MeV Fe, 131 MeV Xe, etc.)
- Up to 1 pμA ion current
- Multiple sample stages supporting irradiation temperature ranging from RT to 900C.



Active Cooling Sample Stage (RT to 300C)



Passive Cooling Sample Stage

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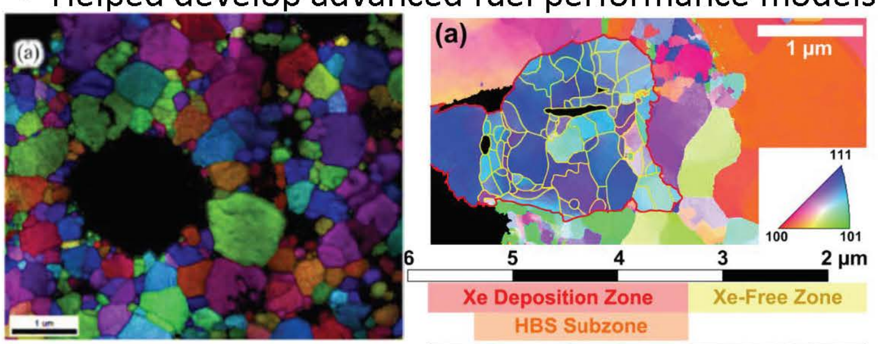
UO_2: REPLICATE MICROSTRUCTURES AT HIGH BURNUP

- **Xe Implantation & PIEs**
  - 84 MeV Xe at 300°C
  - Up to 7.2E17 ions/cm^2 (1379 dpa)
  - TEM+TEM orientation microscopy
- **Fission Gas Behavior**

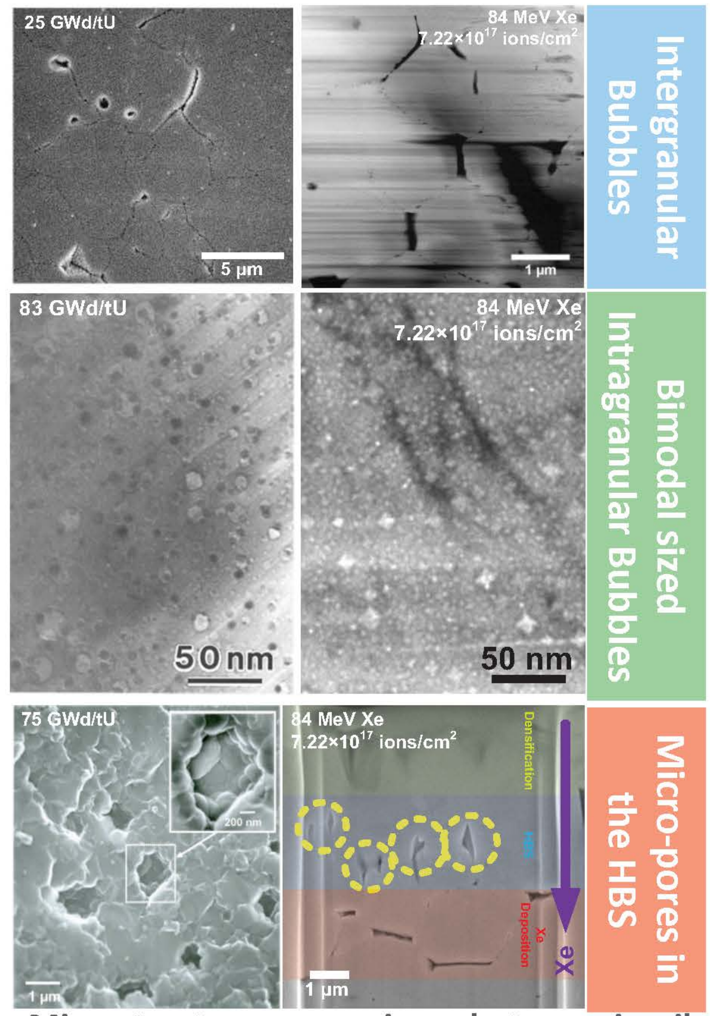
  Replicated intragranular bubbles with bimodal size distribution and intergranular bubbles
- **High Burnup Structure (HBS)**

  Replicated both micro-pores and nanocrystalline grains in the HBS formed in high-burnup UO_2
- **Support Advanced Modeling**
  - Clarified HBS formation mechanism
  - Helped develop advanced fuel performance models



HBS in in-pile irradiated UO_2 and 84 MeV Xe implanted UO_2[1][2].

[1] T.J. Gerczak et al, JNM, 2018 [2] Y. Miao et al., Scripta Materialia, 2018
[3] I. Zacharie et al., JNM, 1998 [4] K. Nogita et al., NIMB, 1994



Microstructure comparisons between in-pile and 84 MeV Xe ion irradiations [3][4].

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U-MO: HIGH-DENSITY RESEARCH REACTORS FUELS

- **Xe Implantation & PIEs**
  - 84 MeV Xe at 50~300C
  - Up to 2.9E17 ions/cm^2
  - TEM+µXRD+XTM
- **Fission Gas Behavior**
  - Intra- and inter-granular

Replicated size and number density of bubbles in in-pile irradiated U-Mo

- **Phase Stability**
  - Radiation-induced recovery of γ-U-Mo within the Xe ion range

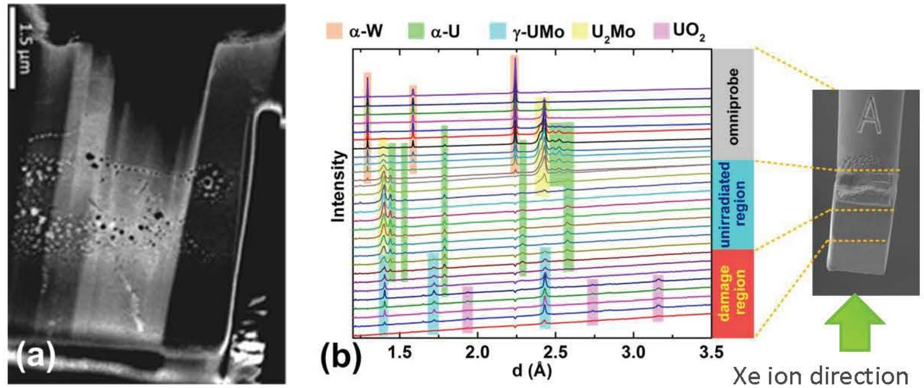
Replicated the γ-UMo phase stabilization by neutron irradiation

- **Recrystallization**
  - Nano-grains formation

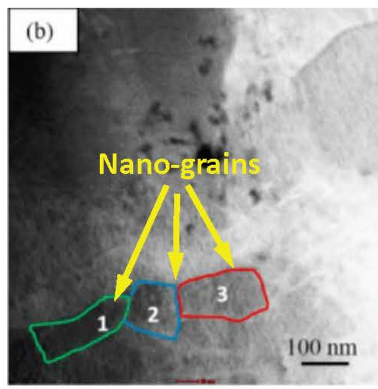
Consistent with in-pile irradiation

- **Interaction Layer**
  - Amorphous IL (T<200C)

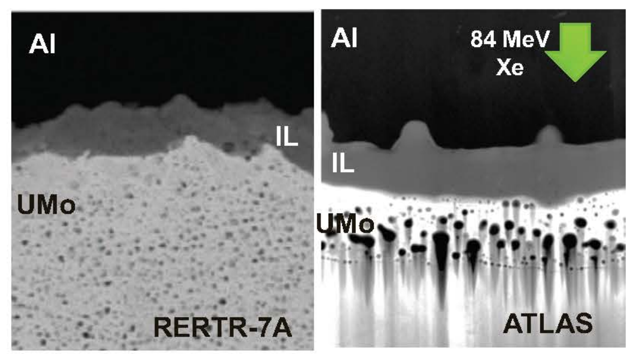
Consistent with in-pile irradiation



Synchrotron µXRD showing the recovery of γ-UMo from α-γ' mixture under Xe ion irradiation



Recrystallization induced by 84 MeV Xe irradiation



Al-UMo IL and Xe bubbles in in-pile (left) and Xe (right) irradiated fuels

[1] B. Ye et al., JNM, 2017 [2]D.D.Keiser et al., Nucl. Eng. Technol. 2014

U_3SI_2: NEW FUEL WITH ENHANCED ACCIDENT TOLERANCE

▪ Novel Fuel for LWRs

- Successful applications at low temperatures in research reactors (RERTR)
- Limited in-pile experience at high temperatures in LWRs
- Ion irradiation needed for accelerated fuel performance evaluation & qualification

• Xe Implantation & PIEs

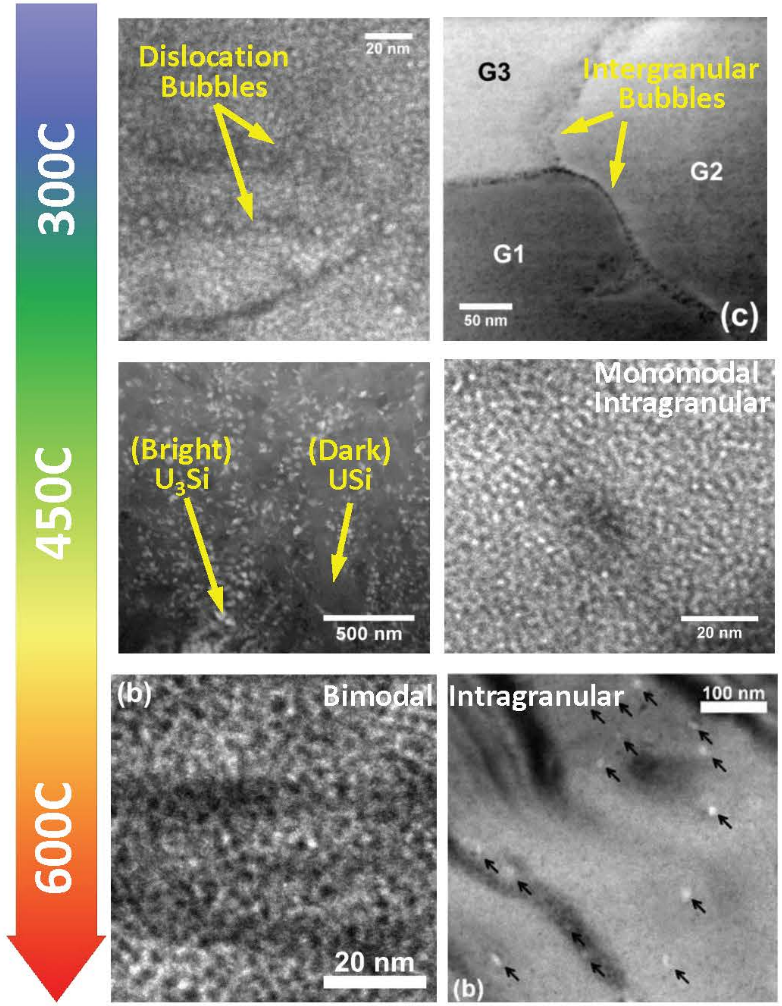
- Exactly same U_3Si_2 batch as irradiated in ATR
- 84 MeV Xe at 300/450/600C
- Up to 1.4E17 ions/cm^2
- TEM+µXRD

▪ Fission Gas Behavior

- Lo Temp → Monomodal intragranulr bubbles
- Hi Temp → Bimodal intragranular bubbles
- Intergranular bubbles with size dependent on the GB type

Consistent with preliminary PIE results of ATF-1 campaign (no prominent swelling at ~20 GWd/tU)

[1] Y. Miao et al., JNM 2017 [2] Y. Miao et al., JNM 2018
[3] Y. Miao et al., JNM 2019



Radiation-induced microstructure modifications in U_3Si_2 implanted by 84 MeV Xe at LWR temperatures

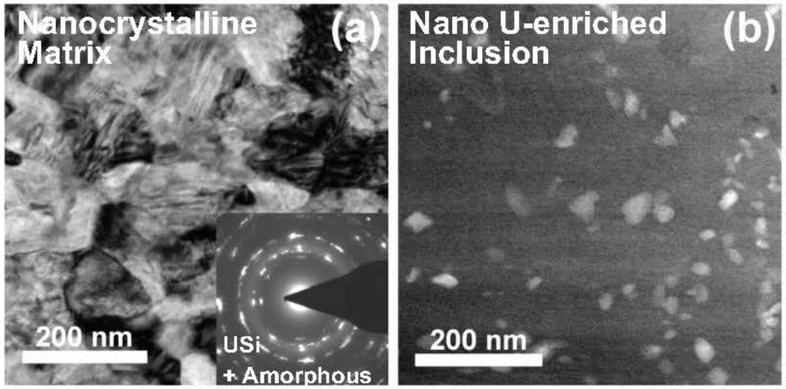
U_3SI_2: NEW FUEL WITH ENHANCED ACCIDENT TOLERANCE

- **Xe Implantation & PIEs**
  - 84 MeV Xe at 450C
  - >200 dpa
  - TEM+µXRD
- **Phase Stability**
  - Phase decomposition at 450C (>200 dpa)
  - Nanocrystalline USi matrix
  - Amorphous U-enriched inclusions

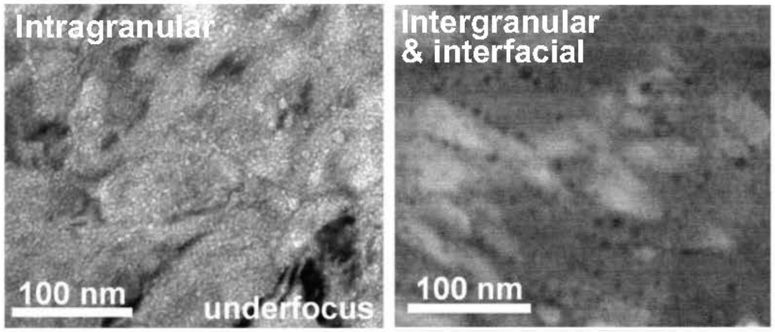
Predicted the occurrence of phase decomposition under certain irradiation conditions
Need confirmation from in-pile irradiation & PIE

- **Bubbles in Decomposed U_3Si_2**
  - Intragranular/intergranular/phase boundary
  - Limited swelling due to the nano-grains
- **Support Model Development**
  - Reference for rate theory parameterization
  - Fission gas correlation implemented into BISON

[1] Y. Miao et al., JNM 2019



Phase decomposition of U_3Si_2 into a U-enriched inclusion and a nanocrystalline USi matrix



Xe bubbles in decomposed U_3Si_2

U-10ZR: BINARY FAST REACTOR FUEL

▪ Xe Implantation & PIEs

- 84 MeV Xe at 700C (~centerline temp)
- Up to 2.19E17 ions/cm^2
- TEM

▪ U-Zr Phases

- Irradiated at γ_1+ γ_2 phase field
- Mainly $\gamma_1 \rightarrow \alpha$; $\gamma_2 \rightarrow \omega/\delta$ during cooling

Consistent with phase diagram

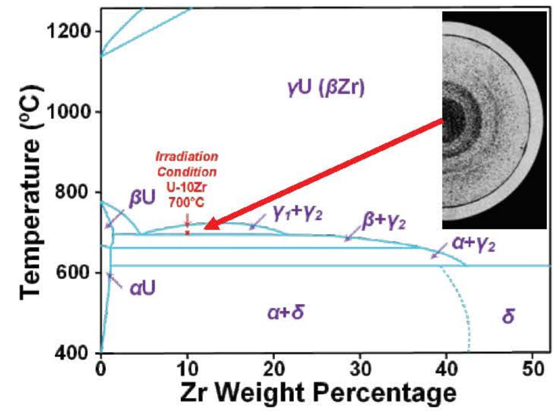
▪ Fission Gas Behavior

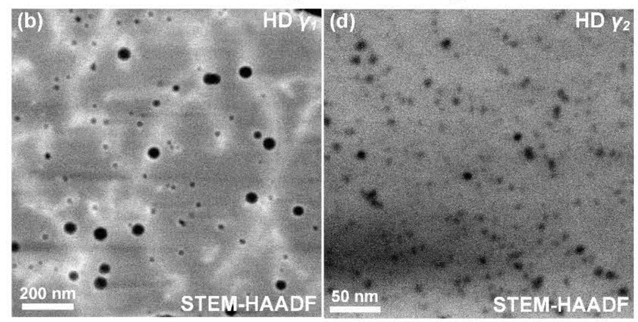
- U-enriched γ_1
  - Bimodal bubble size distribution
  - Large bubbles on dislocations
  - Lower bubble density
- Zr-enriched γ_2
  - Monomodal bubble size distribution
  - Small bubbles, high density

Dissimilar fission gas behavior in different phases

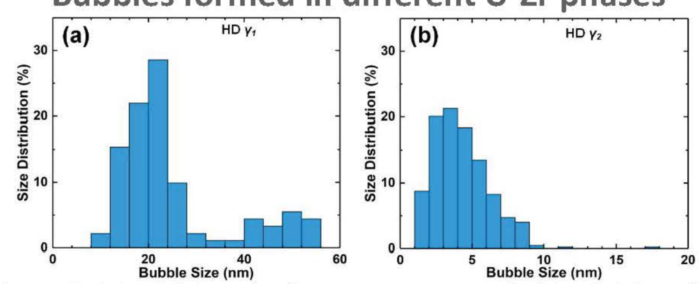
▪ Support Model Development

- Help develop/validate fission gas models for separate U-Zr phases.





Bubbles formed in different U-Zr phases



Bimodal bubbles (γ_1) vs. monomodal bubbles (γ_2)

13

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SUMMARY: HEAVY ION IRRADIATION USING A LINAC (ATLAS) FOR SUPPORT OF AFQ

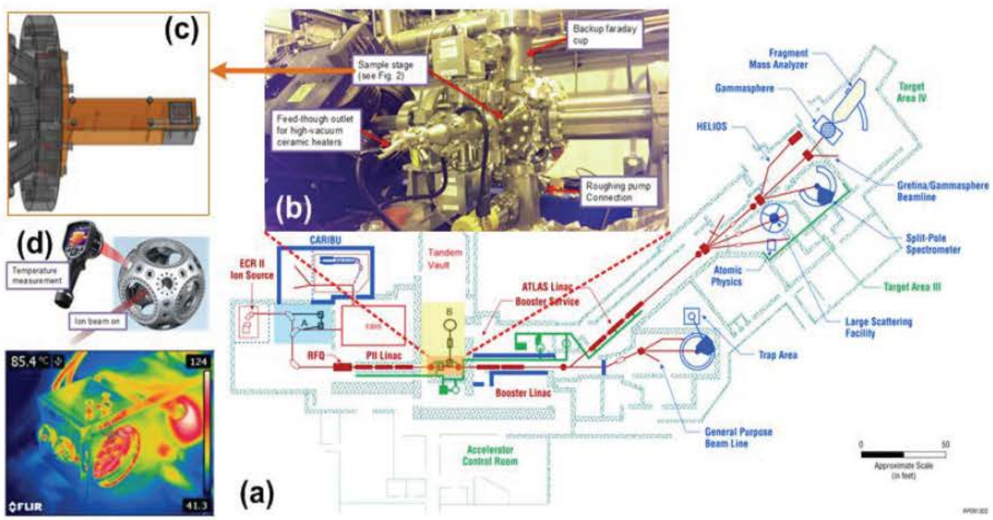
High-energy ion irradiation produced by LINACs is capable of

- replicating a series of microstructural modifications observed in in-pile irradiated materials to help understand the mechanisms;
  - Fission gas bubbles in UO_2 and U-Mo
  - Al-ZrN IL in U-Mo dispersion fuel with ZrN coated particles
  - Radiation-induced dislocations in steels
- providing microstructural modifications data of new nuclear materials before in-pile data are available;
  - Bubble morphology and phase stability data of U_3Si_2
- creating a deep radiation damage profile that enables the application of advanced characterization techniques;
  - Phase stability in U-Mo and U_3Si_2 (µXRD)
  - Dislocations effect on mechanical properties (in situ synchrotron tensile test)

Key Issue: ATLAS is a DOE Science user facility with limited availability for other users. **How to allow for more beam time at ATLAS for accelerated fuel materials testing ?**

ATLAS MATERIALS IRRADIATION STATION (AMIS)

- A beam switching capability which alternate between an intense stable ion beam (to be used for materials research) and a radioactive ion beam (CARIBU – used by DOE office of nuclear physics users – ONP) or vice versa (for tracer studies)
- Utilize the pulsed time structure of the recent ATLAS upgrade, CARIBU, which delivers accelerated beams of radioactive fission fragments from a spontaneous fission source of 252Cf (only pulsed 3% of beam time)
- The materials irradiation beam will be pulsed in between the CARIBU pulses, so it will not interrupt the main mission of the ONP facility

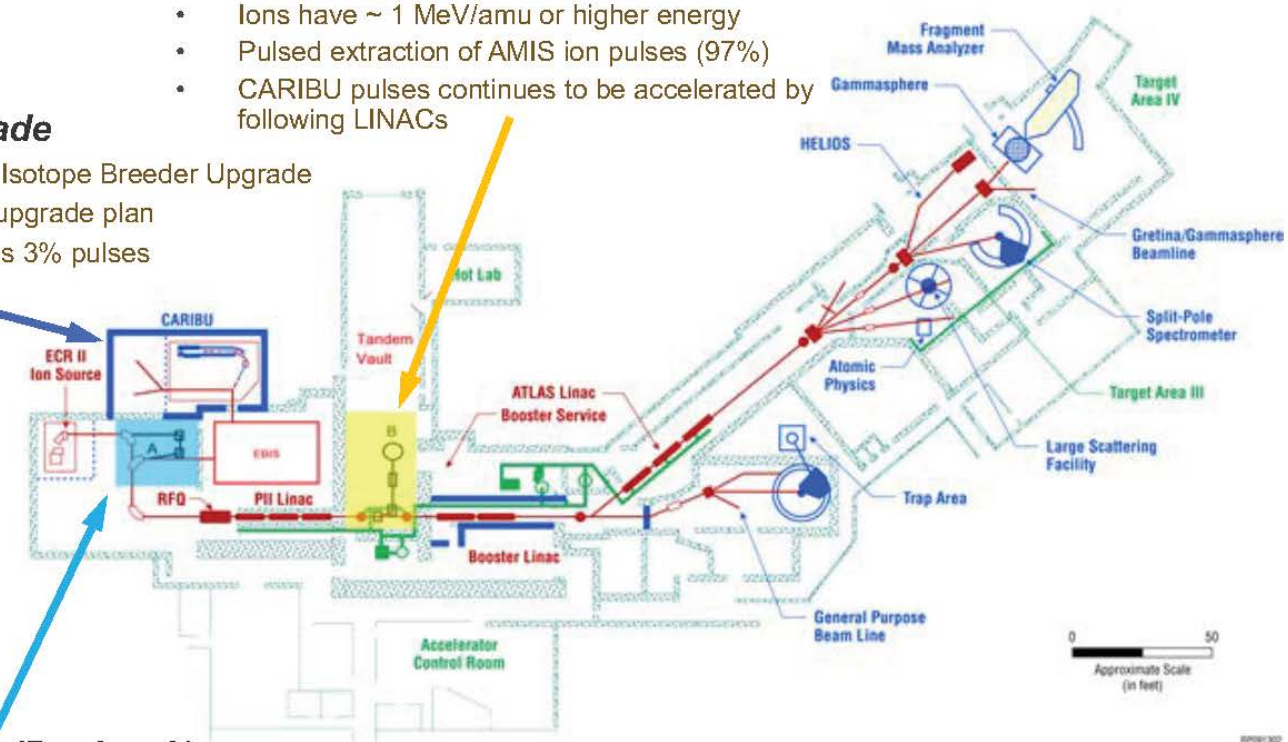


Upgrade plan of establishing AMIS at ATLAS: (a) floor plan of ATLAS after CARIBU and AMIS upgrade; red region is the current irradiation chamber used to validate the feasibility of AMIS; blue(A) and yellow(B) regions indicate the upgrade needed for AMIS. (b) current irradiation chamber operating during maintenance period. (c) sample stage of the current irradiation chamber. (d) temperature control of the current irradiation chamber.

UPGRADE PLAN OF AMIS: OVERVIEW

- ***AMIS Beam Extraction (Region B)***
  - In Tandem Vault after the Injector LINAC
  - Ions have ~ 1 MeV/amu or higher energy
  - Pulsed extraction of AMIS ion pulses (97%)
  - CARIBU pulses continues to be accelerated by following LINACs

- ***CARIBU Upgrade***
  - Californium Rare Isotope Breeder Upgrade
  - Recently funded upgrade plan
  - CARIBU only uses 3% pulses

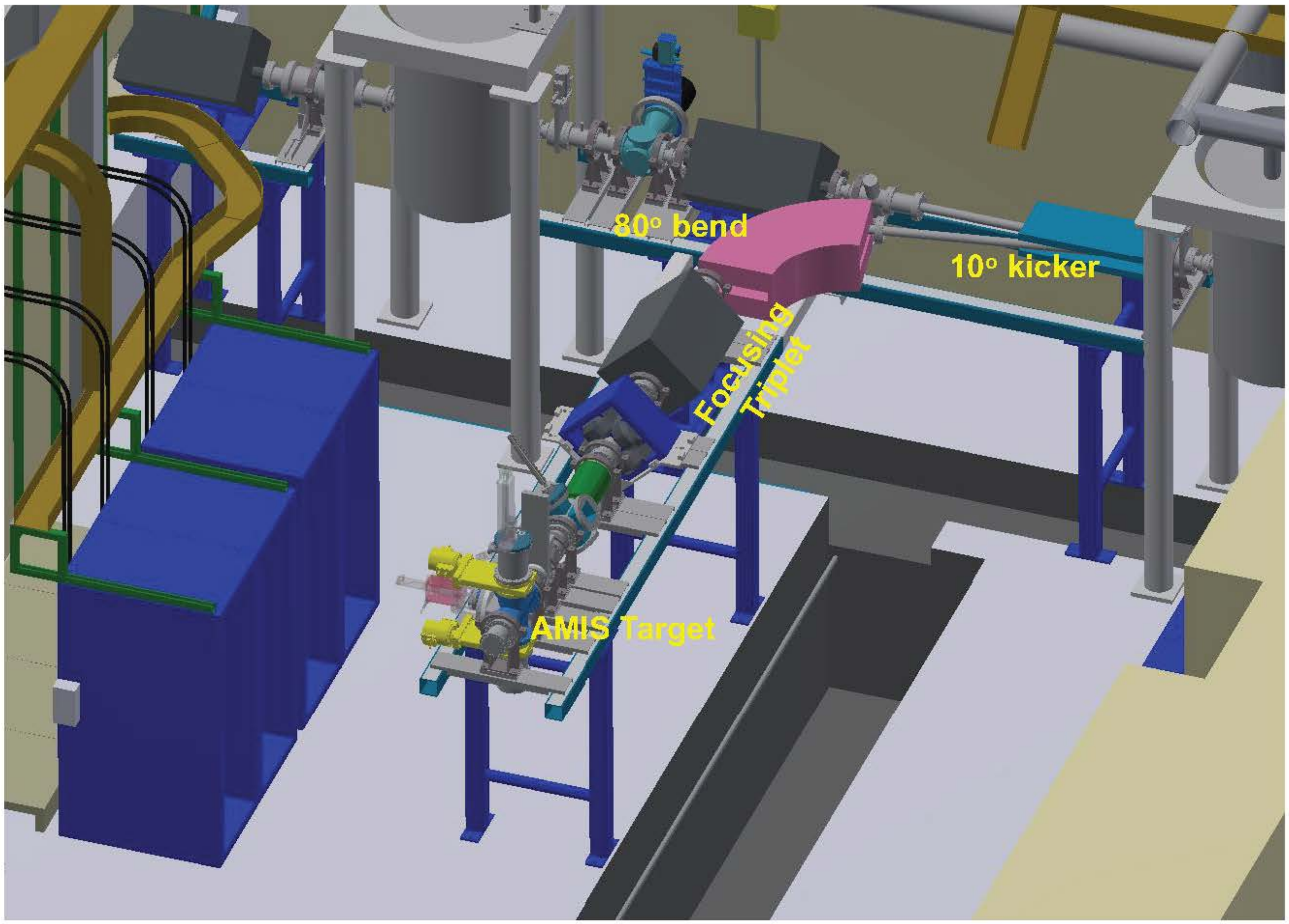


- ***Beam Combiner (Region A)***
  - Combining CARIBU and AMIS ion sources
  - Time allocation: 97% AMIS and 3% CARIBU
  - Both beams share ATLAS acceleration capability simultaneously

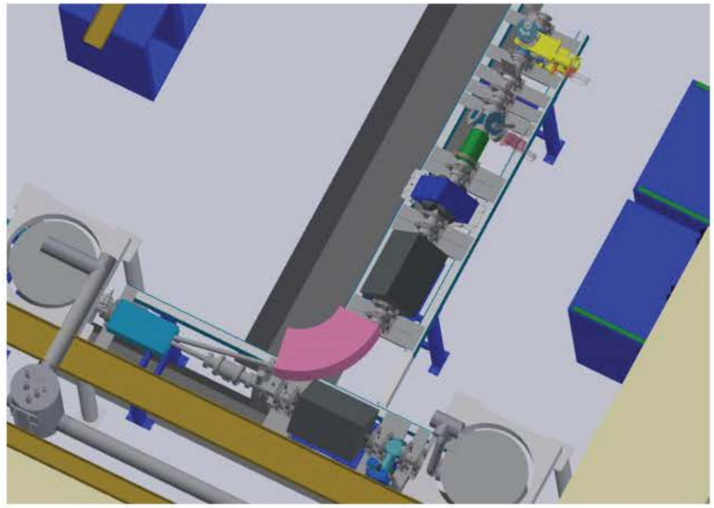
AMIS (ATLAS MATERIALS IRRADIATION STATION)

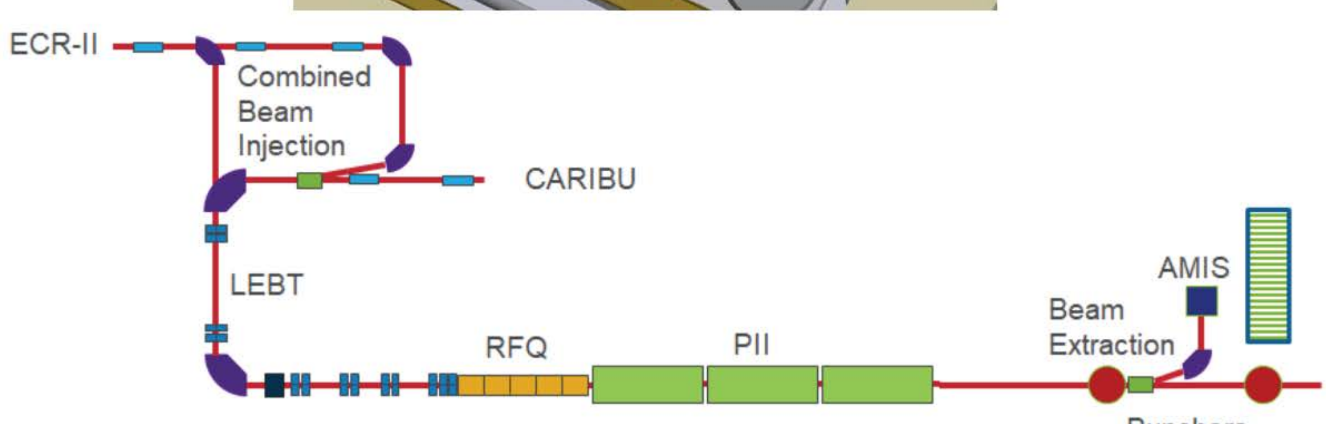
- **Advantages:**
  - Accelerated testing of fuel materials to support down-selection of fuel material over a short period of time (1 to 2 years time frame)
  - Will enhance already existing inter-laboratory and university collaborations on heavy ion irradiation
  - Moderate investment to gain extended access to a unique world class facility
  - Leverage already existing office of science investment in ATLAS
  - Potential for becoming a NSUF user facility for the nuclear materials community providing more access time for national labs and universities

AMIS STATION LAYOUT



AMIS STATION LAYOUT





Extraction Beamline Design

SUMMARY

- ~ 100 MeV fission fragments produced during fission are responsible for majority of damage and changes in fuel microstructure during irradiation
- High Energy Heavy Ion Irradiation with key fission fragments types and energies can simulate those fission products
- High burnup &1000's of dpa in fuel materials can be simulated
- Accelerated testing was performed at ATLAS accelerator on different fuel materials at different operating conditions (U-Mo, UO2, U3Si2, U10-Zr) and structural materials
- Accelerated testing using high energy heavy ions can support the accelerated fuel qualification approach, based on the positive results of testing on different fuel materials
- A dedicated materials irradiation station (AMIS) at ATLAS will provide extended access to the facility (more beam time)

BACKUP

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PROPOSAL – EXTREME MATERIALS BEAMLINE (XMAT)

A new beamline at the Advanced Photon Source (APS) for in situ studies of materials under irradiation, temperature, stress, environmental, etc.

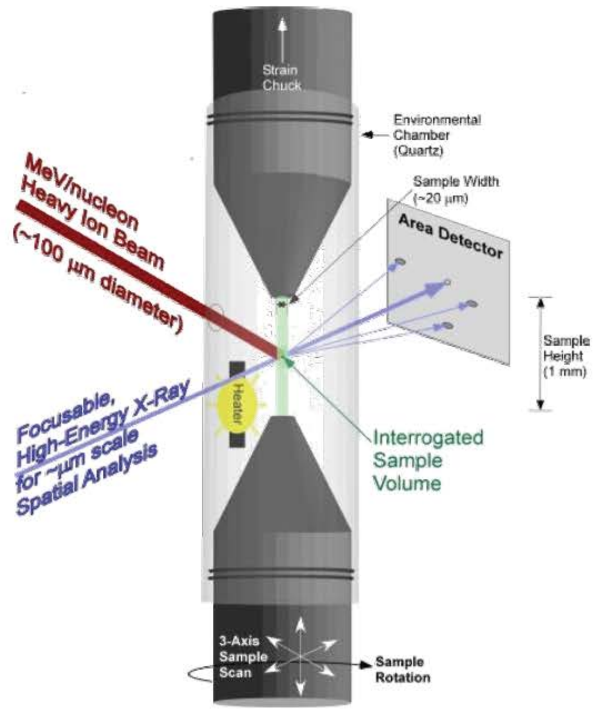
XMAT will provide x-ray probes for *in-situ* study of materials in simulated extreme radiation environments, enabling rapid evaluation of materials performance under extreme service conditions including structural materials and in particular for nuclear fuels.

XMAT is made possible by combining the technology of Argonne's unique capabilities:

1.Energetic, Heavy Ion Beams (ATLAS)

2.Focusable, High Energy X-Rays (APS)

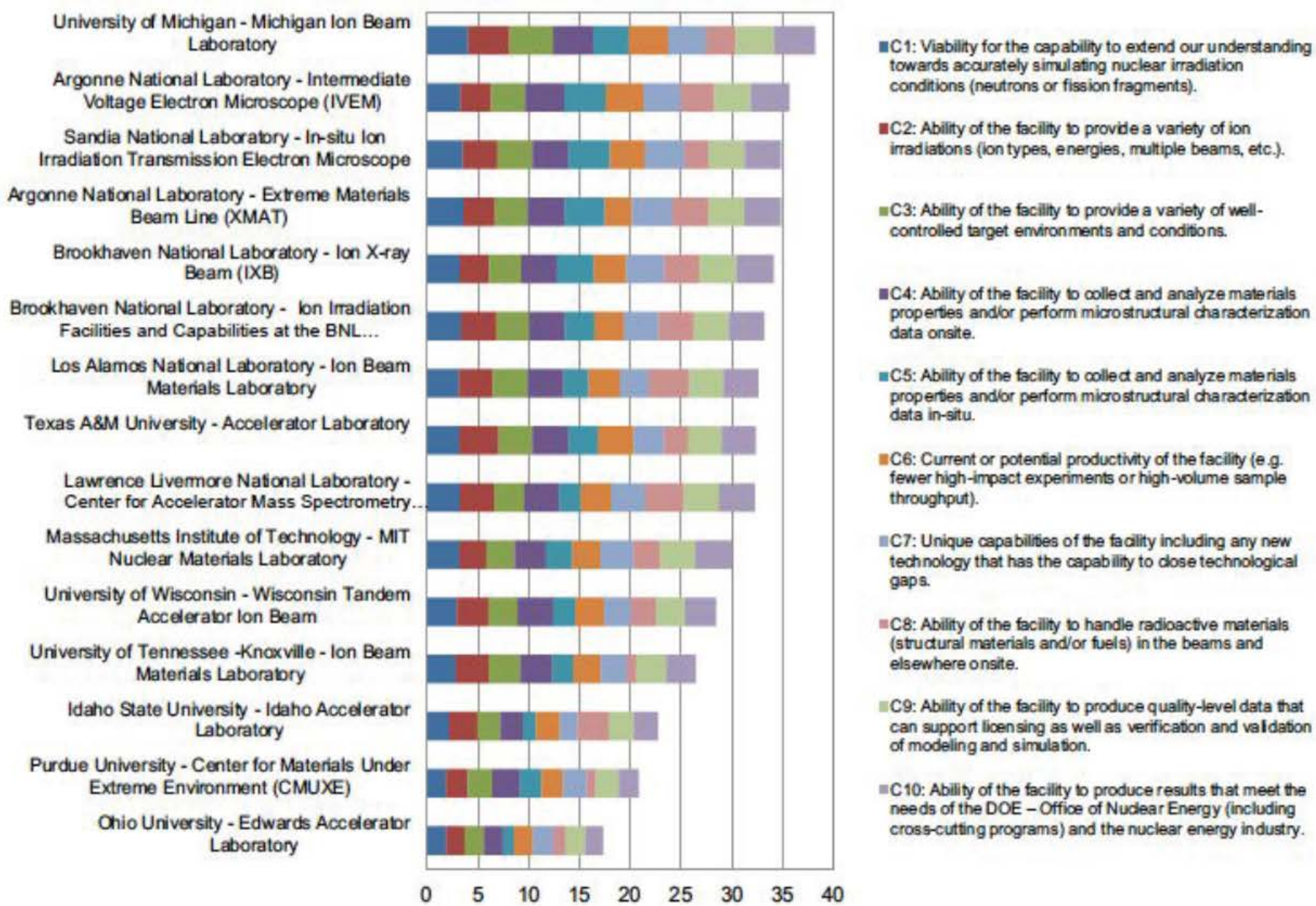
3.Multi-modal Imaging (APS)



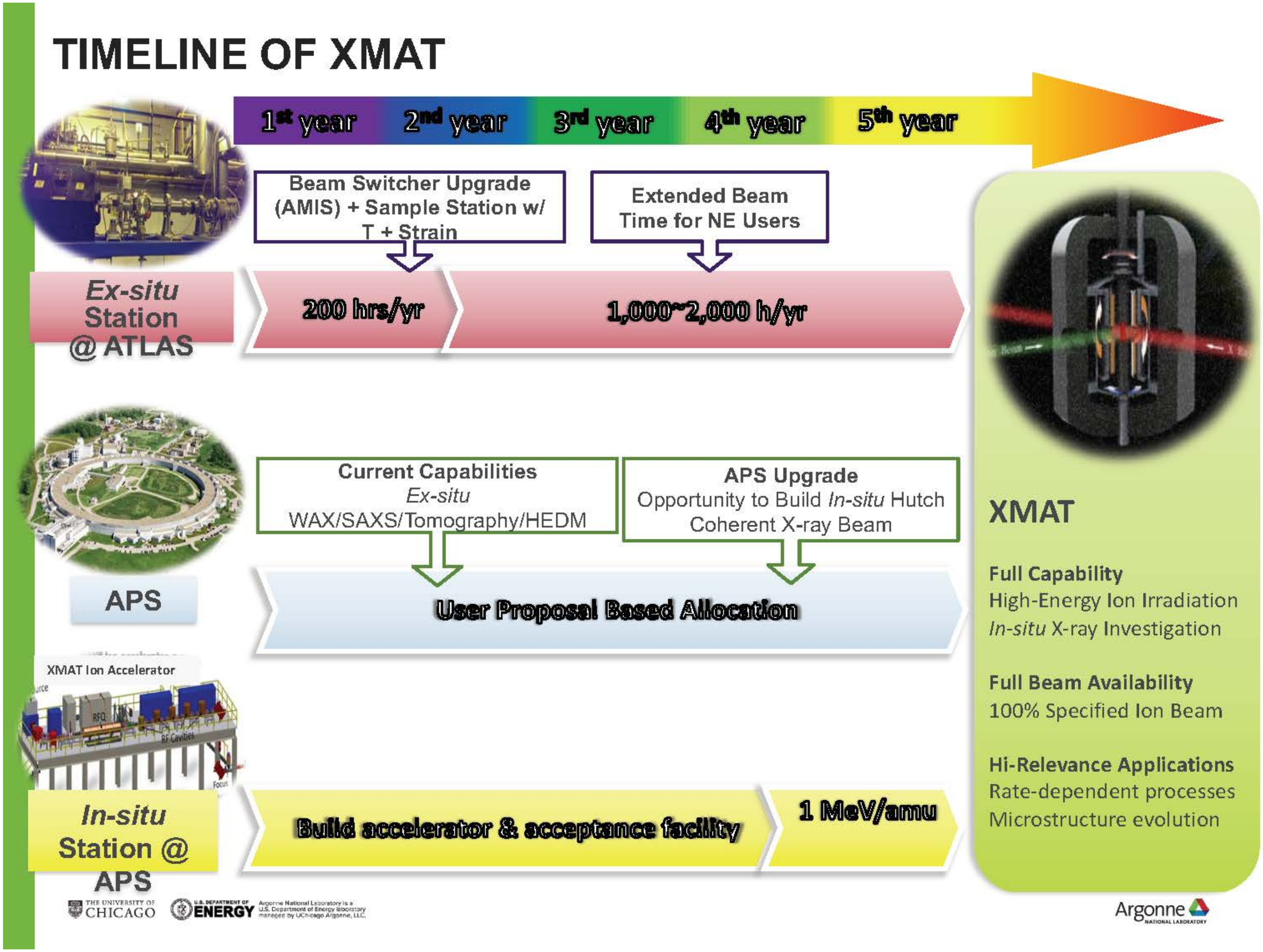
In-situ monitoring the changes in mechanical properties, and microstructures during ion irradiations

Opportunity Window -> APS/ATLAS Upgrades

RANKING OF XMAT IN RELATION TO OTHER ION IRRADIATION FACILITIES IN THE US



Overall score and ranking of the ion beam facilities, "NSUF ION BEAM INVESTMENT OPTIONS WORKSHOP," INL/EXT-16-38957, March 22-24, 2016


TIMELINE OF XMAT
1st year
2nd year
3rd year
4th year
5th year
Beam Switcher Upgrade (AMIS) + Sample Station w/ T + Strain
Extended Beam Time for NE Users
Ex-situ Station @ ATLAS
200 hrs/yr
1,000~2,000 h/yr
Current Capabilities
Ex-situ
WAX/SAXS/Tomography/HEDM
APS Upgrade
Opportunity to Build In-situ Hutch
Coherent X-ray Beam
APS
User Proposal Based Allocation
XMAT Ion Accelerator
RFQ
RF Cavities
Focus
In-situ Station @ APS
Build accelerator & acceptance facility
1 MeV/amu
XMAT
Full Capability
High-Energy Ion Irradiation
In-situ X-ray Investigation
Full Beam Availability
100% Specified Ion Beam
Hi-Relevance Applications
Rate-dependent processes
Microstructure evolution
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Argonne

KEY XMAT ADVANCES

In comparison to most existing ion irradiation capabilities, the XMAT ion energies and currents are ~100 times higher. The increased ion irradiation energy (e.g., 133 MeV for xenon) enables several critical advances:

- It provides a unique opportunity to simulate the effects of fission fragments in nuclear fuels, where ions of all elements can be accelerated to fission fragment energies, while being characterized *in situ*.
- For cladding and structural materials, the increased penetration depth of energetic ions allows the "bulk behavior" to be examined, eliminating surface-sink effects, and allows understanding of individual physics of ion damage including electronic, collisional, & added interstitial
- The in situ penetrating ability of the APS focusable hard x-rays, applied during ion irradiation, is another key advancement of XMAT that allows the interrogation of individual grains within solid material samples during irradiation.
- With this information and related computational modeling, the differences between ion and neutron irradiation as well as the impact of fission products damage become much more understandable.

XMAT can close the design loop for the entire nuclear materials community in two ways:
1)It provides accelerated testing for hundreds to thousands of samples (24; 7)
2)It reveals the key "single" physics dependences required for accurate computational modelling

APPENDIX D - Fission Accelerated Steady-State Testing (FAST) in Nuclear Fuel Development

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Fission Accelerated Steady-State Testing (FAST) in Nuclear Fuel Development

Geoffrey (Boone) Beausoleil, Kyle Paaren, Matthew Kerr, and Steve Hayes
Nuclear Fuels and Materials Division, Idaho National Laboratory

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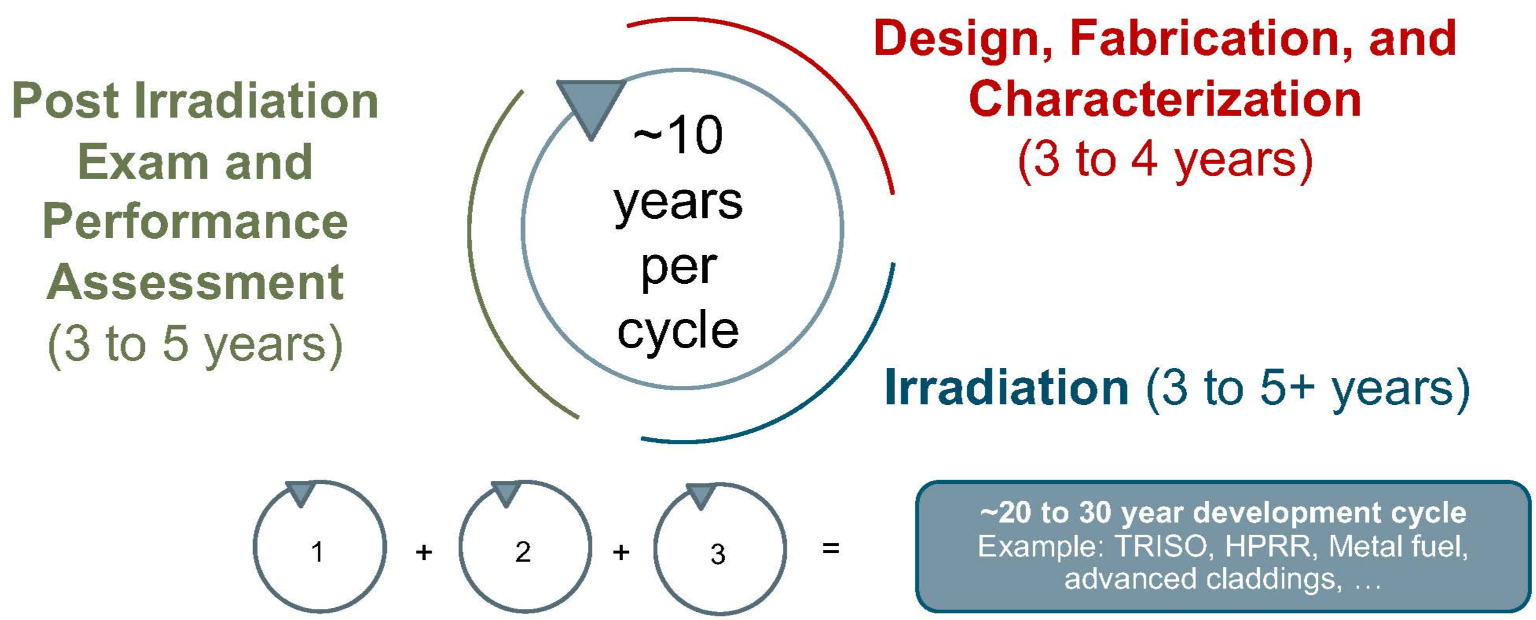
Current Nuclear Development Cycle



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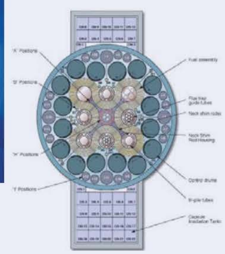
DOE's Standard Fuel Testing Reactors

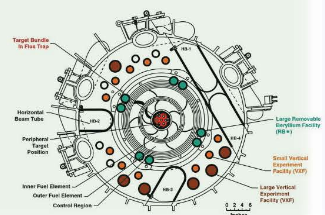


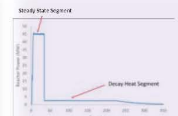
ATR:

- Water-cooled plate-type MTR started 1967, still one of the newest and most advanced MTRs today
- Serpentine driver core creates nine flux traps and numerous other test positions
- High flux, large useable test geometries (1.2 m long core), and high capacity factor (for an MTR, ~200 day/yr)
- Rich history of burnup accumulation in capsules, instrumented lead outs, & pressurized water loops
- Transient power-cycling via specimen insertion/removal device

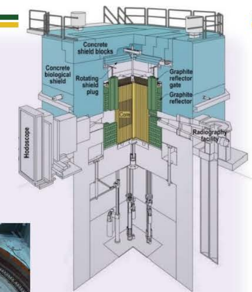
HFIR:

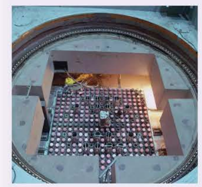
- Water-cooled plate-type MTR started 1965
- Two involute plate rings create very high flux in center trap and other reflector positions
- Unrivalled isotope production and neutron beamline capabilities
- Unique material/fuel irradiation capabilities for properties evolution, separate effects, and model validation

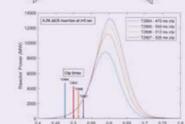




LOCA Transient







RIA Transient

TREAT:

- Graphite-based transient reactor started in 1959
- Unparalleled transient shaping capability (milliseconds to minutes)
- Operated until 1994 focused largely on SFR testing
- Restarted 2018, demonstrated transient capabilities for LWR (RIA & LOCA)
- First fueled water capsule irradiated just weeks ago

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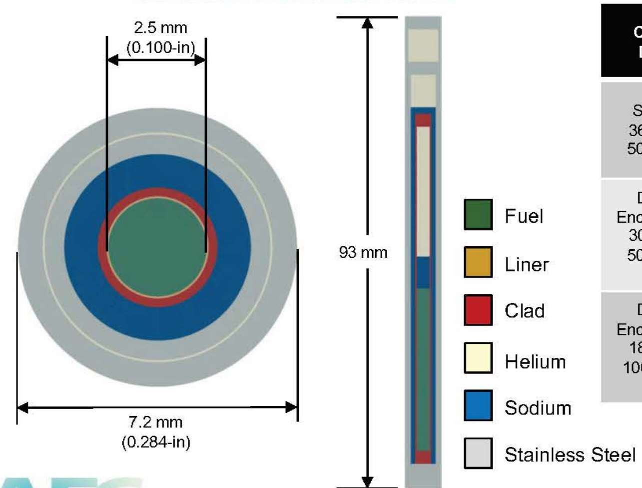
Nuclear Energy

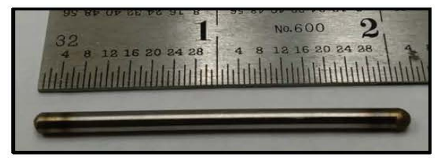
Approach to Accelerated Integral Fuel Testing (Fission Accelerated Steady-state Testing)

- **Revised Capsule Design Objectives:**
  1) Increase burnup rate for fuel experiments: reduce time to achieve high burnup
  2) Improve experiment reliability: reduced sensitivity to fabrication tolerances and capsule/pin eccentricity
  3) Double capsule design allows experiment tenability to variety of prototypic conditions and fuel forms

Fabrication and assembly for FAST Phase 1 is underway



Capsule Design	Cases	Max. Inner Clad Temp (C)	Min. Inner Clad Temp (C)	Peak Fuel Temp (C)
Standard 365 W/cm 50 μm gap	0 μm offset	572	572	709
	25 μm offset	605	483	695
	Difference	+33	-89	-14
Double-Encapsulated 300 W/cm 50 μm gap	0 μm offset	570	570	684
	25 μm offset	567	523	664
	Difference	-3	-47	-20
Double-Encapsulated 180 W/cm 100 μm gap	0 μm offset	566	566	637
	25 μm offset	566	556	629
	Difference	0	-10	-8



One-half diameter pins could achieve ~5% burnup/ATR 55-day cycle and reach 30% burnup in less than 3 years.

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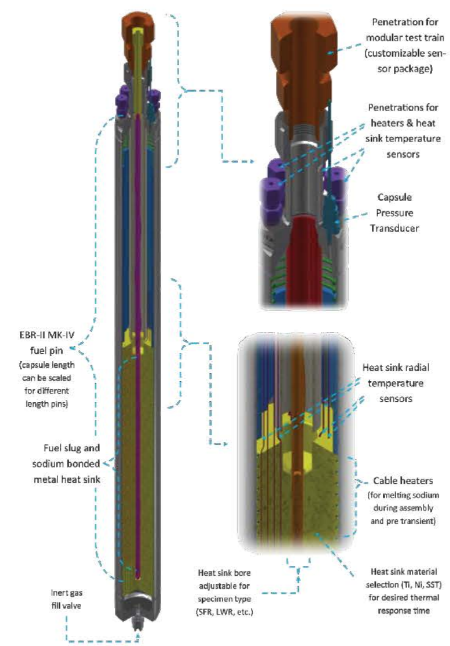
TREAT-THOR Testing

Temperature Heat-sink Over-power Response (THOR) capsule

- **Thick wall heat sink capsule with liquid metal bond (sodium) to specimen**
- **Easy way to get heat transfer without the cost of a full loop**
- **Concerted with TREAT transient power shaping to created desired temperature response (milliseconds to minutes)**

AFC, JAEA, and NSUF efforts underway for FY21 testing

- **SFR fuel temperature response during early stages of overpower transients**
- **Phase-based radial thermal conductivity measurement (oscillating transient)**
- **Power to melt studies for SFR fuel**



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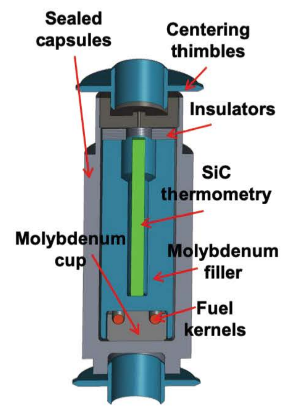
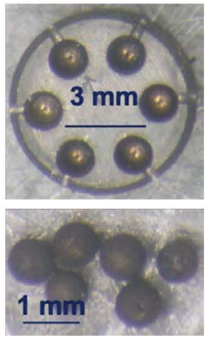
HFIR: MiniFuel Testing Capabilities

- **Recently commissioned MiniFuel Capability**
  - Burnup accumulation of small specimens (~1mm particle and disc scale)
  - More for microscopists than engineers, clever way to produce specimens for small-scale phenomena PIE
  - Specimen to “filler” hardware volume ratio yields ~constant temperature irradiations relatively independent of fission rate
  - Gamma-heated filler design can affect different target temperatures, life avg measured in PIE by passive SiC thermometry
- **Current efforts already underway**
  - First UN irradiations recently performed
  - AFC U-Zr irradiations presently under preparation
- **Value potential to be evaluated**
  - RUSL experiments can give the first look at fresh fuel phase stability vs. temp/fission-rate
  - MiniFuel can add the fission damage effect





MiniFuel capsule (left) and PIE of UN fuel kernels irradiated to ~10 MWd/kg U (right)

Images courtesy of C. Petri

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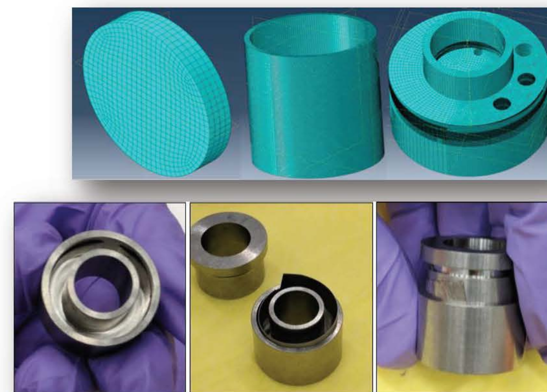
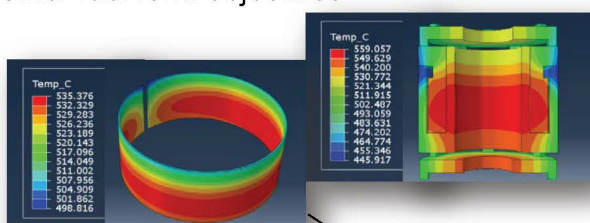
DISECT Separate Effects Testing at BR-2

NSUF project that can be adopted into ATR

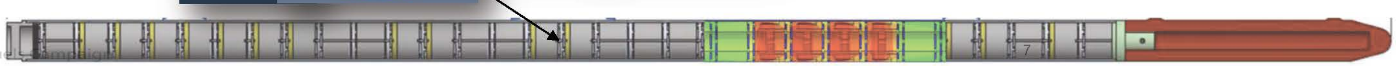
- Separate effects irradiation test at BR-2 in Belgium
- PIE planned at INL
- DISECT vehicle allows for customization of sample holder to meet the needs of the experiment
- Two approaches are being used for this irradiation
  - U-Zr foils are placed in a zirconium housing with customized internal volume to accommodate swelling and act as a plenum for fission gasses.
  - U-Mo 3mm diameter TEM punches are placed in an aluminum holder.
- Can be tailored to meet other fuel form objectives

DISECT sample holders.
Top) Illustration of U-Mo TEM punches in aluminum housing.
Bottom) U-Zr foil in zirconium housing





Abaqus thermal rendering of U-Zr housing (Top) and U-Zr foil (Bottom)



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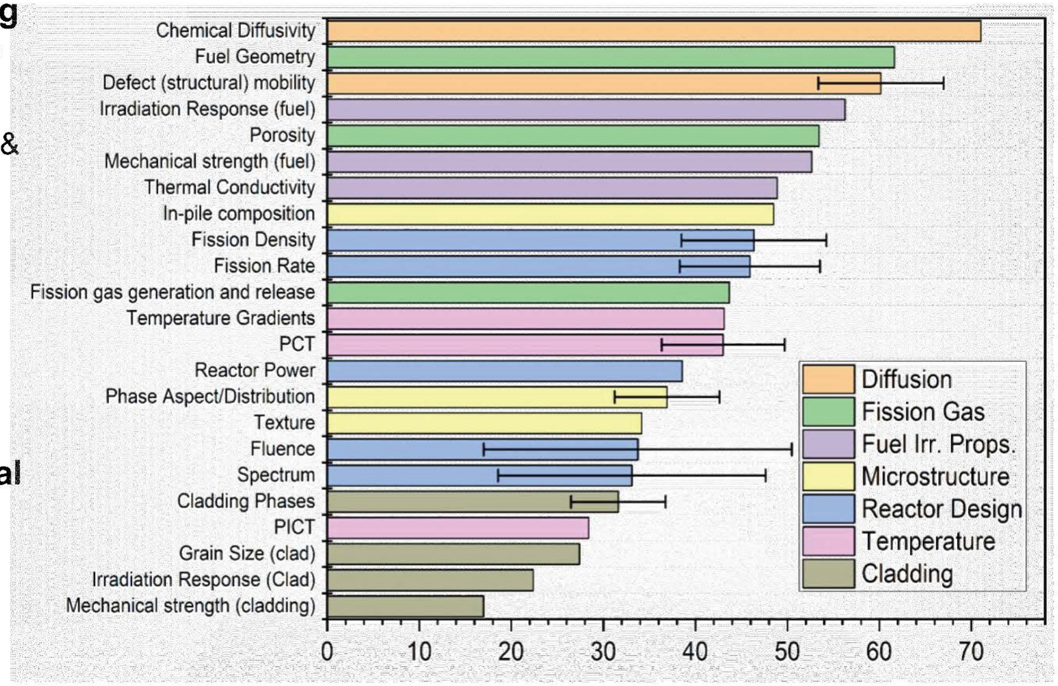
PIRT Analysis and Prioritized Strategy

- **INL stood up an accelerated testing working group that spans multiple laboratories and programs**
  - Contributors from across INL, LANL, & ORNL as well as AFC and NEAMS
- **Phenomenon Identification and Ranking Table analysis was performed**
- **Identified key focus areas for modelling and simulation needs**
- **Provided guidance for experimental objectives and data acquisition**
- **Coordinated AFC-NEAMS milestones based on results**



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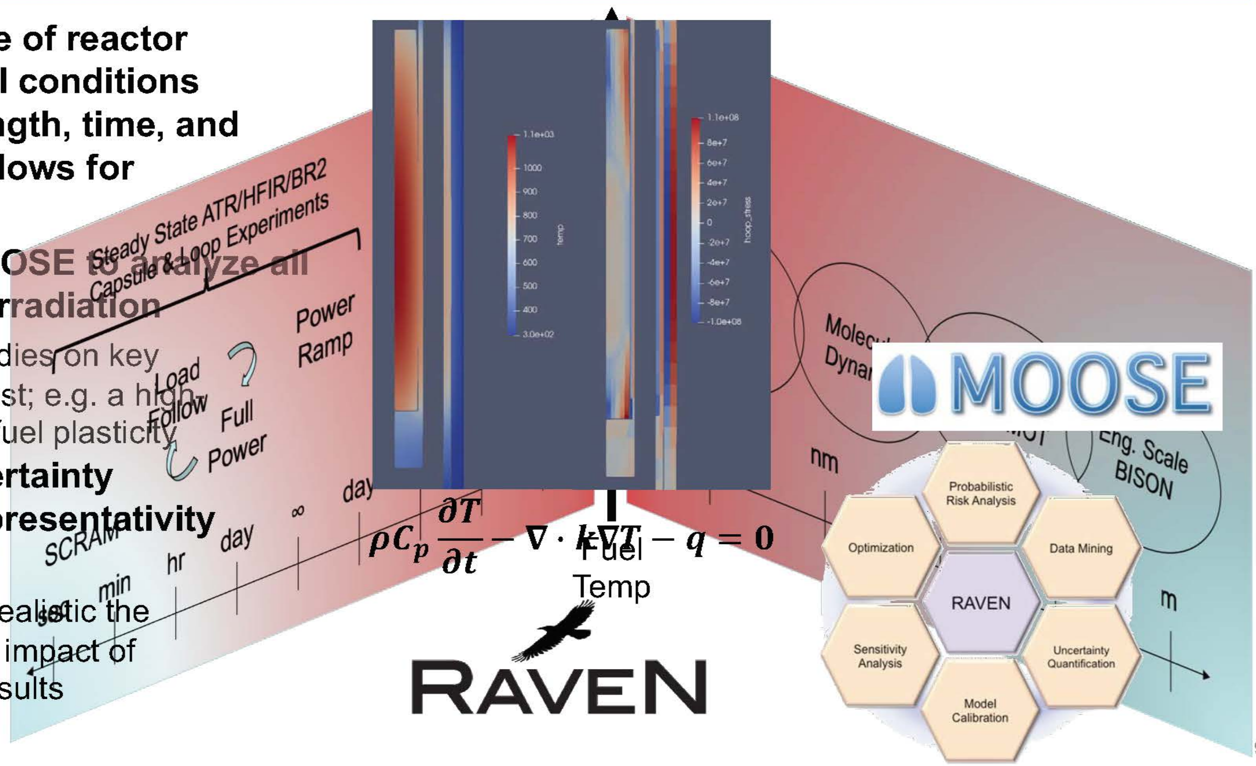
Experiment & Model-Simulation Synergy

- **Coupling a wide range of reactor conditions with model conditions across a variety of length, time, and temperature scales allows for optimized R&D**
- **Utilize BISON and MOOSE to analyze all experiments prior to irradiation**
  - Perform bounding studies on key phenomenon of interest; e.g. a high-medium-low study of fuel plasticity
- **Utilize Raven for uncertainty quantification and representativity analysis**
  - Able to quantify how realistic the experiment is and the impact of uncertainties to the results



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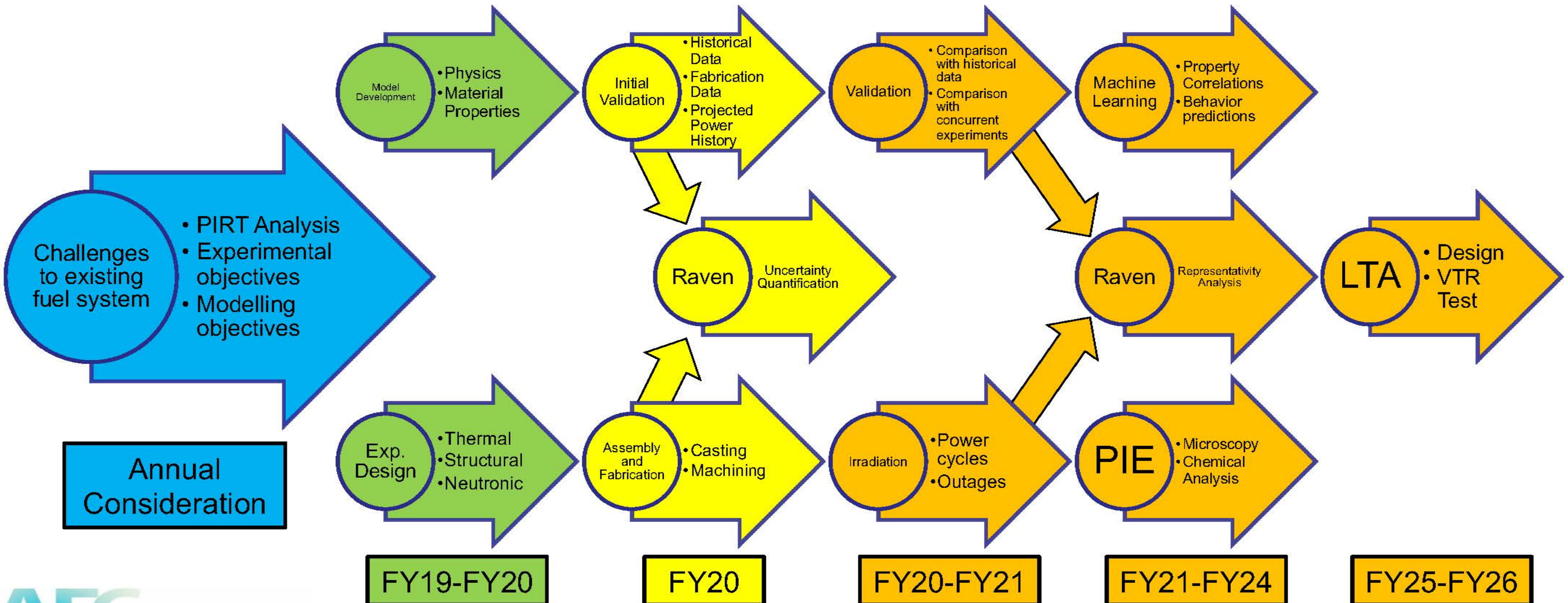
Accelerated Testing within AFC

- AFC-ATWG relationship between experimental programs and modelling/simulation



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Experiment Schedule Strategy for Metal Fuels

2020 | 2021 | ATR Core Internal Change-out | 2022 | 2023 | 2024 | 2025 | 2026 | 2027

AFC-3, -4, -IRT Cont.

FAST Phase-1

FAST Phase-3: SI & H

FAST Phase-2

Post-Irradiation Furnace Tests on FAST Phase-1

Na-Loop Fresh Tests

Fresh fuel tests THOR Capsule

Pre-irradiated fuel tests, THOR Capsule

Na-Loop Pre-Irr. Tests (baseline fuel)

Na-Loop Pre-Irr. Tests (Advnaced fuel)

MiniFuel Metallic Fuel Test, ORNL

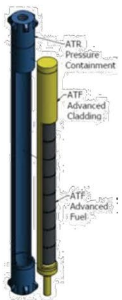
DISECT Fuel Test (BR-2)

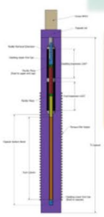
MiniFuel-Metal PIE, INL

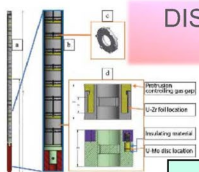
DISECT Fuel PIE, BR-2 and INL

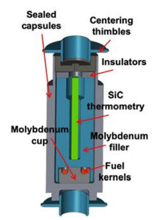
Begin VTR Loop Tests →

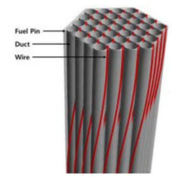
Begin VTR G2 LTA →

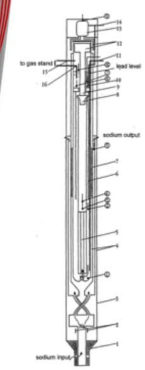












5 Year Period of AFC's Transformation toward Industry-Endorsed Fuel Qualification Framework

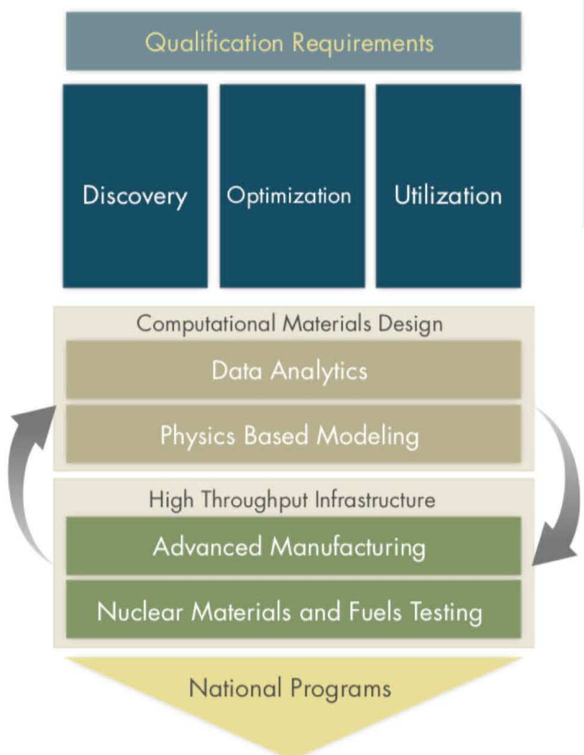
AFC Advanced Fuels Campaign

FAST is Beyond Metal Fuel…

- **FAST is performing extensive metal fuel irradiations**
  - But FAST was originated to support more than just SFR metal fuel development
- **Vendor Support**
  - Being adopted for UC irradiations with GA via LDRD
  - Scoping studies for supporting Oklo fuel concepts
- **Supporting pre-irradiation of novel LWR fuel concepts from LANL for TREAT testing**
- **Adopted as irradiation platform for the NNSA Advanced LEU concepts**

NMDQi Nuclear Materials Discovery and Qualification Initiative

Idaho National Laboratory



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.

APPENDIX E - Appendix E: Fuel Performance Modeling and Fuel Qualification at TerraPower

Fuel Performance Modeling and Fuel Qualification at TerraPower

James Vollmer and Sam Miller

Tight Integration Between Testing and Modeling

- One of TerraPower's strengths has been the tight integration between modeling and testing activities
  - Often a necessity due to aggressive performance and schedule targets
  - Pushing the envelope for fuel burnup, lifetime, and fast fluence
  - Need to make design decisions with limited information
  - Needed to start testing early to achieve targets
- Small teams forced integration of activities
  - Fuel performance model development
  - Fuel performance assessments to support core design
  - Fuel and material fabrication development
  - Fuel and material testing (in-pile and out-of-pile)
  - Overall support of fuel qualification

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Flow Down of Requirements

- Established fuel regulatory acceptance criteria that correspond to what is covered in the Standard Review Plan, making revisions as necessary to cover sodium fast reactors
- Revised fuel design criteria/bases to assure one-to-one coverage of the established fuel regulatory acceptance criteria
- Fuel Qualification Plans prepared to assess testing and analysis activities required to justify and assess compliance with fuel design criteria

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Fuel Qualification Plans

- Fuel qualification plans prepared to identify activities needed to:
  - Justify fuel system damage criteria
  - Justify fuel pin failure criteria
  - Justify fuel coolability criteria
  - Justify control rod insertability criteria
  - Establish fuel system description
  - Establish and validate methods for fuel system design evaluation

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Fuel Qualification Plans (cont.)

- Establish testing and inspection plans/specifications for new fuel
- Establish methods and programs for online fuel system monitoring
- Establish post irradiation surveillance plans/programs

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Justifying Fuel Design Limits & Evaluation Methods Have Been Main Priority

- Evaluated and summarized available data to set and justify initial fuel design limits
- Wherever practical identify additional testing to verify acceptability of established limits using TerraPower materials
- Develop correlations and computational methods to analyze designs to verify limits are met
  - Correlations/methods to cover high impact phenomena
  - Identify validation needs for phenomena correlations and methods

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Phenomena Identification Ranking Tables (PIRTs) Help Guide the Process

For each design limit and targeted condition list all phenomena required to assess performance.
Rank importance and knowledge for each phenomenon.

Importance Rank	Definition
Low (L)	Variation of parameter has minimal impact on assessment of design criterion
Medium (M)	Variation of parameter has moderate impact on assessment of design criterion
High (H)	Variation of parameter has significant impact on assessment of design criterion

Knowledge Level	Definition
High (H)	Known
Medium (M)	Partially Known
Low (L)	Unknown

PIRT process ensures that key fuel phenomena are identified and understood

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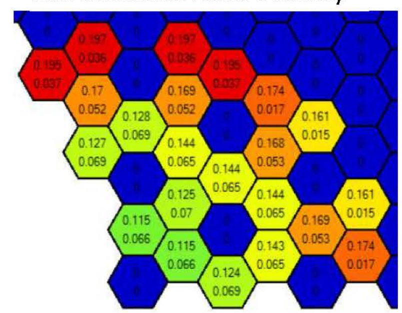
PIRT Evaluation Identifies Key Fuel Phenomena

Design Criteria (Limits)	Purpose of Limit	Key Parameters that Influence Criteria
Thermal Creep Strain in Cladding	Prevent cladding rupture or coolant flow blockage	• HT9 Properties/Constituent Model • FCCI Clad Wastage • Fission Gas Release
Total Strain (Thermal plus Irradiation Enhanced Creep and Swelling)	Prevent mechanical interaction and coolant flow blockage	• Fission Gas Release • HT9 Properties/Constituent Model
Peak Fuel Temperature	Prevent fuel melting	• Fuel Thermal Conductivity • Axial Growth
Peak Cladding Temperature	Prevent cladding failure due to fuel-clad eutectic reactions	• Coolant Temperature
Cladding Wastage	Prevent cladding rupture or coolant flow blockage	• FCCI Clad Wastage

Fuel Performance Tools at TerraPower

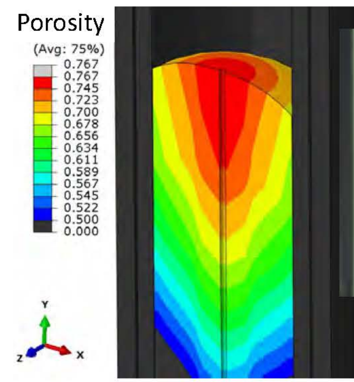
Crucible – Fast, integrated with ARMI®, aimed at key design criteria during normal operation for all assemblies:

- Sodium-bond transport
- Fission gas release transport
- Fuel axial growth
- Cladding wastage
- Temperatures
- Cladding Strain



ALCHEMY® – FEA model for high-fidelity calculations

- Steady-state and transient behavior
- High-fidelity strain and temperatures
- Cladding damage models
- Capsule models for ATR/MITR/TREAT testing
- Absorber pin models (B_4C)
- "Structural" material models are used elsewhere
  - OXBOW
  - Pin attachment hardware (pin rails, endcaps, etc.)



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Fuel Performance Model Philosophy

Focus:

- Modeling key criteria necessary for design and licensing
- Collecting and analyzing experimental data
- Automation and efficiency of tools

Use fundamental equations and models where appropriate:

- General thermo-mechanical FEA models (ALCHEMY®)
- Structural materials creep and swelling models
- Fuel deformation

Use empirically-based models and avoid overly complex models: (*minimize number of unknown model constants*)

- Gas release model
- FCCI model
- Creep damage model
- Axial growth model
- Fuel conductivity change due to irradiation

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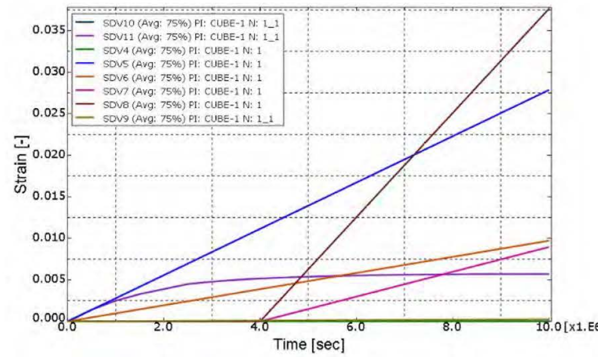
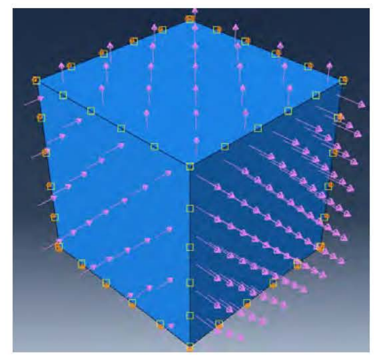
ALCHEMY® Verification: Separate & Mixed Effects Testing

Constitutive Model Benchmark Tests:

- Model tests use a variety of 2D and 3D element types and geometries, under various loading conditions
- Structural material models
  - Thermal & Irradiation Creep
  - Stress-free and Stress-Enhanced Swelling
  - Irradiation Hardening
- Fuel constitutive models
  - Porous Plasticity & Creep
  - Fission Gas Behavior
  - Thermal Behaviors



Plot of an integration test showing the complex HT9 strain behavior



3D Triaxial Load Creep Integration Test

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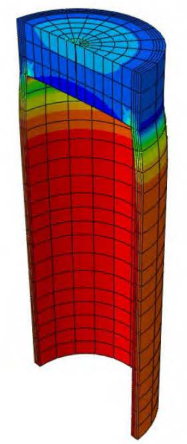
Cladding Deformation Mechanisms

Models for HT9 (multiple), SS316, D9, other steels & materials

8 mechanisms of deformation:

- Stress-Free Swelling — $f(dpa, T)$
- Stress-Enhanced Swelling — $f(dpa, T, \sigma)$
- Linear Irradiation Creep — $f(dpa, \sigma)$
- Non-linear Irradiation Creep — $f(dpa, T, \sigma)$
- Primary Thermal Creep — $f(T, \sigma, \varepsilon)$
- Diffusional Thermal Creep — $f(T, \sigma)$
- Power-Law Thermal Creep — $f(T, \sigma)$
- Visco-Plasticity — $f(T, \sigma)$



❖Each of these mechanisms has an effective regime where the mechanism has a strong effect.

❖Models informed by recent TerraPower testing

❖During *steady-state operation*, Power-Law Thermal Creep and Visco-Plasticity should <u>not</u> be dominant mechanisms (σ<<Yield Strength)

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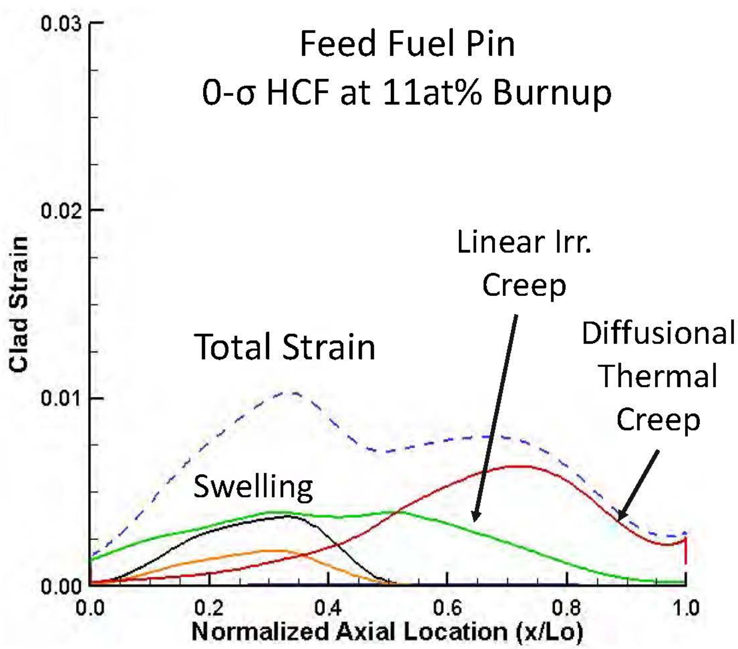
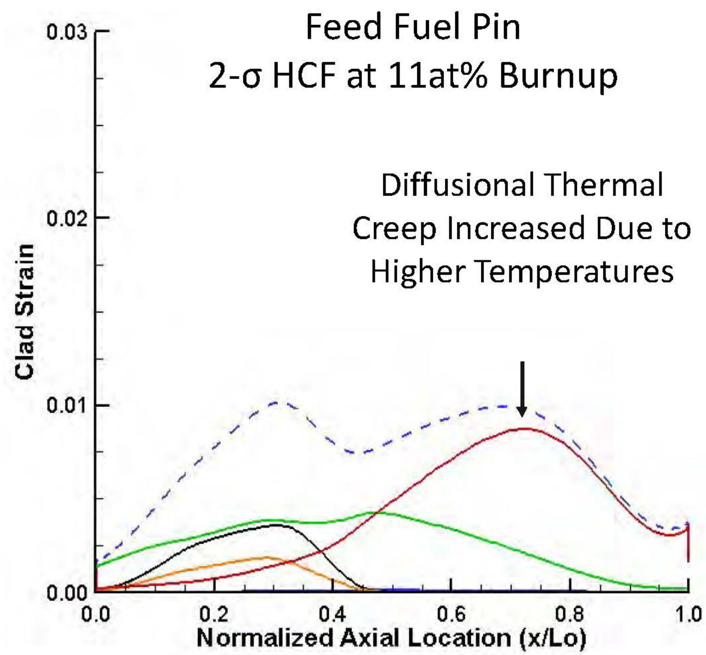
Sample Fuel Pin Clad Strain Profile Predictions





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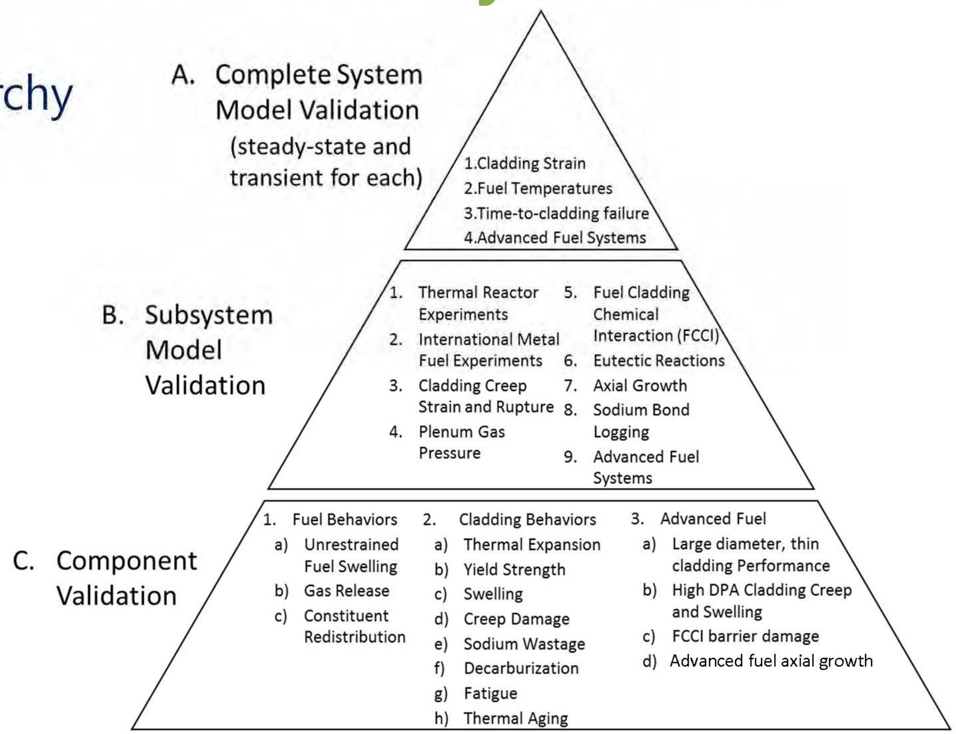
ALCHEMY® Validation Hierarchy & Phases

3 Levels of Validation Hierarchy

- Component
- Subsystem
- Complete system

3 Validation Phases

- Phase 1: Demonstrate general adequacy for modeling sodium-bonded metallic fuel (in this phase)
- Phase 2: Qualify ALCHEMY® for licensing SFR sodium-bonded fuel
- Phase 3: Qualify ALCHEMY® for licensing advanced TWR fuel systems (with additional testing)



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Historic Fuel Reports and Database Effort to Support Validation

- Dedicated effort to compile, digitize, and analyze metallic fuel data from EBR-II and FFTF to create a fuel performance database to support ALCHEMY® validation
- Phased approach to progressively expand the number of benchmark cases as we develop and improve ALCHEMY's functionality
- Primary focus has been HT9-clad pins, but we do have 316 and D9 pins in our plans to validate applicability to other cladding materials
- Topical reports of fuel phenomena have also been prepared to support correlation development and sub-model validation
  - Axial growth, fission gas release, FCCI, eutectic interactions

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Status of Historic HT9-Clad Fuel Pin Reports

Assembly	Fuel Type	As-Built Report	Irradiation History Report	Profilometry Report	Additional PIE Results
X425	U-10Zr, U-8Pu-10Zr, U-19Pu-10Zr	X	X	X	X
X430	U-10Zr, U-19Pu-10Zr, U-22Pu-10Zr, U-26Pu-10Zr	X	X	X	X
X431	U-2Zr, U-6Zr, U-10Zr			X	X
X432	U-2Zr,U-6Zr,U-10Zr			X	X
X441	U-19Pu-6Zr, U-19Pu-10Zr, U-19Pu-12Zr	X	X	X	X
X447	U-10Zr	X	X	X	X
X496	U-10Zr				X
MFF-2	U-10Zr	X	X	X	X
MFF-3	U-10Zr	X	X	X	X
MFF-5	U-10Zr	X	X	X	X
MFF-6	U-10Zr	X	X	X	X
X448	U-10Zr				X
X451	U-10Zr				X

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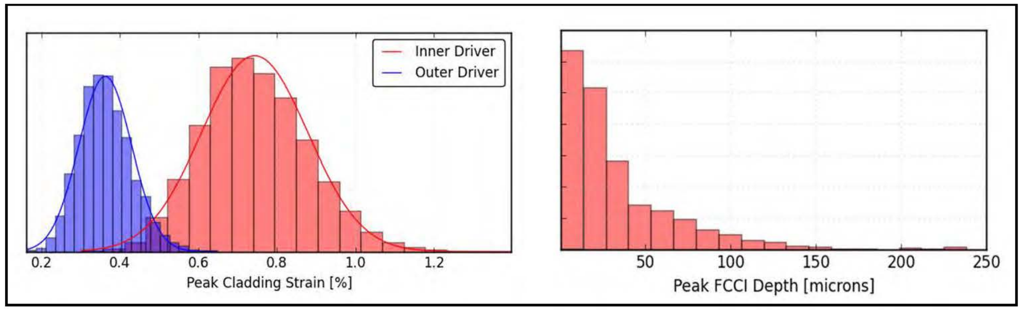
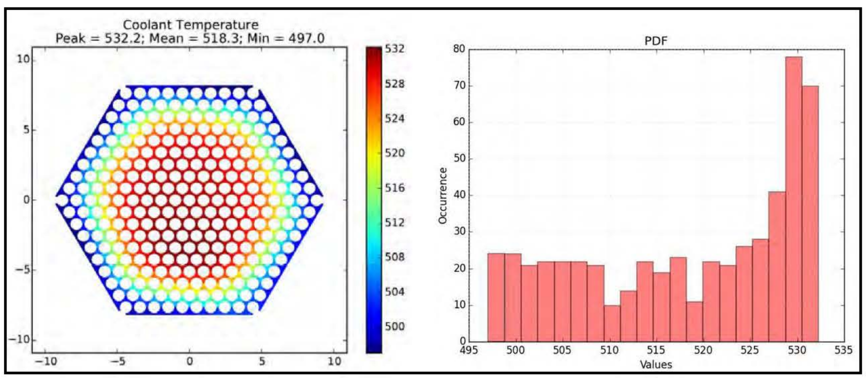
Uncertainty Propagation – Core Assessment

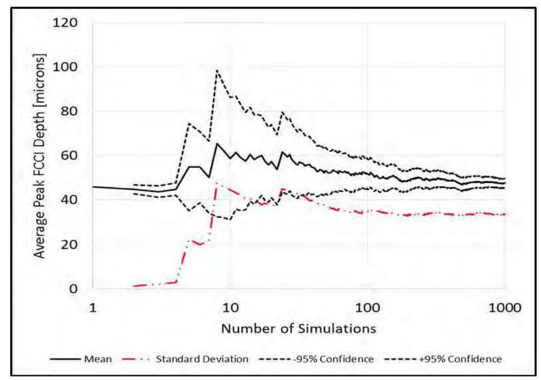
Probability distributions developed for key model inputs/parameters

- Coolant temperature distribution
- FCCI wastage
- Fission Gas Release

Parameters sampled stochastically to determine prediction intervals for key design criteria







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Conclusions

- Rely heavily on PIRT process to prioritize testing and modeling needs to provide high confidence in overall fuel performance
- Using a phased approach for fuel performance validation, including validation of sub-models for key phenomena
  - Account for all key phenomena in fuel performance
  - Quantify uncertainties for these sub-models
- Uncertainty propagation methodology allows us to assess the impacts of these uncertainties and tailor the fuel/core design, test program, and/or planned surveillance program to best address the uncertainties

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APPENDIX F - Fuel performance simulations of swelling, fission gas release and creep in U_3Si_2 informed by atomistic simulations

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Fuel performance simulations of swelling, fission gas release and creep in U_3Si_2 informed by atomistic simulations

David Andersson, Michael Cooper, Xiang-Yang Liu, Christopher Matthews, Chris Stanek
MST-8, Los Alamos National Laboratory

Benjamin Beeler, Larry Aagesen, Kyle Gamble, Jason Hales, Giovanni Pastore, Richard Williamson
Idaho National Laboratory

Acknowledgements, goal and outline

- **Acknowledgements:** Work funded under the NEAMS ATF HIP project and CASL (NRC pilot) – **collaboration with WEC** - still ongoing (but being wrapped up) under the Joint Modeling and Simulation program.
- **Goal of presentation:** Demonstrate how lower length scale (LLS) simulations can be used to fill data gaps for new fuels and be applied in qualification relevant fuel performance simulations validated against irradiation tests.
  – Exemplified for U_3Si_2, but much of the methodology and most associated challenges extend to other fuels as well, including metal fuel, UN, UC, etc.
- **Outline of presentation**:
  – Background and problem overview.
  – DFT calculations of U_3Si_2 thermodynamics and intrinsic Xe, U and Si diffusion.
  – MD simulations of species transport due to irradiation induced ballistic mixing.
  – Cluster dynamics simulations of irradiation-enhanced thermally activated diffusion informed by DFT and MD.
  – Phase-field simulations of bubble percolation threshold.
  – Bison implementation of LLS models.
  – Application to U_3Si_2 ATR irradiation tests.
  – Conclusions and lessons learned.

Hierarchic multi-scale modeling

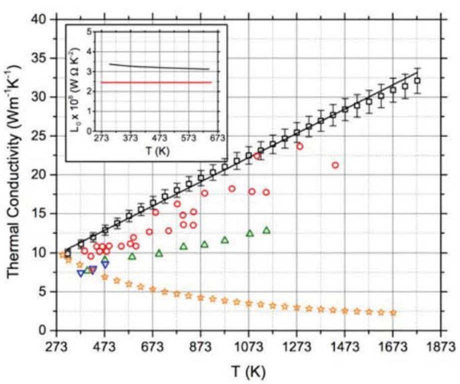
Accelerated fuel qualification and multi-scale fuel performance

- Multi-scale fuel performs modeling and simulation refers to engineering scale fuel analysis performed with models and model parameters derived from a combination of experiments and lower length scale modeling.
- Experiments and modeling are used as complementary tools to improve understanding, model accuracy and ability to use models for extrapolation (predictability) throughout the design and qualification process.
  - Opportunities also exist in discovery and screening space.
- Modeling should be used to derive maximum value; apply to problems where experiments are hard/expensive or where the additional understanding helps qualification.
- Integral testing for validation is still going to be critical, but multi-scale fuel performance may help develop a smaller test matrix.

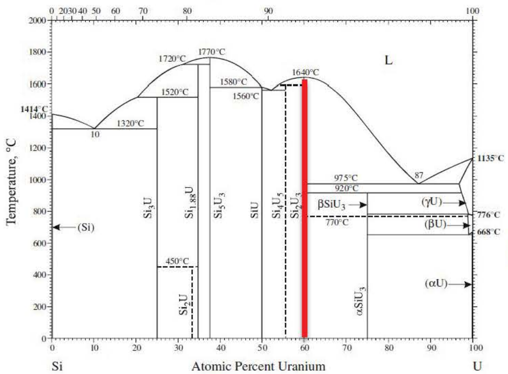
U_3Si_2 as ATF for LWRs

- U_3Si_2 is one of the concepts proposed as Accident Tolerant or Advanced Technology Fuel in response to the Fukushima accident and economic drivers (WEC).
- High thermal conductivity reduces temperature of pellet - less energy stored and increased coping time during an accident – possibly lower fission gas diffusion.
- Higher U density gives economic benefits.
- Oxidation is a concern upon cladding breach.
- The simulation approach would be similar for other fuels.

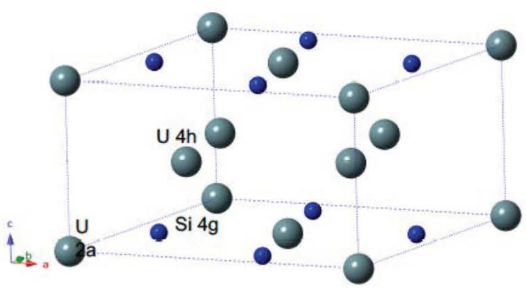
High U_3Si_2 conductivity



U_3Si_2 phase diagram

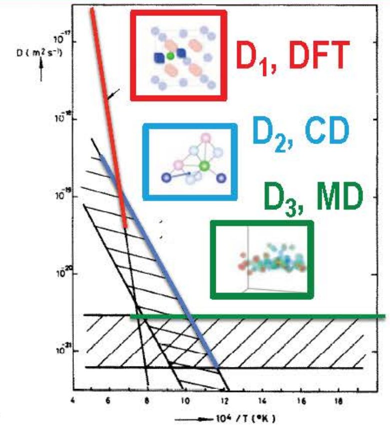


U_3Si_2 crystal structure



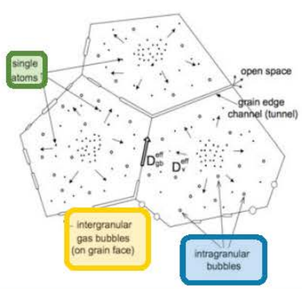
Development of atomistic models for U_3Si_2

- A data poor fuel:
  - Less operational experience than doped UO_2.
  - More material properties will be different relative to standard fuel.
- Study of self-diffusion, point defect mobility, and fission gas diffusion has relevance to:
  - fission gas release,
  - swelling,
  - and creep models for U_3Si_2.
- Like UO_2 bulk diffusion in U_3Si_2 has three regimes (D_1, D_2, and D_3)
  - The same methods that work for UO_2 are being extended to U_3Si_2.
- Investigation of grain boundary diffusion as input to creep and swelling models.
- Results inform engineering scale fuel performance models in Bison.



Fission gas in the grain

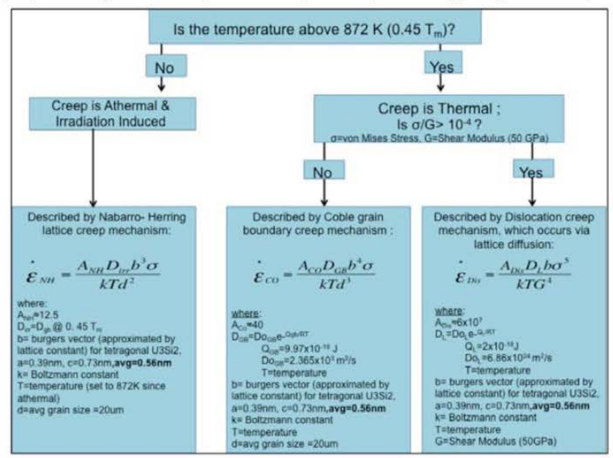
$$\frac{\partial C_t}{\partial t} = D_{eff}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_t}{\partial r}\right) + \beta$$



Bubble growth at grain boundaries

$$\frac{dn_v}{dt} = \frac{(2\pi D_v \delta_g)}{kTS}(p - p_{eq})$$

U_3Si_2 creep model, developed by Metzger (UofSC)



Modeling point defects, self-diffusion and Xe diffusion

Atomic/electronic scale

- DFT to calculate defect formation and migration energies.
  - 2x2x3 supercell, GGA+U to stabilize the U_3Si_2 crystal structure.
- DFT to calculate phonon spectra and defect entropies.
  - Finite displacement method with 2x2x2 supercell.
  - Only the most important attempt frequencies for diffusion were calculated.
- The tetragonal crystal structure of U_3Si_2 means that the diffusivity is a tensor property.

For details: D. A. Andersson, et al., "Density functional theory calculations of self-and Xe diffusion in U_3Si_2", J. Nucl. Mater. **515**, 312-325 (2019).

Thermodynamic averaging

Defect concentrations from formation energies and entropies (dilute limit):

$$E_{A_B,f} = E\left(A_B, N \pm 1\right) \mp e_B - E\left(N\right)$$

$$S_{A_B,f} = S\left(A_B, N \pm 1\right) \mp s_B - S\left(N\right)$$

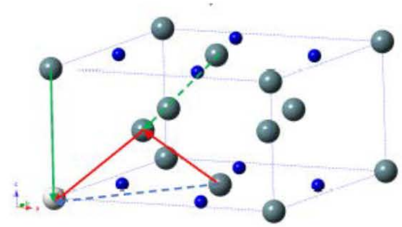
$$c_{A_B} = z_{A_B} \exp\left(-\frac{F_{A_B,f}}{k_B T}\right)$$

- Xe trap incorporation energies, vacancy-trap site binding energies and barriers for interstitial and vacancy assisted migration mechanisms calculated from DFT.
- Entropies from DFT following the approach for point defects.

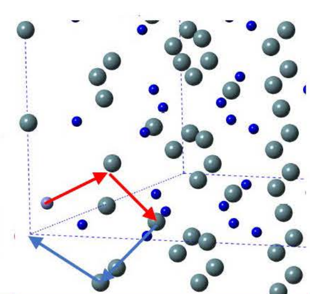
Kinetic theory

The components of the self-diffusion tensor calculated by summing over all possible pathways:

$$D_B^R = \sum_{A_B} u_{A_B} D_{A_B,0}^R \exp\left(-\frac{E_{A_B,m}^R}{k_B T}\right)$$

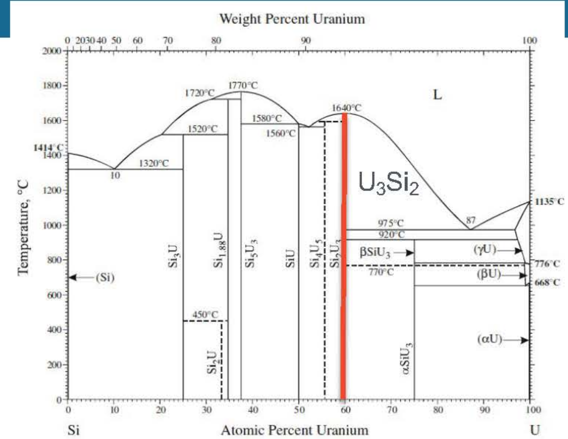


$$D_{Xe}^R = \sum_X y_{Xe_X,Xe} y_{Va} m_{Xe_X,Va} \cdot \exp\left(-\frac{F_{Xe_X,b}}{k_B T}\right) D_{Xe_X,0}^R \exp\left(-\frac{E_{Xe_X,m}^R}{k_B T}\right)$$

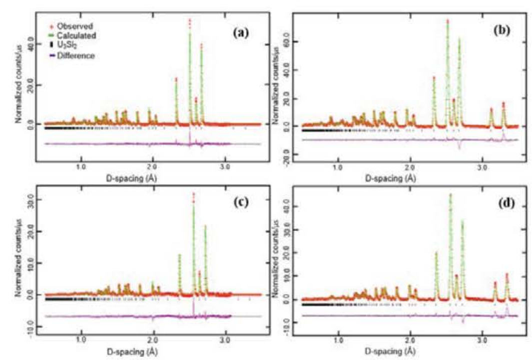


Defect concentrations from DFT

Experiments



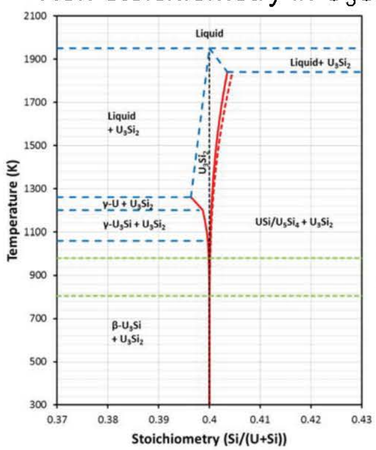
Neutron diffraction by T.L. Wilson et al.[3]



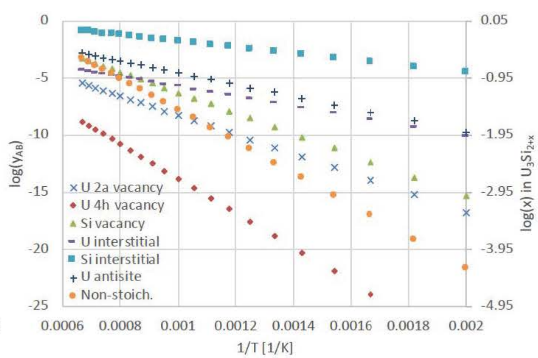
- **High concentration of Si interstitials** predicted from DFT (energy+entropy)[1], even higher non-stoichiometry than in Middleburgh et al.[2]
- Non-stoichiometry disagrees with the available phase diagram, but recently confirmed by neutron diffraction experiments on $U_3Si_{2.01}$[3].
- Non-stoichiometry of U_3Si_{2+x} matters, because of burnup evolution.

Predictions from atomic scale simulations

Non-stoichiometry in U_3Si_2[1]



Defect concentrations and non-stoichiometry in "nearly" stoichiometric U_3Si_2

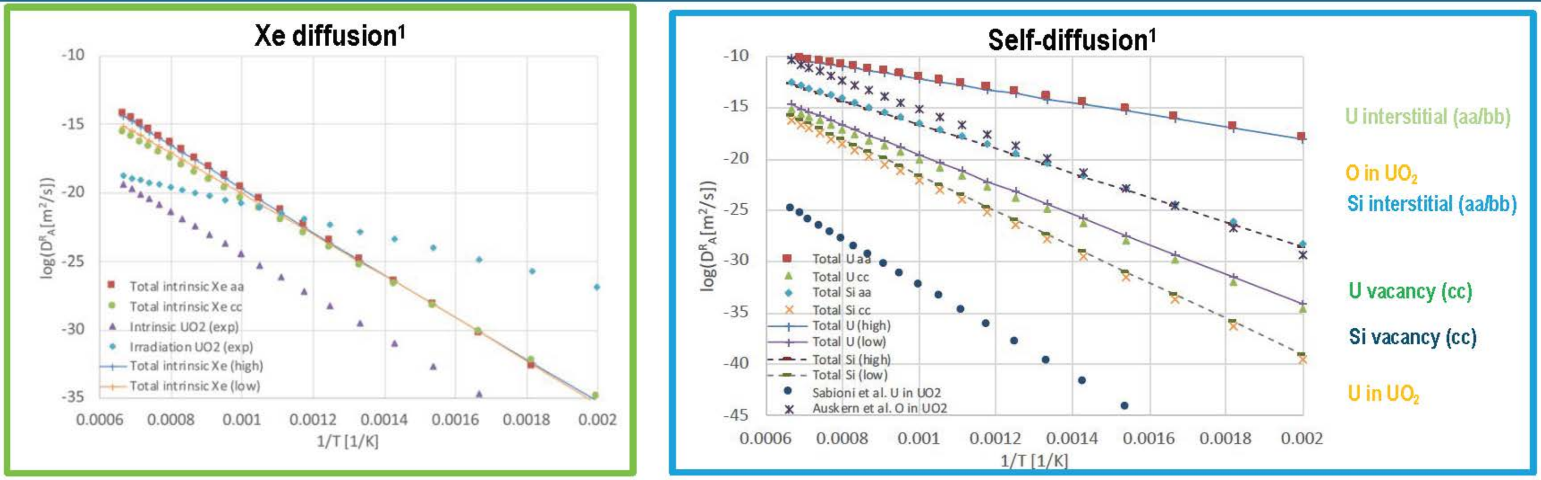


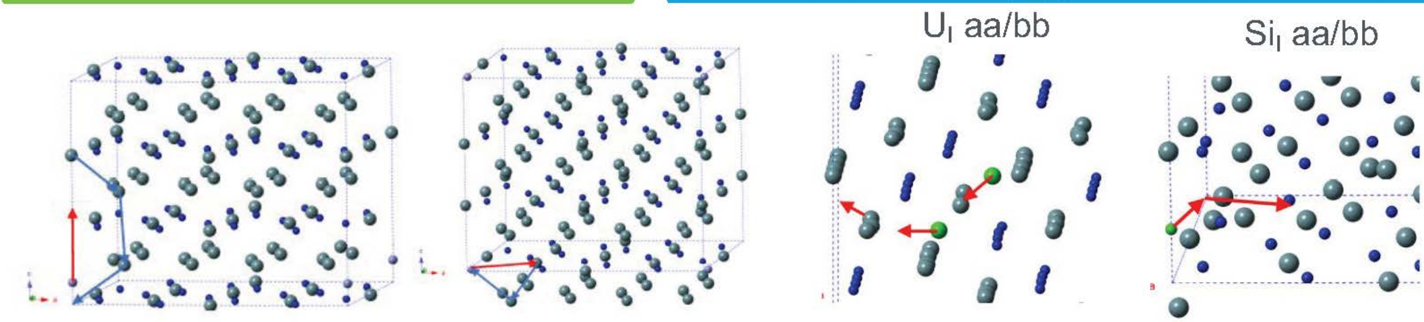
[2]S. C. Middleburgh, et al., "Non-stoichiometry in U_3Si_2", J. Nucl. Mater. **482**, 300 (2016).

[1]D. A. Andersson, et al., "Density functional theory calculations of self-and Xe diffusion in U_3Si_2", J. Nucl. Mater. **515**, 312-325 (2019).

[3]T. L. Wilson et., S.C. Vogel et al., "Temperature-Dependent Crystal Structure of U_3Si_2 by High Temperature Neutron Diffraction", Materialia (2020).

Intrinsic Xe and self-diffusion from DFT (D_1)





- Xe diffusion in c direction is U vacancy assisted.
- Xe diffusion in a-b plane is Si vacancy assisted.
- Intrinsic Xe diffusion is higher than in UO_2.

- Self-diffusion due to highly anisotropic interstitial mechanisms.
- Very low barrier for U_I.
- High concentration for Si_I.

[1]D. A. Andersson, et al., "Density functional theory calculations of self-and Xe diffusion in U_3Si_2", J. Nucl. Mater. **515**, 312-325 (2019).

Athermal diffusion in U_3Si_2 from MD (D_3)

Electronic excluded for U_3Si_2
Important for UO_2

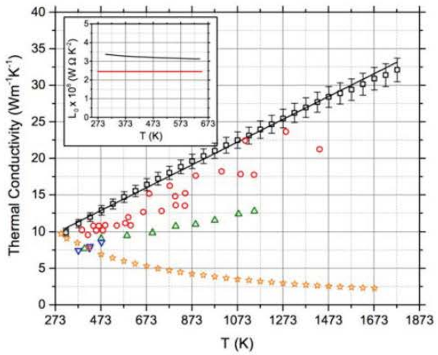
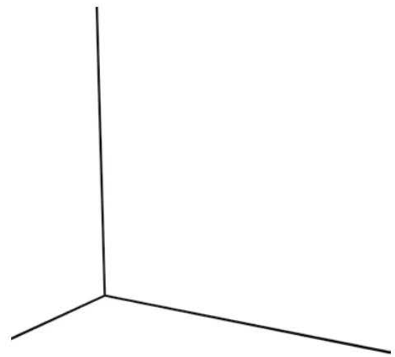
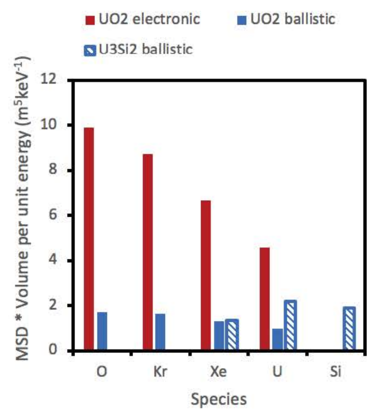


Fig. 6. Calculated thermal conductivity data for U_3Si_2 as a function of temperature to 1773 K collected in this study (□). Reference data from Shimizu [17] is represented by (○), (▽), and (△). Literature values for UO_2 (☆) are included from [26]. An inset is provided to compare the expected Lorenz values (—) with calculated values (—).

White *et al.*, *J. Nucl. Mater.* **464** 275-280 (2015)

Ballistic included for U_3Si_2





- High thermal conductivity in U_3Si_2 means that heat deposited electronically is dissipated before it can melt the lattice – 90% of the energy fission is removed in this way.
- All atomic mixing is assumed to come from ballistic stopping (10% of fission energy)
- The ballistic part is similar to the same contribution in UO_2, but much lower than transport due to electronic stopping (thermal spikes).

[2] Beeler, Baskes, Andersson, Cooper, Zhang, *J. Nucl. Mater.*, **495** (2017) 267-276

Cluster dynamics model for irradiation enhanced diffusion (D_2)

- Using the same FECD framework developed by Matthews et al.[1] for cluster dynamics on UO_2, a CD model is developed for U_3Si_2.
- Parameterized using the DFT data from Andersson.
- Assumptions:
  - Given that the two U vacancies have the same migration saddle point they are both described using only the more stable 2a vacancy.
  - Anisotropy in diffusion is treated by taking the fastest direction and modifying the number of dimensions in pre-exponential of diffusion coefficient.
  - Anti-sites have been omitted to reduced the number of solved defects and coupled ODEs.

Solved point defects: $U_i, V_U, Si_i, V_{Si}, Xe_i$
Solved clusters: $Xe_U, Xe_{Si}, Xe_{2U}, Xe_{2Si}, Xe_{USi}$
Dependents: U_U, Si_{Si}

[1]C. Matthews et al., "Cluster Dynamics Simulation of Uranium Self-diusion During Irradiation in UO_2", J. Nucl. Mater. (2019).

$$sink + U_i \leftrightarrow sink + V_i \quad (1)$$
$$sink + Si_i \leftrightarrow sink + V_i \quad (2)$$
$$sink + V_U \leftrightarrow sink + U_U \quad (3)$$
$$sink + V_Si \leftrightarrow sink + Si_{Si} \quad (4)$$
$$U_i + V_U \leftrightarrow U_U + V_i \quad (5)$$
$$Si_i + V_{Si} \leftrightarrow Si_{Si} + V_i \quad (6)$$
$$U_i + Xe_U \leftrightarrow Xe_i + U_U \quad (7)$$
$$V_i + Xe_U \leftrightarrow Xe_i + V_U \quad (8)$$
$$U_i + Xe_{2U} \leftrightarrow Xe_U + U_U + V_i \quad (9)$$
$$Xe_{2U} \leftrightarrow Xe_U + V_U \quad (10)$$
$$Si_i + Xe_{Si} \leftrightarrow Xe_i + Si_{Si} \quad (11)$$
$$V_i + Xe_{Si} \leftrightarrow Xe_i + V_{Si} \quad (12)$$
$$Si_i + Xe_{2Si} \leftrightarrow Xe_{Si} + Si_{Si} + V_i \quad (13)$$
$$Xe_{2Si} \leftrightarrow Xe_{Si} + V_{Si} \quad (14)$$
$$Xe_{USi} \leftrightarrow Xe_{Si} + V_U \quad (15)$$
$$Xe_{USi} \leftrightarrow Xe_U + V_{Si} \quad (16)$$
$$Si_i + Xe_{USi} \leftrightarrow Xe_U + Si_{Si} + V_i \quad (17)$$
$$U_i + Xe_{USi} \leftrightarrow Xe_{Si} + U_U + V_i \quad (18)$$

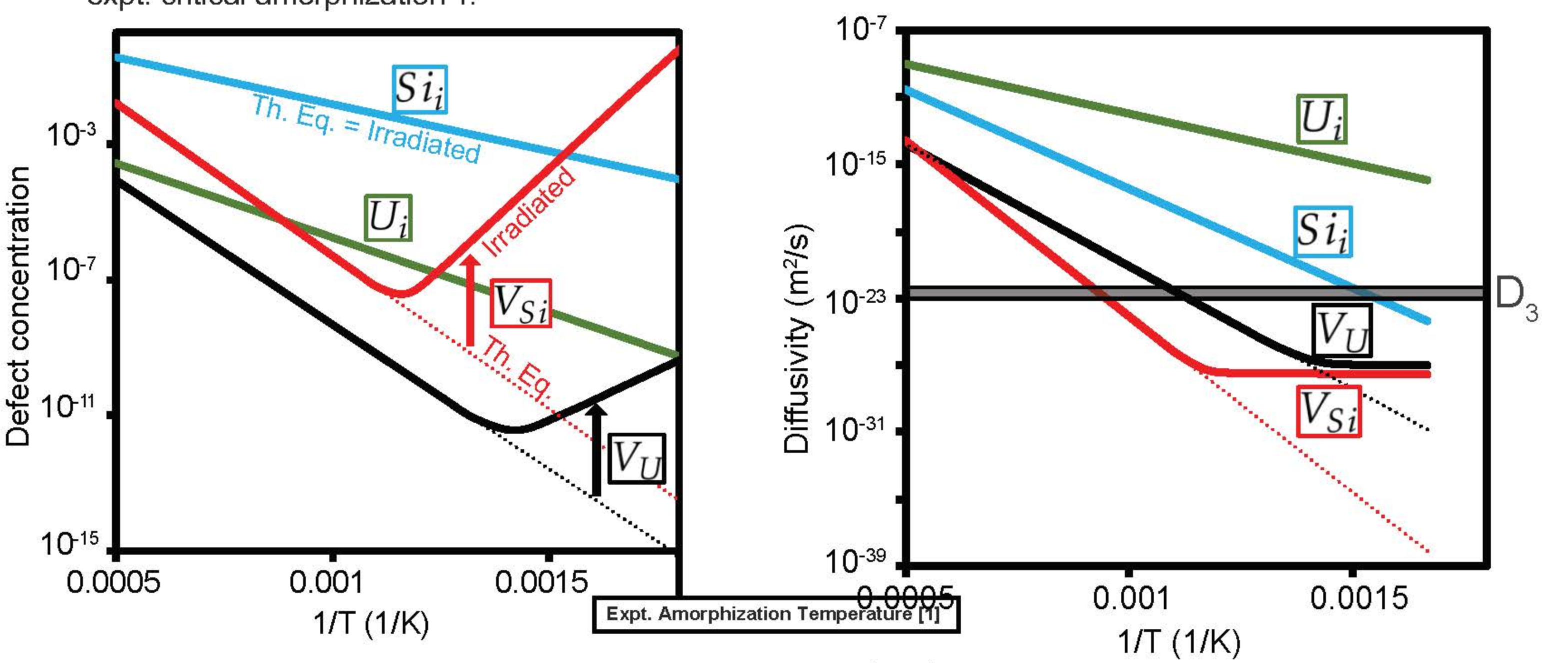
Irradiation enhanced self-diffusion (D_2)

Concentrations of U and Si defects:

- No enhancement of U or Si interstitial concentrations – still high at thermal equilibrium.
- Enhancement of V_{Si} and V_U at low T.
- Very high V_{Si} concentration as approaches expt. critical amorphization T.

Self-diffusion:

- No enhancement of U or Si interstitial diffusivity: – Highly mobile U interstitials are now fastest.
- Enhancement of V_{Si} and V_U at low T.
- All self-diffusion coefficients are wiped out by athermal D_3.



[1] Birtcher et al. JNM **230** (1996) 158-163

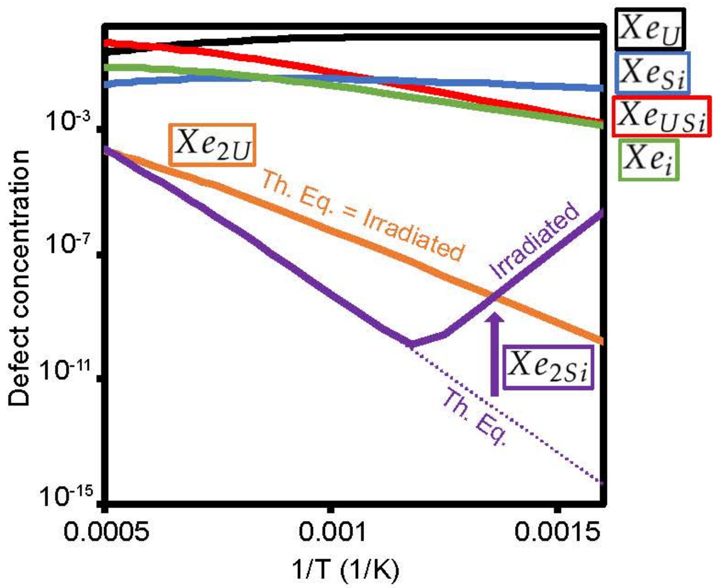
Irradiation enhanced Xe diffusion (D_2)

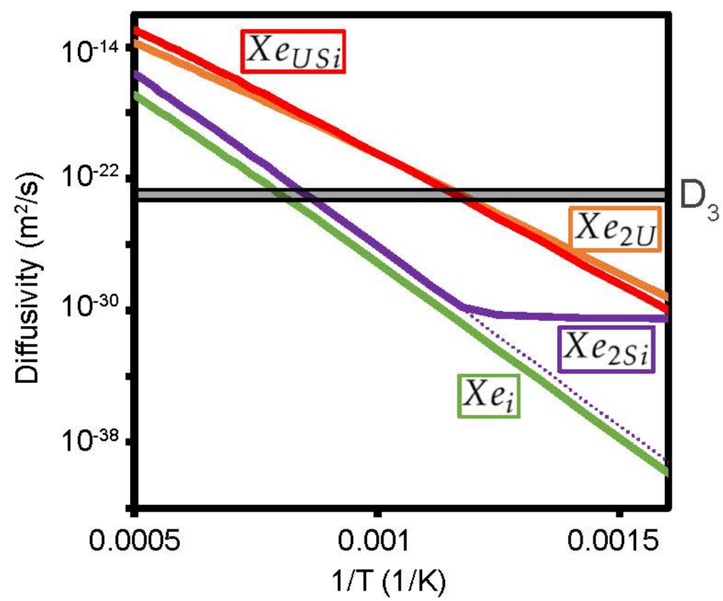
Xe concentrations (normalized):

- Xe_{2Si} defect concentration enhanced due to higher V_{si} concentration at low T.
- All other defects are unaffected by irradiation.
- Fast interstitial defects are thought to recombine with Xe_{USi} and Xe_{2U} driving them back to equilibrium despite enhanced V_{si}.

Xe diffusivity:

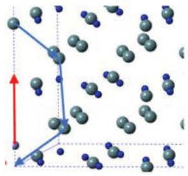
- As before only Xe_{2Si} diffusion is enhanced.
- However, is much lower diffusivity than for Xe_{2U} or Xe_{USi} which are at equilibrium.
- Furthermore, athermal D_3 diffusion dominates over D_2 .





Bison implementation of gas and self-diffusion in U_3Si_2

DFT used to describe the high T intrinsic regime of diffusion (D_1)



Migration pathway

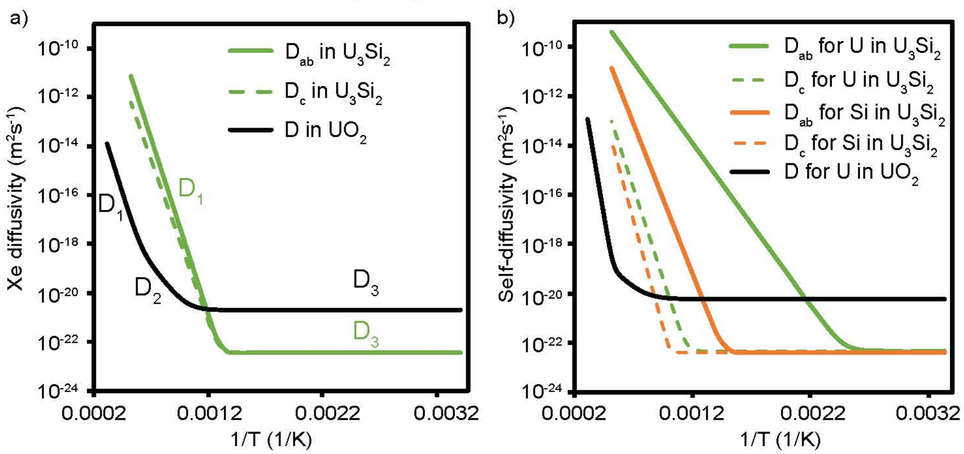
- Thermally activated diffusion of point defects
- Anisotropic due to non-cubic structure of U_3Si_2

Molecular dynamics simulations of athermal diffusion (D_3)

Displaced atoms in cascade

- Atomic mixing during damage event
- Homogeneous process

Andersson, *Liu, Beeler, Middleburgh, Claisse, Stanek, J. Nucl. Mater.* **337** 271-278 (2018)



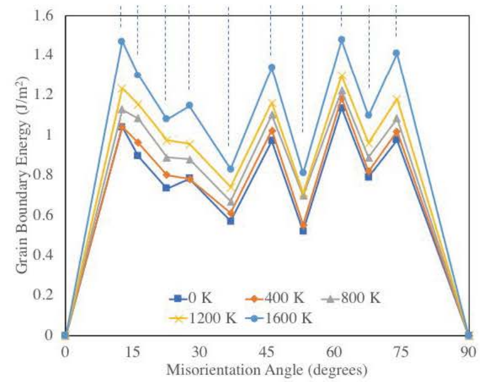
- Predicted fission gas diffusion and self-diffusion coefficients for U_3Si_2 (comparison is made with UO_2).
- Significant anisotropy for self-diffusion.
- Analytical expressions for implementation in Bison for Xe and Si vacancy diffusion.

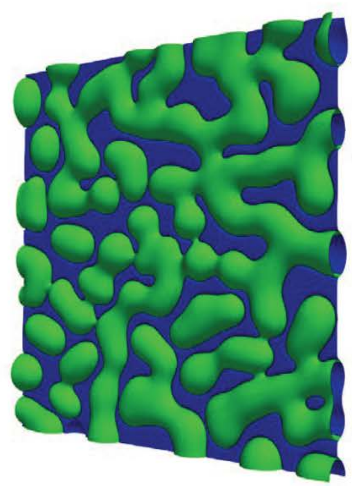
$$D_{U_3Si_2} = 2.95\times 10^{-4}\exp\left(\frac{-2.92}{k_BT}\right) + 3.58\times 10^{-42}\dot{F}$$

$$D = 9.40\times 10^{-4}\cdot\exp\left(\frac{-4.17}{k_BT}\right) + 3.01\times 10^{-47}\cdot\dot{F}$$

Mesoscale simulations for U_3Si_2 (L. Aagesen, INL)

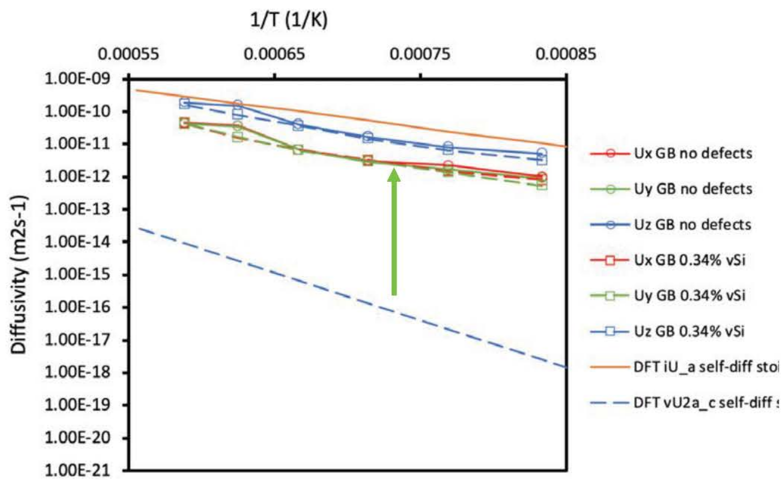
- Fission gas bubble dihedral angle, U_3Si_2/gas surface energy determined from MD calculations of surface and grain-boundary energies (*B. Beeler, M. Baskes, D. Andersson, M. Cooper, Y. Zhang, JNM 514, 290, 2019*).
- Used Marmot simulations to calculate grain boundary coverage at saturation ($F_{c,sat}$):
  - $F_{c,sat}$ = 0.54, much closer to observed experimental value for UO_2 (0.5) than theoretical value that was previously used ($\pi/4$).
  - Considered effect of minimum spacing between bubbles and other parameters by sensitivity analysis.
- All implemented in the Bison fission gas model
  - Large impact on Bison fission gas release and gaseous swelling predictions.



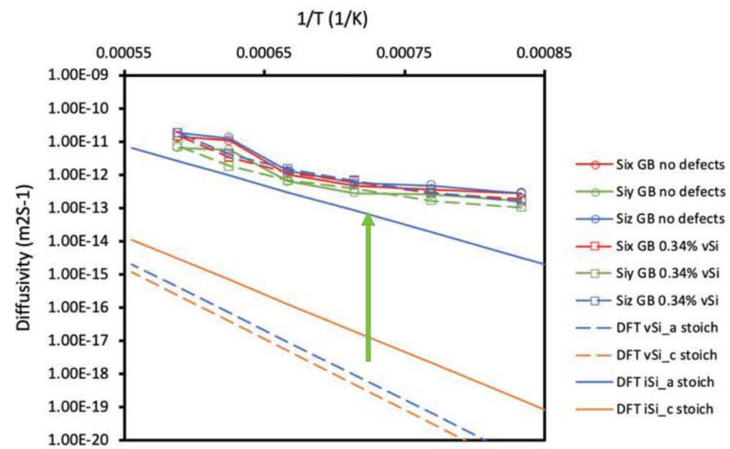


Grain boundary self-diffusion

U diffusion at grain boundaries

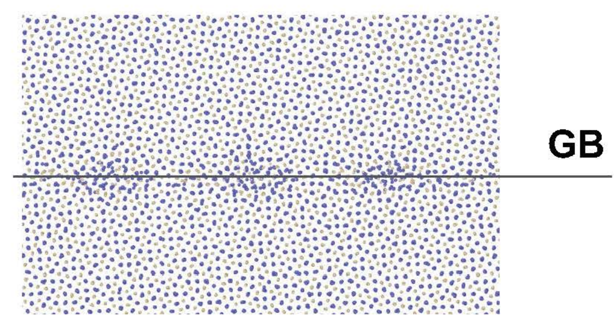


Si diffusion at grain boundaries



- Classical MD simulation of diffusion at a 530 tilt grain boundary.
- Slightly higher diffusion for U at grain boundaries than for Si.
- Diffusion at grain boundaries is approx. 6 orders of magnitude higher than vacancy diffusion in the bulk lattice, although with weaker temperature dependence – this validates current assumption in BISON.
- The addition of vacancies to the grain boundary was predicted to have negligible effect on the diffusivity.

Lines show atomic displacement



Atomic scale diffusional U_3Si_2 creep model

Nabarro-Herring creep

- Using the bulk diffusivity of Si interstitials (faster than Si vacancies but slower than U defects) the Nabarro-Herring creep rate is predicted using the following equation:

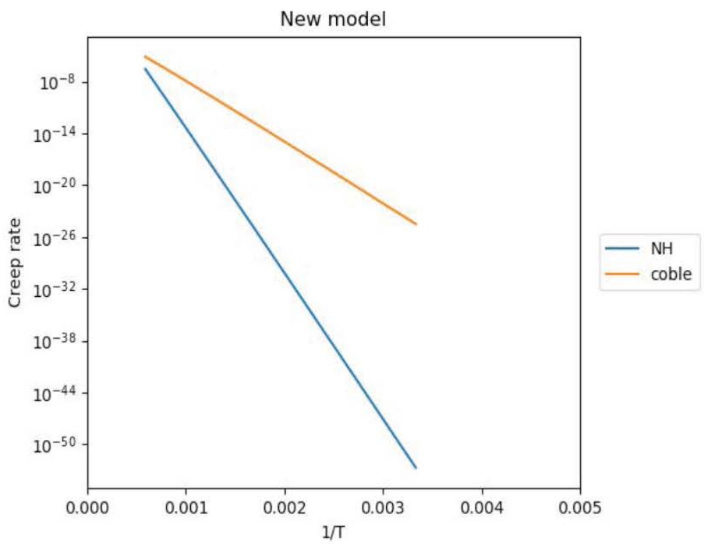
$$\dot{\epsilon} = \frac{42\sigma_s\Omega}{k_B T d^2} D$$

Coble creep

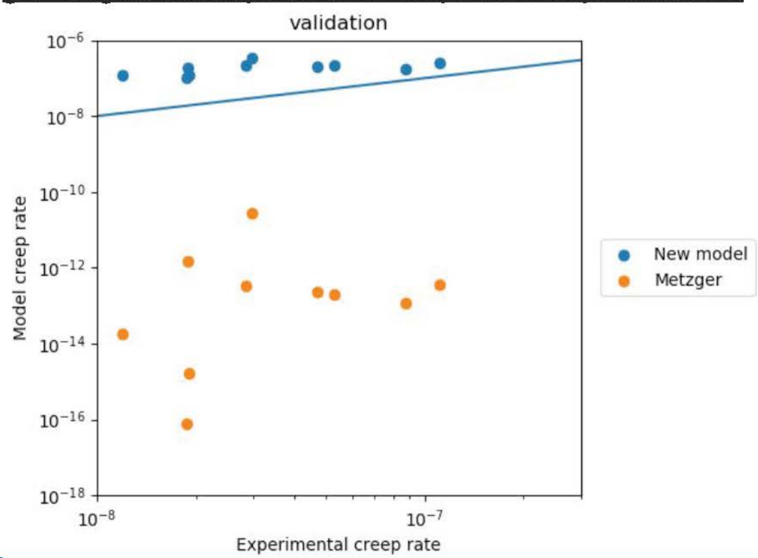
- Using the grain boundary diffusivity from classical MD the Coble creep rate is predicted using the following equation:

$$\dot{\epsilon} = \frac{42\sigma_s\Omega\delta}{k_B T d^3} D$$

Coble > NH Creep

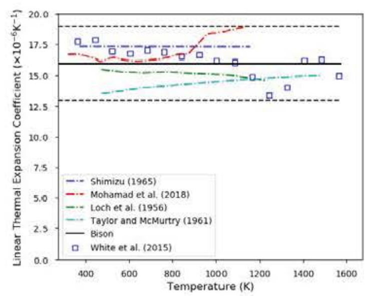


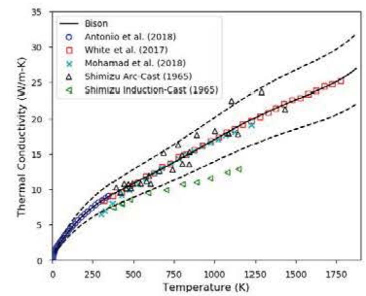
Similar approach to Metzger but with atomic scale diffusivities gives significant improvement compared to Expt. from USC



U_3Si_2 material and behavioral models in Bison (K. Gamble, INL)

- Bison contains the following material and behavioral models for U_3Si_2 (from best available source, experiments or modeling):
  - Thermal Properties
    - Thermal Conductivity (4 options + degradation)
    - Specific Heat (2 options)
  - Elasticity
    - Porosity dependent Young's Shear moduli
  - Thermal and Irradiation Creep (2 options)
  - Thermal Expansion
  - Gaseous Swelling (3 options)
  - Solid Swelling
  - Densification
  - Fission Gas Release
    - Stoichiometric and Si-rich





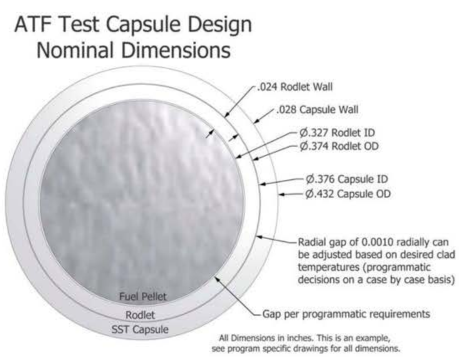
Model	Range of Applicability	Uncertainty
Thermal Conductivity	$13 \leq T \leq 1500$ K	± 18.2 %
Thermal Conductivity Degradation	$390 \leq T \leq 1190$ K	$\pm 10\%$ Intra.
	$0 \leq G \leq 160$ K/mm	$\pm 10\%$ Inter.
	$0 \leq f \leq 2.5755\times 10^{21}$ fissions/cm^3	
Specific Heat	$293 \leq T \leq 1500$ K	$\pm$ 3%
Young's Modulus	$1.5 \leq p \leq 10\%$	$\pm$ 29.1%
Shear Modulus	$1.5 \leq p \leq 10\%$	$\pm$ 26.8%
Creep	$300 \leq T \leq 1900$ K	$\pm$ a factor of 1.83
Thermal Expansion	$273 \leq T \leq 1473$ K	$(16.0\pm 3.0)\times 10^{-6}$
Solid Swelling	All burnups	$\pm$ 20 %
Fission Gas Release	Normal Operating Conditions	See SA and UQ
Gaseous Swelling	Normal Operating Conditions	See SA and UQ
Densification	Normal Operating Conditions	Needs Further Work

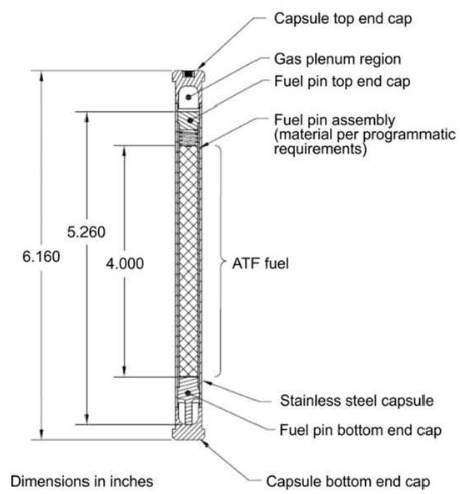
LLS results available to inform Bison, being implemented

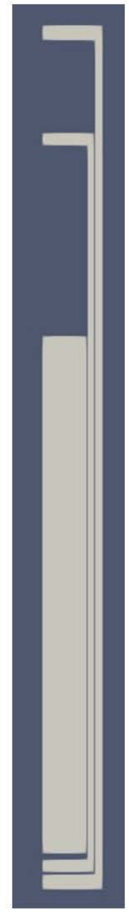
Informed by LLS simulations

Validation of Bison (U_3Si_2) against ATR experiments

- Two U_3Si_2 fueled experiments with ZIRLO™ (WEC)
  - ATF-13 R4 filled with helium
  - ATF-15 R6 filled with helium/argon mixture
- Available data includes:
  - Fission Gas Release
  - Fuel axial elongation (inferred from neutron radiographs)
  - Clad profilometry



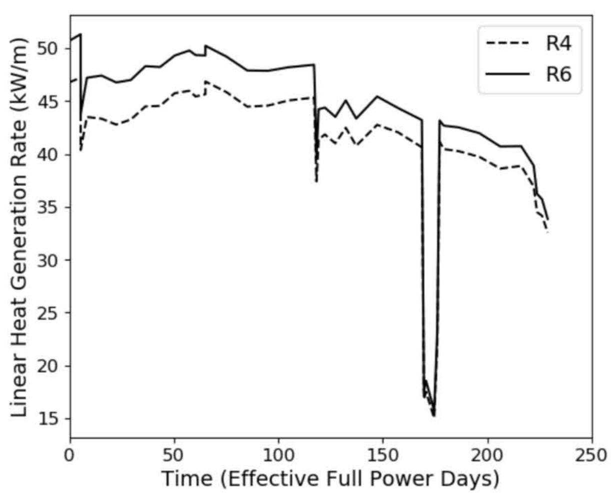




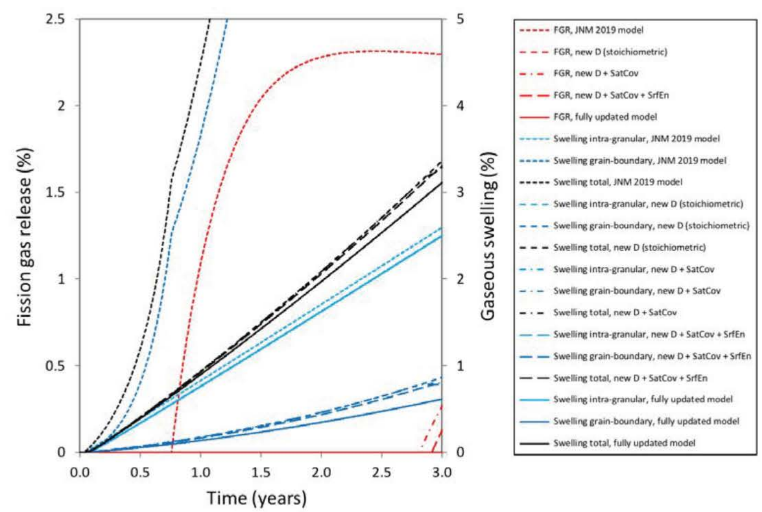
Bison geometry used. Axial direction scaled by 0.5.

Validation results

- Using the nominal models Bison underpredicts swelling for R4 and overpredicts for R6.



Swelling predictions for different gas diffusion models



Bison comparisons to ATF-13 R4 and ATF-15 R6 PIE data

	Bison R4	Experiment R4	Bison R6	Experiment R6
Fuel Elongation (mm)	-0.0784	0.0	0.0128	0.0
Fission Gas Release (%)	0.0	0.06	0.19	0.06

Sensitivity analysis and uncertainty quantification (K. Gamble, INL)

- Using the uncertainty defined in the individual material models, perform an SA and UQ analysis on the ATF-13 R4 case.

Parameters varied in the sensitivity analysis and uncertainty quantification

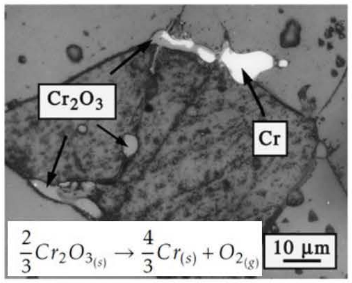
Parameter	Nominal value	Scaling factor range	Distribution
Thermal conductivity ($W{\cdot}m^{-1}K^{-1}$)	See Equation 29	[0.82; 1.18]	Normal
Coefficient of thermal expansion (K^{-1})	16.0×10^{-6}	[0.8125;1.1875]	Normal
Young's modulus (GPa)	See Equation 39	[0.709; 1.291]	Normal
Shear modulus (GPa)	See Equation 40	[0.732; 1.268]	Normal
Solid swelling (/)	See Equation 68	[0.8; 1.2]	Normal
Nucleation factor of intra-granular bubbles (/)	10^{-6}	$[10^{-3}; 10^{4}]$	Uniform
Re-solution rate of intra-granular bubbles (s^{-1})	$2.80 \cdot 10^{-25} \left(5 \cdot 10^{-10}/R_{ig}\right)^{0.23} \cdot \dot{F}$	[0.1; 10]	Uniform
U_3Si_2/gas specific surface energy ($J{\cdot}m^{-2}$)	1.7	[0.5; 1.5]	Uniform
Inter-granular diffusion coefficient of vacancies ($m{\cdot}s^{-2}$)	$10^{6} \cdot D^{v}_{ig}$	$[10^{-2}; 10^{2}]$	Uniform
Initial number density of inter-granular bubbles ($bbl{\cdot}m^{-2}$)	$2 \cdot 10^{12}$	$[10^{-3}; 10^{3}]$	Uniform
Semi-dihedral angle of inter-granular bubbles (deg)	72.9	[0.5; 1]	Uniform
Saturation coverage of grain boundaries (/)	0.5	$[1; \pi/2]$	Uniform

Bison comparisons to ATF-13 R4 PIE data including $\pm 2\sigma$

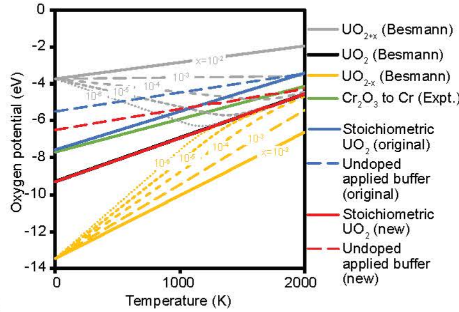
	Bison Stoichiometric	Bison Si-Rich	Experiment
Fuel Elongation (mm)	-0.135 to 0.132	-0.1305 to 0.0567	0
Fission Gas Release (%)	0.0 to 1.412	0.0 to 0.902	0.06

Doped UO_2 fission gas diffusivity model

Hypothesis is that Cr_2O_3 to Cr reaction governs oxygen potential in doped UO_2



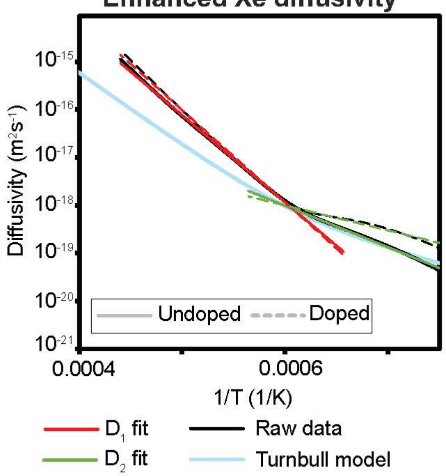
Bourgeois et al., *J. Nucl. Mater.*, **297** (2001) 313-326



CD model calibrated to Besmann data

Defect	ΔH (eV)	ΔS (k_B)
I_O	-0.437	-1.002
V_O	0.337	1.002
V_U	-0.674	-2.005
I_U	0.674	2.005
h	0.136	-0.366
e	0.614	0.366
E_{mig} V_U	-0.338	0

Enhanced Xe diffusivity



Turnbull et al., *J. Nucl. Mater.*, **107** (1982) 168-184

New enhanced diffusivity equation for use in Bison FGR model

$$D^{doped} = \exp\left(-\frac{\Delta H_1}{k_B}\left[\frac{1}{T}-\frac{1}{T_1}\right]\right)D_1^{undoped} + \exp\left(-\frac{\Delta H_2}{k_B}\left[\frac{1}{T}-\frac{1}{T_2}\right]\right)D_2^{undoped} + D_3^{undoped}$$

where $T_1 = T_2 = 1673$ K, $\Delta H_1 = 0.316$ eV, and $\Delta H_2 = -0.684$ eV.

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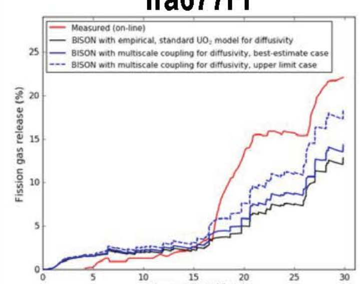

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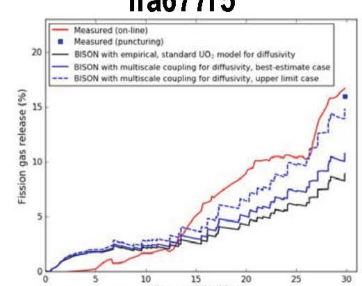

Model made available to MIT IRP team (K. Shirvan) for additional testing.

Summary and conclusions

- Demonstrated application of a hierarchical multi-scale simulation approach for U_3Si_2:
  - Relied on DFT calculations, MD simulations, cluster dynamics and phase field simulations.
  - Informed engineering scale gas release, swelling and creep models in BISON (hierarchical information exchange, no concurrent coupling).
  - LLS informed models are combined with empirical models derived from experiments to complete a Bison U_3Si_2 simulation capability.
  - Bison simulations of ATR U_3Si_2 irradiations compare well with experimental data.
  - UQ and SA are important tools for guiding development and assessing results in a qualification context.
- Although exemplified for U_3Si_2, methodology, challenges and lessons-learned are expected to extend to other fuel types as well.
- Multi-scale modeling and simulations are a valuable tool to develop material models where experimental data is missing and difficult/expensive to acquire – provides valuable understanding.
- M&S work must be performed in parallel with experiments for both “fine-calibration” and validation based on rigorous UQ.

APPENDIX G - TCR fuel design and development towards qualification

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AFQ Case Study: TCR fuel design and development towards qualification

Jan 16, 2019

Kurt Terrani
Transformational Challenge Reactor Technical Director

Contributors: B. Betzler, Brian Ade, D. Scappel, J. Weinmeister, Luke Scime

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

U.S. DEPARTMENT OF ENERGY

Outline

- What is the **Transformational Challenge Reactor** demonstration program?
- **AFQ approach** and application to **TCR** core design and development
- Concluding thoughts

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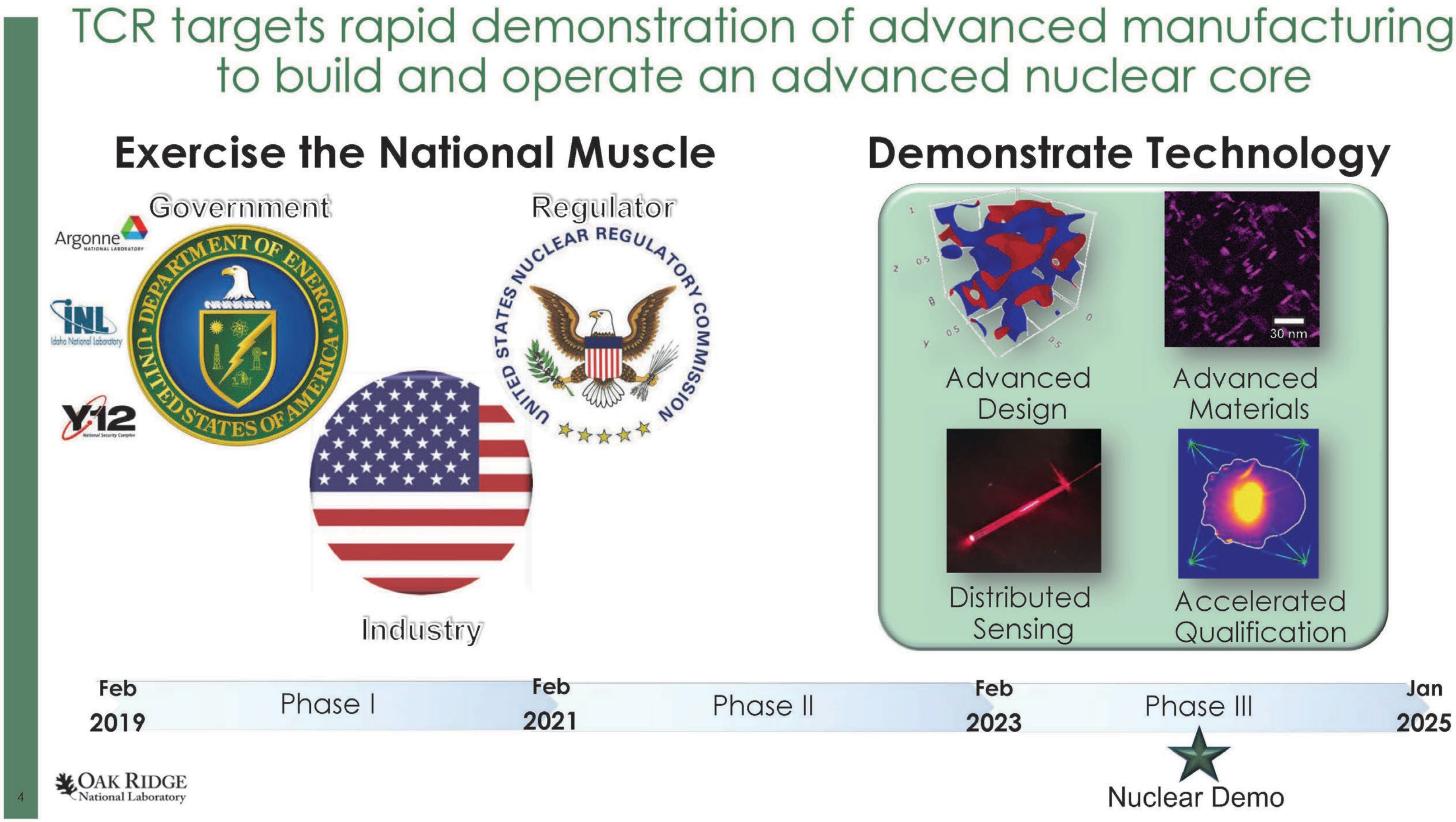
What is TCR?


TCR targets rapid demonstration of advanced manufacturing to build and operate an advanced nuclear core
Exercise the National Muscle
Government
Argonne
INL
Idaho National Laboratory
Y-12
DEPARTMENT OF ENERGY
UNITED STATES OF AMERICA
Regulator
UNITED STATES NUCLEAR REGULATORY COMMISSION
Industry
Demonstrate Technology
Advanced Design
30 nm
Advanced Materials
Distributed Sensing
Accelerated Qualification
Feb 2019
Phase I
Feb 2021
Phase II
Feb 2023
Phase III
Jan 2025
Nuclear Demo
4
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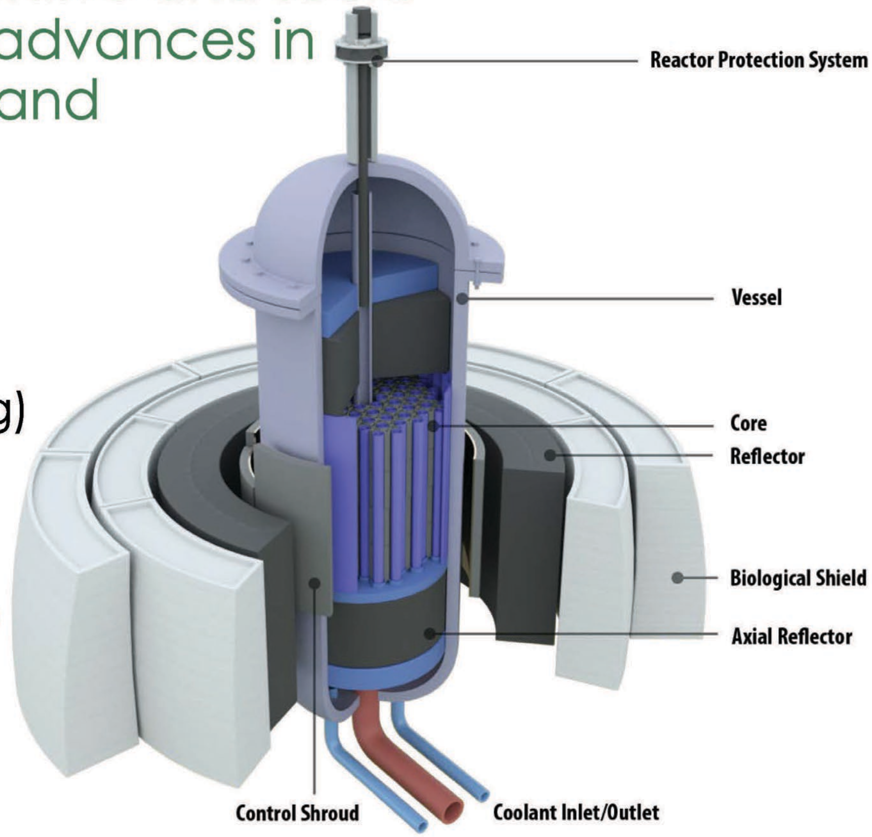
The TCR core design is inventive and seeks to bring to bear the latest advances in manufacturing, materials, and computational sciences

- Compact (<0.4 m^3), highly optimized, and inventive core design
- Resourceful with HALEU (<250 kg)
- Fueled with uranium nitride in silicon carbide
- Moderated with yttrium hydride
- Cooled with helium



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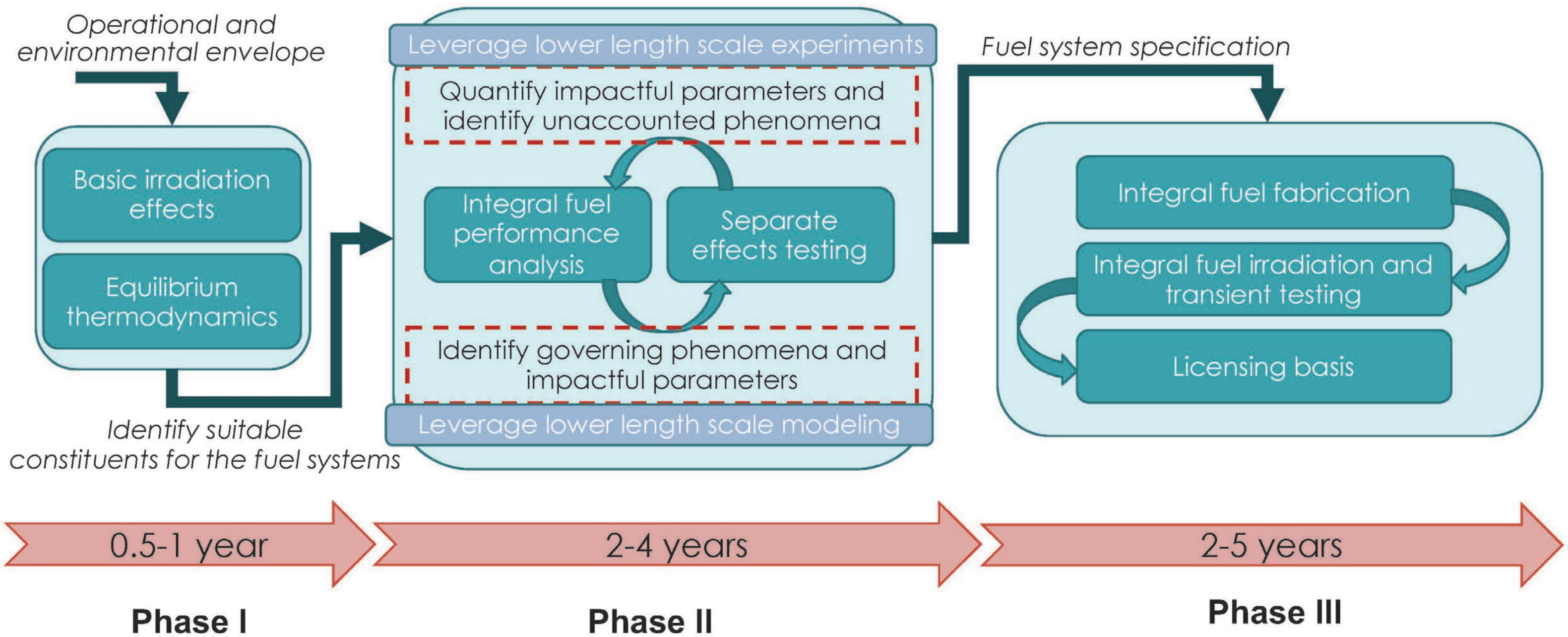
AFQ approach applied to TCR core development

An accelerated scheme for nuclear fuel (core) development and qualification



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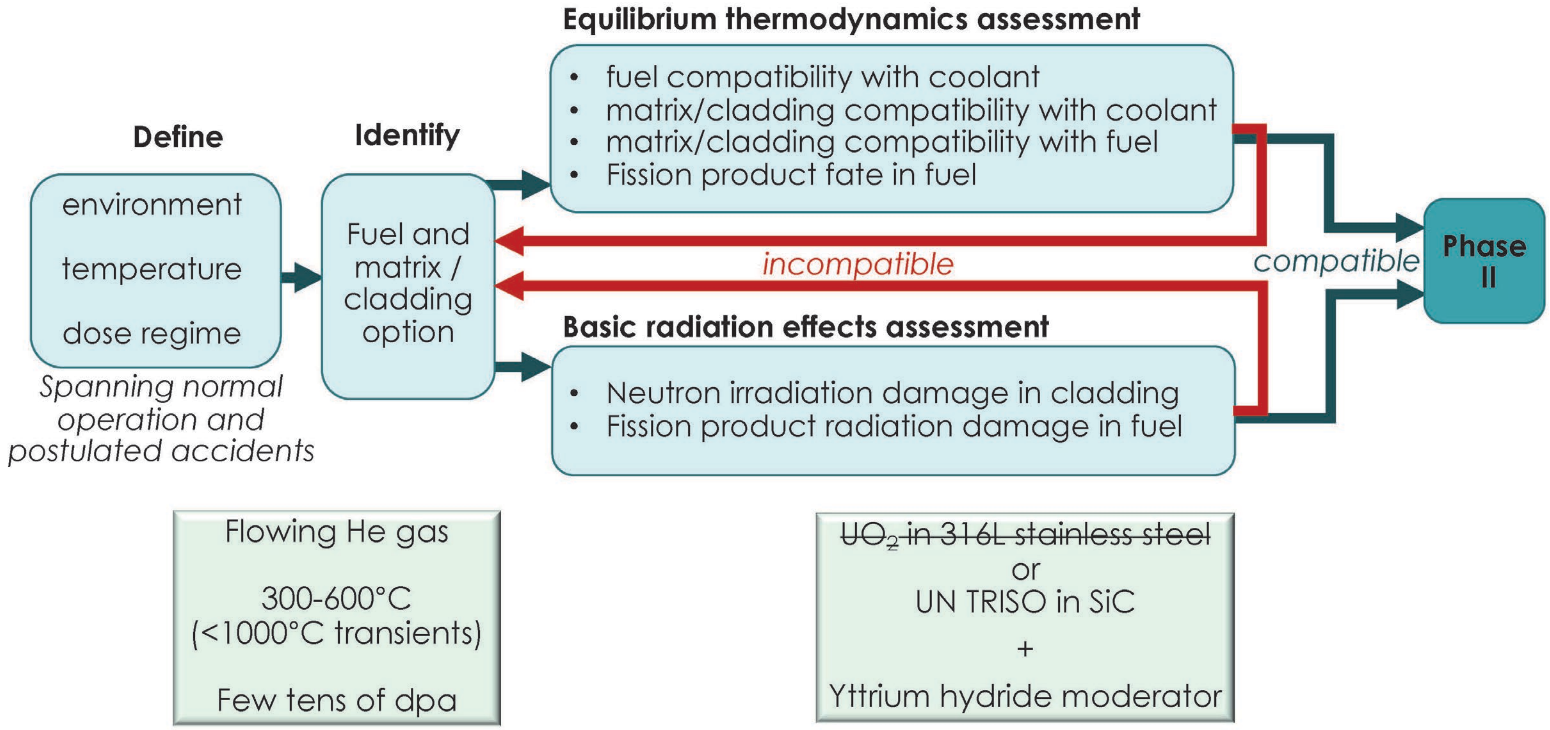
K.A. Terrani, N.A. Capps, M.J. Kerr, C. Back, A.T. Nelson, B.D. Wirth, S.L. Hayes, C.R. Stanek, "Accelerating Nuclear Fuel Development and Qualification: Engineering-Scale Modeling and Simulation Integrated with Separate Effects Testing," *J. Nucl. Mater.*, submitted (2020)

Phase I: Informed Constituent Downselection



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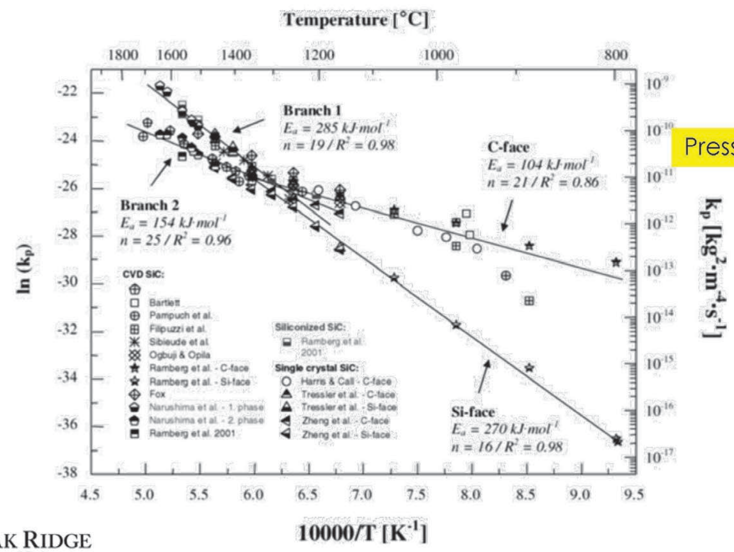
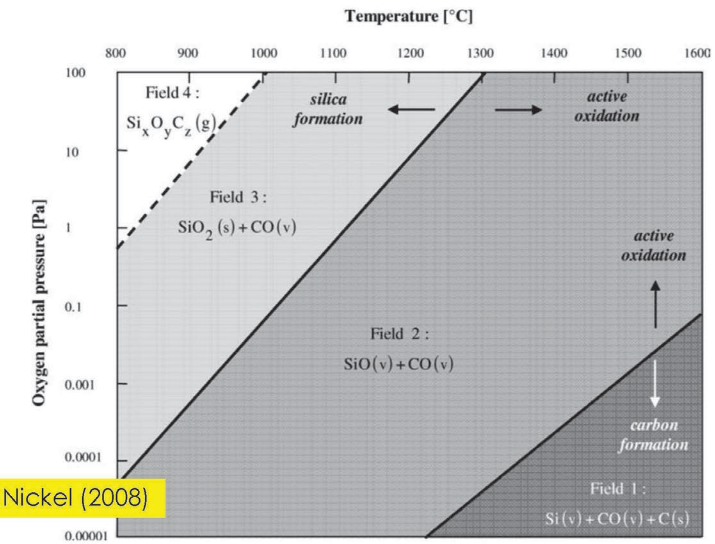
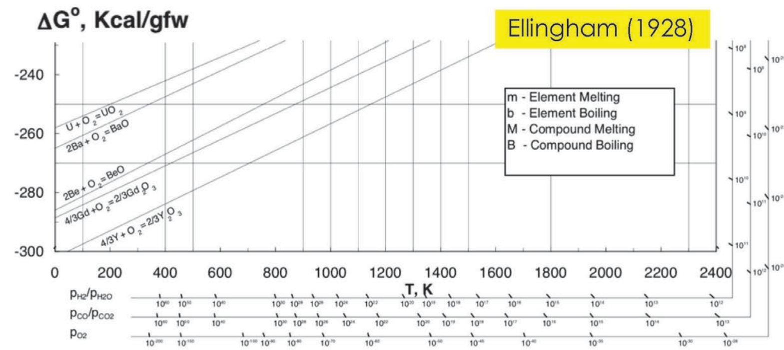
Phase I: Informed Constituent Downselection

- Fuel/matrix/cladding compatibility with coolant
- Matrix/cladding compatibility with fuel
- Fission product fate in fuel
- Neutron irradiation damage in cladding
- Fission product radiation damage in fuel





Presser and Nickel (2008)



Ellingham (1928)

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Phase I: Informed Constituent Downselection

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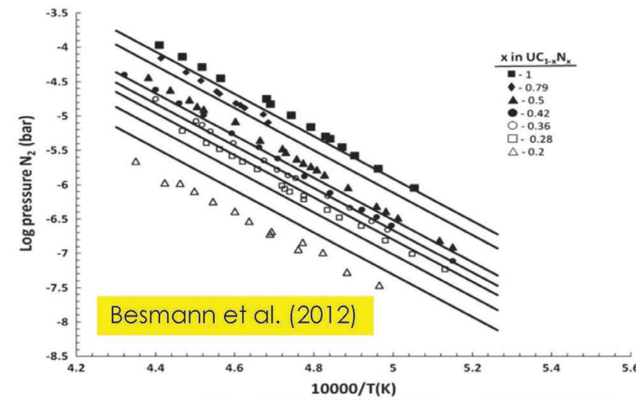
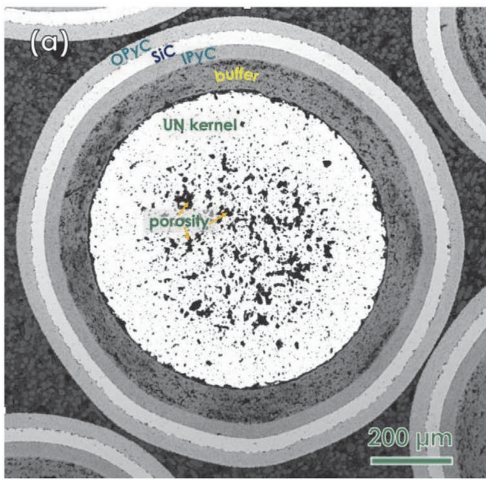
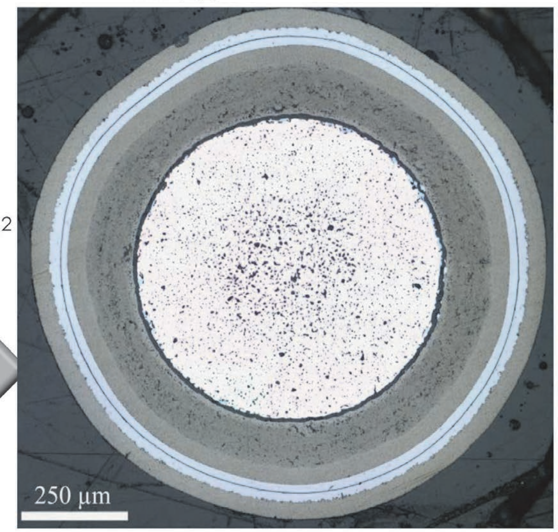




HFIR Irradiated
~460°C, ~0.7% FIMA
fast fluence (E > 0.1 MeV): 3.2×10^{20} n/cm^2
power-per-particle 120-545 mW
power density 450-2030 W/cm^3

Terrani et al. (2020)



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Phase I: Informed Constituent Downselection

- Fuel/matrix/cladding compatibility with coolant
- Matrix/cladding compatibility with fuel
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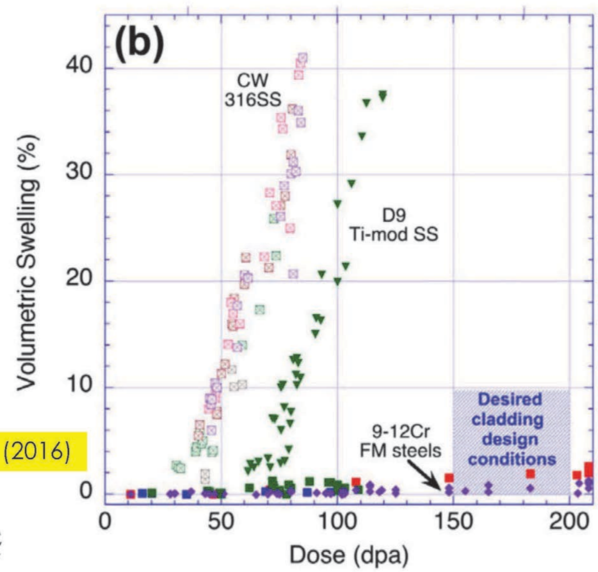
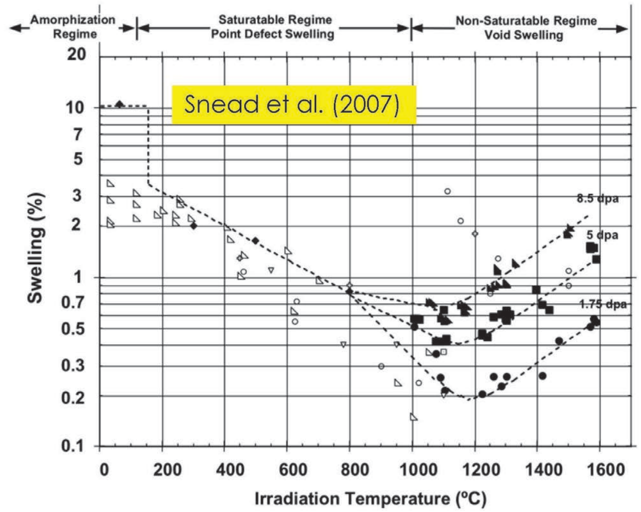
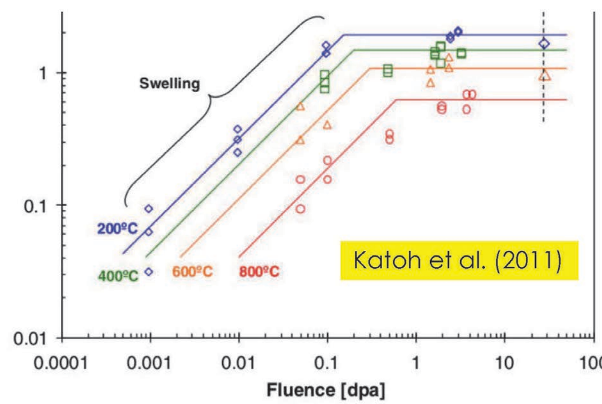


Zinkle et al. (2016)



Snead et al. (2007)



Katoh et al. (2011)

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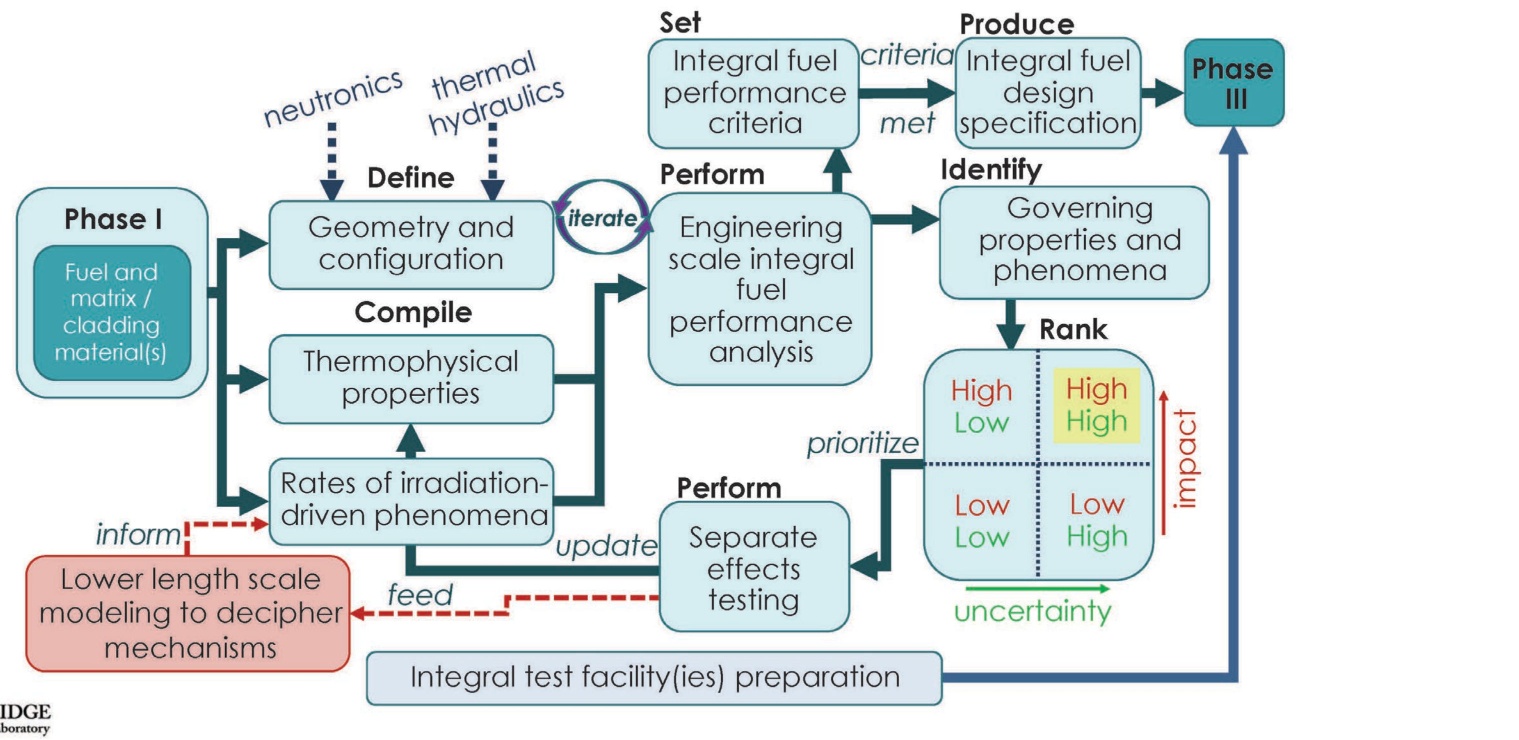
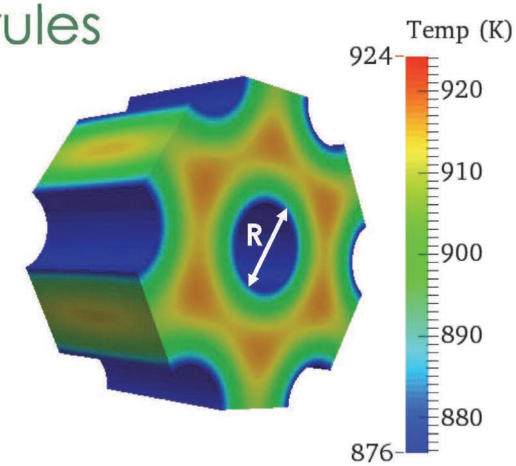
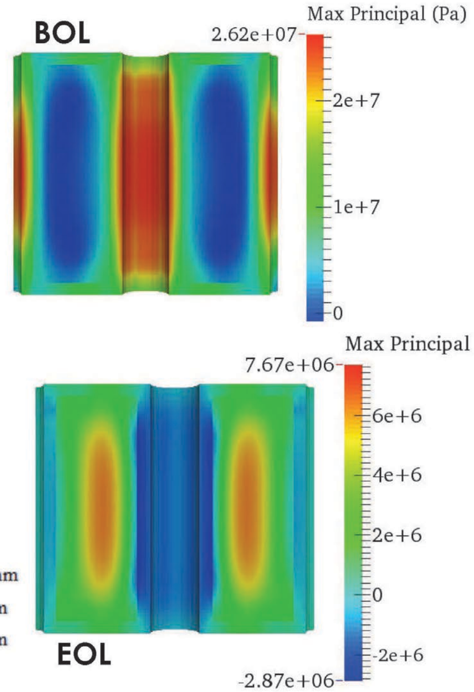
Phase II: iteration of engineering-scale modeling and simulation tools combined with separate-effects testing

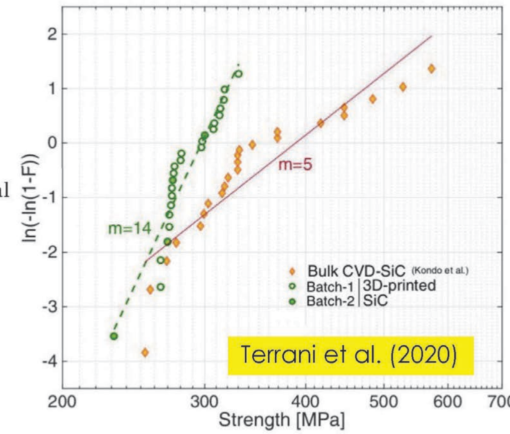


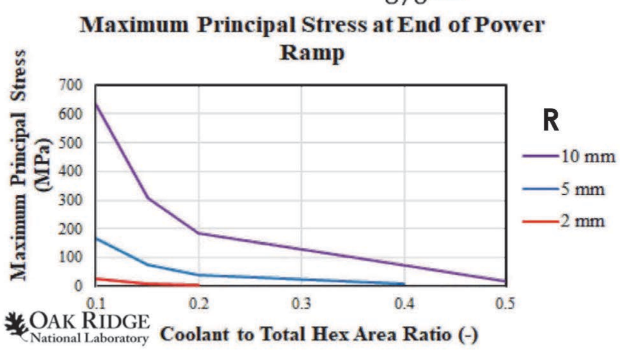
Defining geometry and configuration – start with design rules

~1500 Y-shaped elements needed









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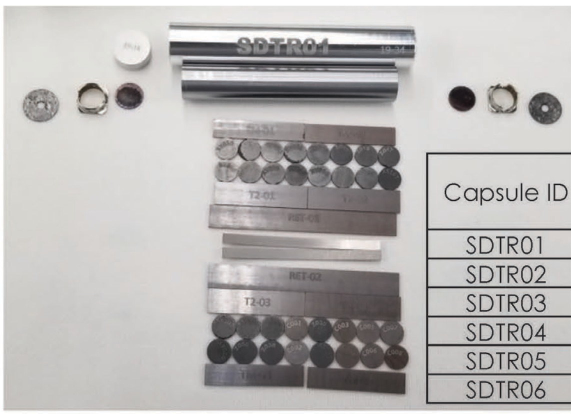
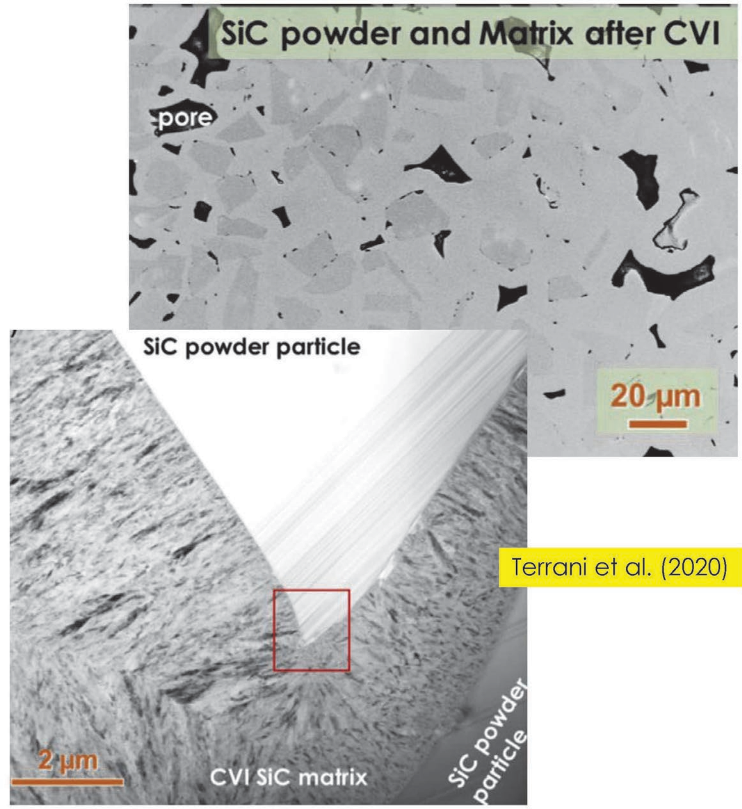
Thermophysical properties database development and ranking

Property	SiC Can and Fueled Region
Thermal Conductivity	Moderate
Interface HTC Ratio	-
Coefficient of thermal expansion	Moderately Low
Swelling	High
Elastic Modulus	Moderately High
Poisson's Ratio	Low

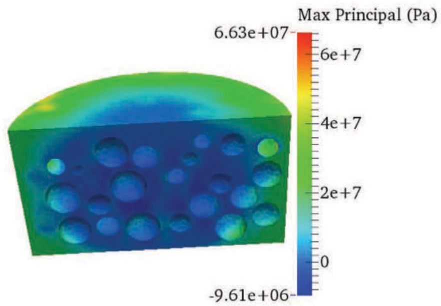


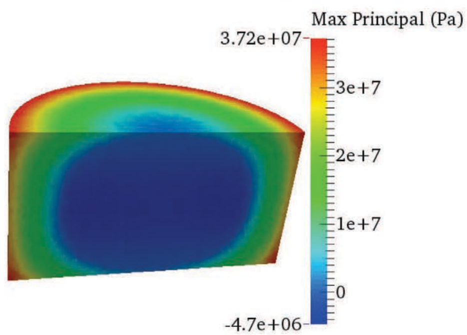
Capsule ID	Irradiation temperature
SDTR01	400°C
SDTR02	650°C
SDTR03	900°C
SDTR04	400°C
SDTR05	650°C
SDTR06	900°C

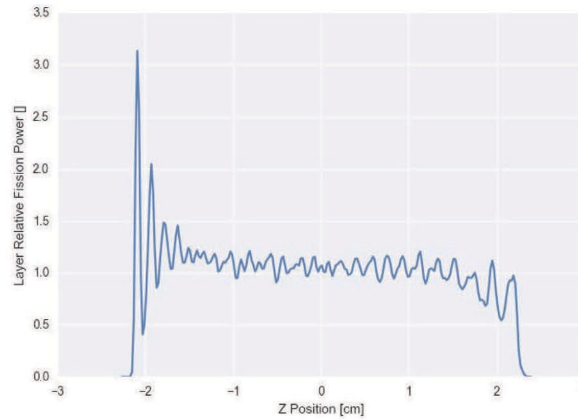


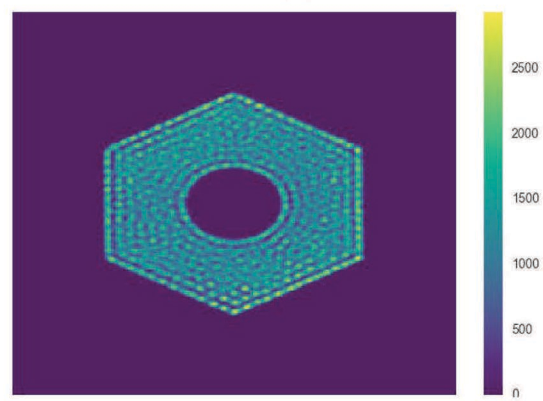
Terrani et al. (2020)

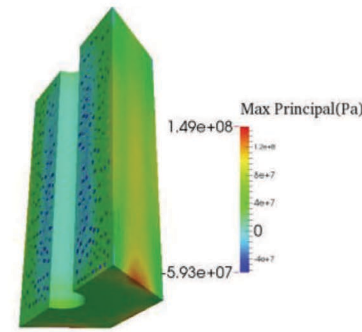
Learn and answer questions: do I need to discretely model the particles?

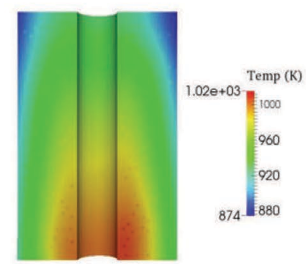












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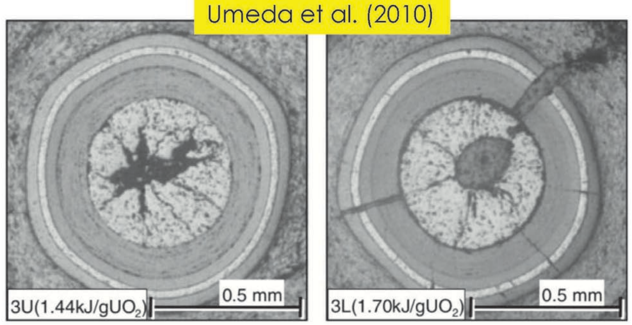
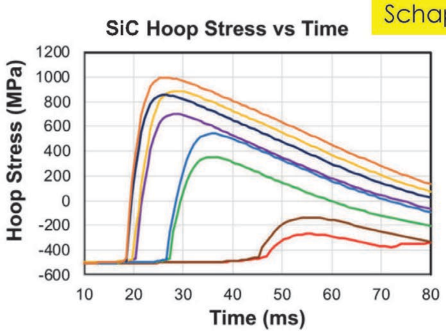
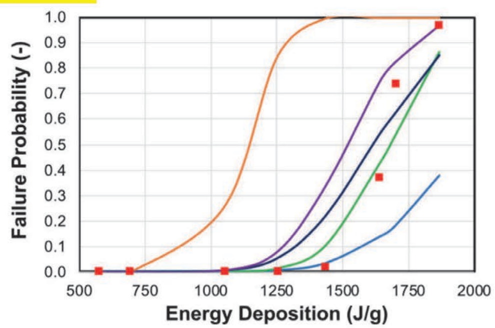
Learn and answer questions: "does TRISO pop like popcorn under an RIA?" - "When particles touch fuel fails?"

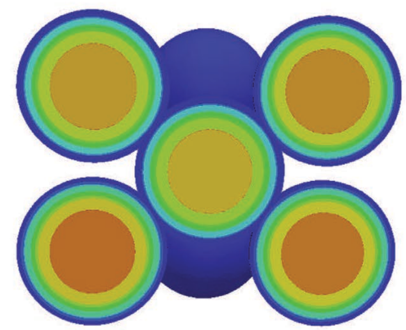
Umeda et al. (2010)

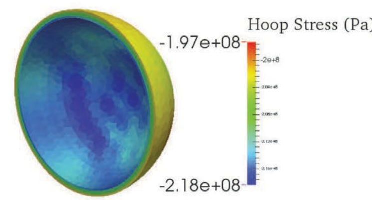


Schappel et al. (2020)









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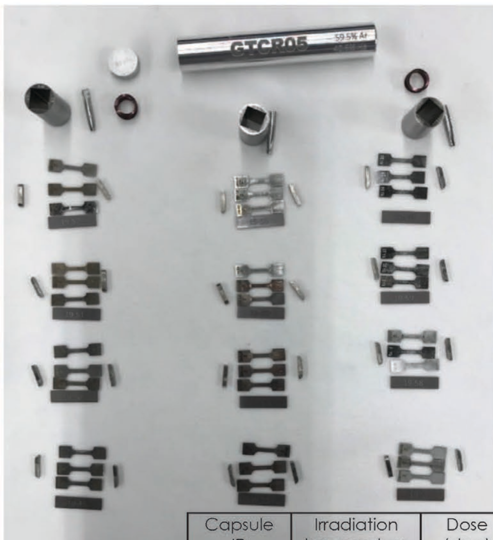
Separate effects testing to inform dose and temperature dependent phenomena

Advanced manufactured 316L



Capsule ID	Irradiation temperature	Dose (dpa)	Material
GTCR01	300°C	0.2	Wrought 316L and 3D-printed 316L (as-printed, or printed+650°C or 1050°C heat treatment)
GTCR02		2	
GTCR03		8	
GTCR04	600°C	0.2	
GTCR05		2	
GTCR06		8	

Yttrium hydride

Capsule ID	Irradiation temperature	Dose (dpa)	Material
YHXT01	600°C	0.1	$YH_{1.72}$
YHXT02		1	
YHXT03		2	
YHXT04	900°C	0.1	
YHXT05		1	
YHXT06		2	
YHXT07	600°C	0.1	$YH_{1.87}$
YHXT08		1	
YHXT09		2	
YHXT10	900°C	0.1	
YHXT11		1	
YHXT12		2	

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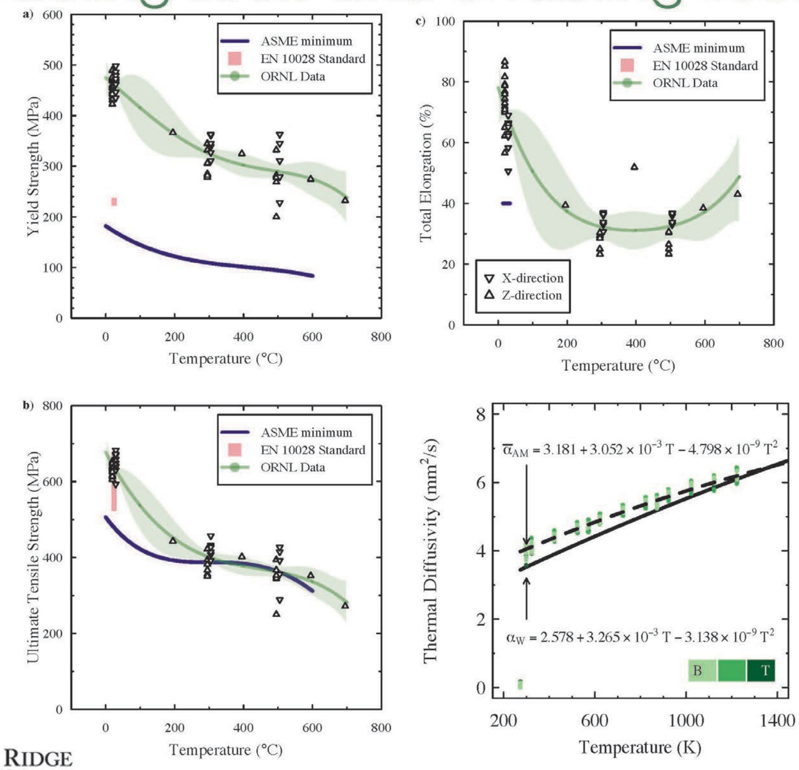
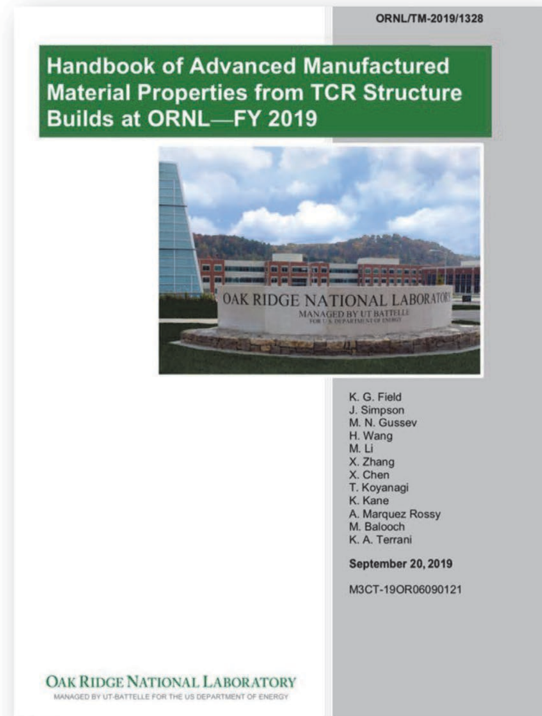
High quality property handbooks are key in informing modeling tools and enabling licensing and deployment





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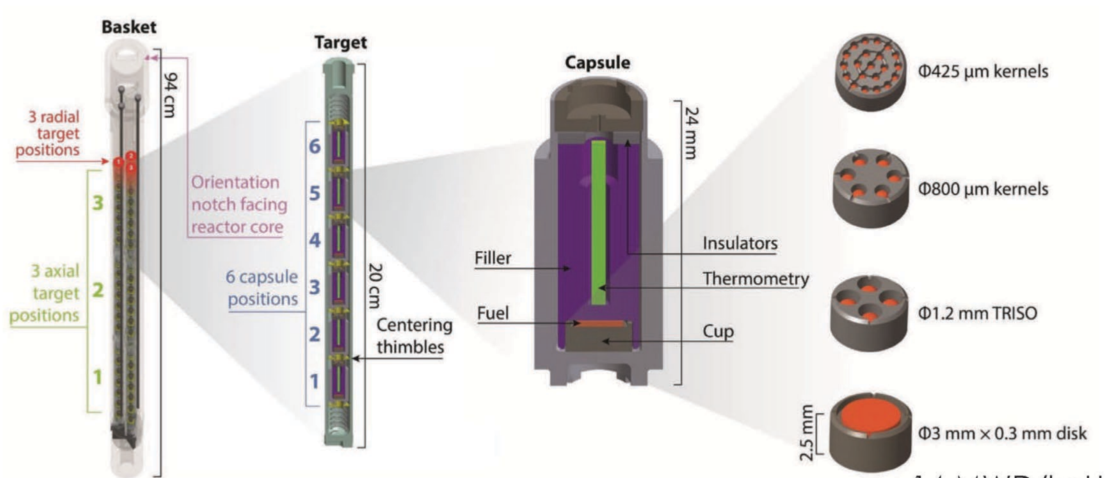
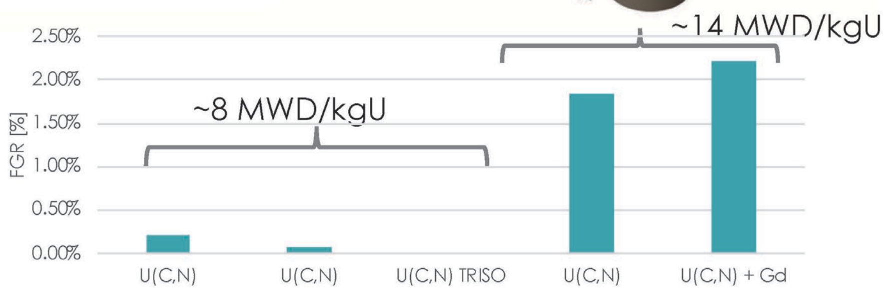
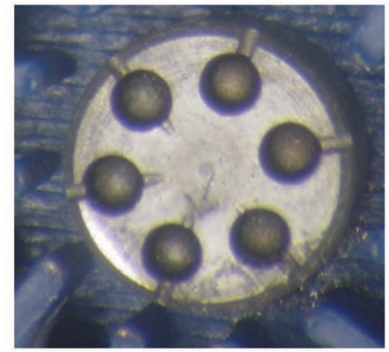
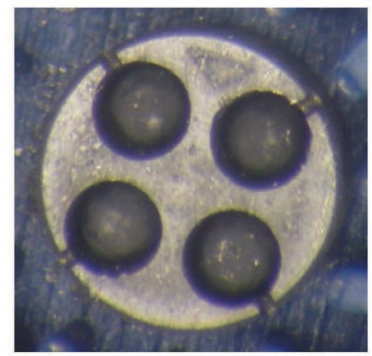
Separate effects testing to inform burnup and temperature dependent fuel constituent behavior









Petrie and Harp (2019)

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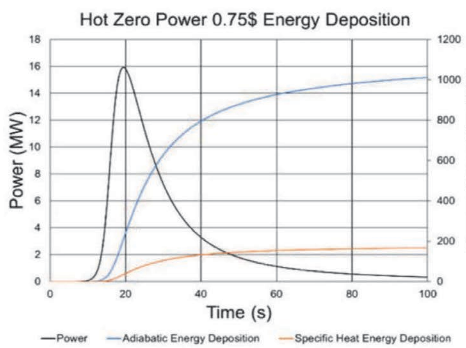
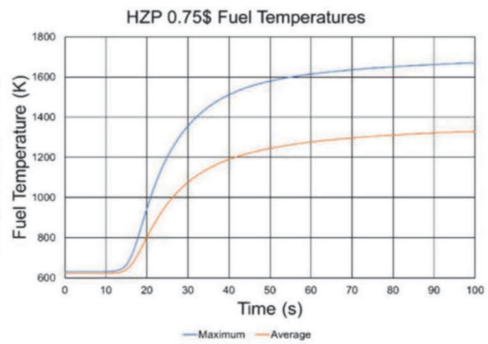
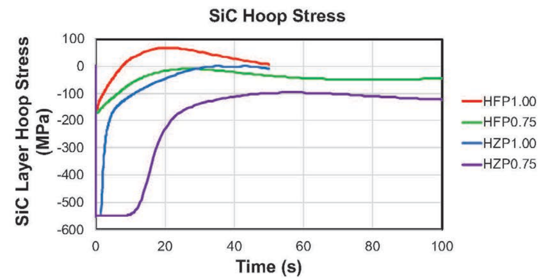
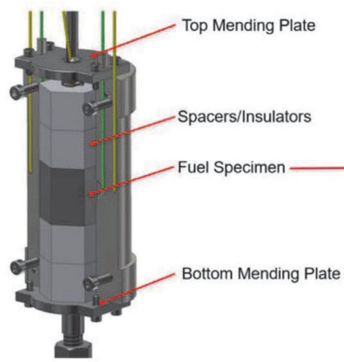
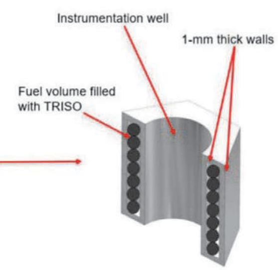
Separate Effects Transient Testing coupled with Modeling inform Integral Fuel Simulations

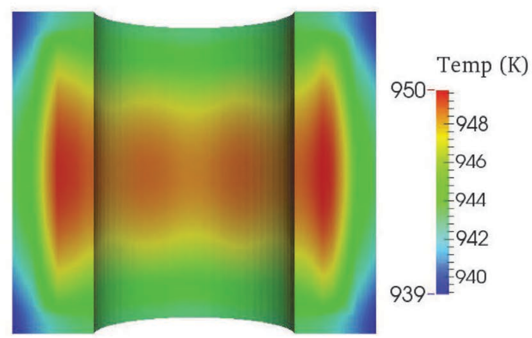












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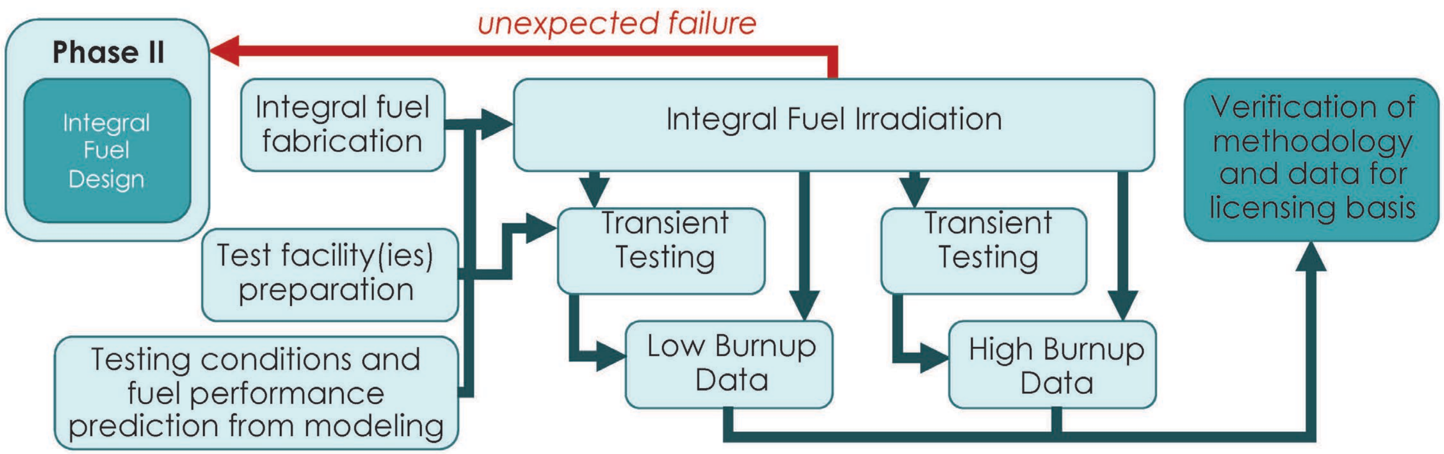
Phase III: minimal integral fuel testing to verify models and capture (if any) unaccounted integral effects



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Concluding thoughts

Engineering-Scale Modeling and Simulation Informed by and Integrated with Separate-Effects Testing will Greatly accelerate Fuel Development and Qualification

- TCR is building on the full breadth of the national capability and complex to deliver on its mission

- Modeling tools (e.g. NEAMS) are mature and knowledge of fuels and materials behavior (e.g. AFC/AGR/ART) are ample to facilitate an informed AFQ process (methodology + data)

- TCR demonstration will benefit the entire community and deliver new technologies and approaches for industrial adoption

tcr.ornl.gov

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APPENDIX H - Feltus AFQ Workshop II Jan 2020 Presentation on TRISO Fuel Material Properties Study

Evaluating the importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

Dr. Madeline Anne Feltus
Office of Advanced Fuel Technologies, NE-42

U.S. DEPARTMENT OF ENERGY

AFQ Workshop II Jan. 16, 2020

Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

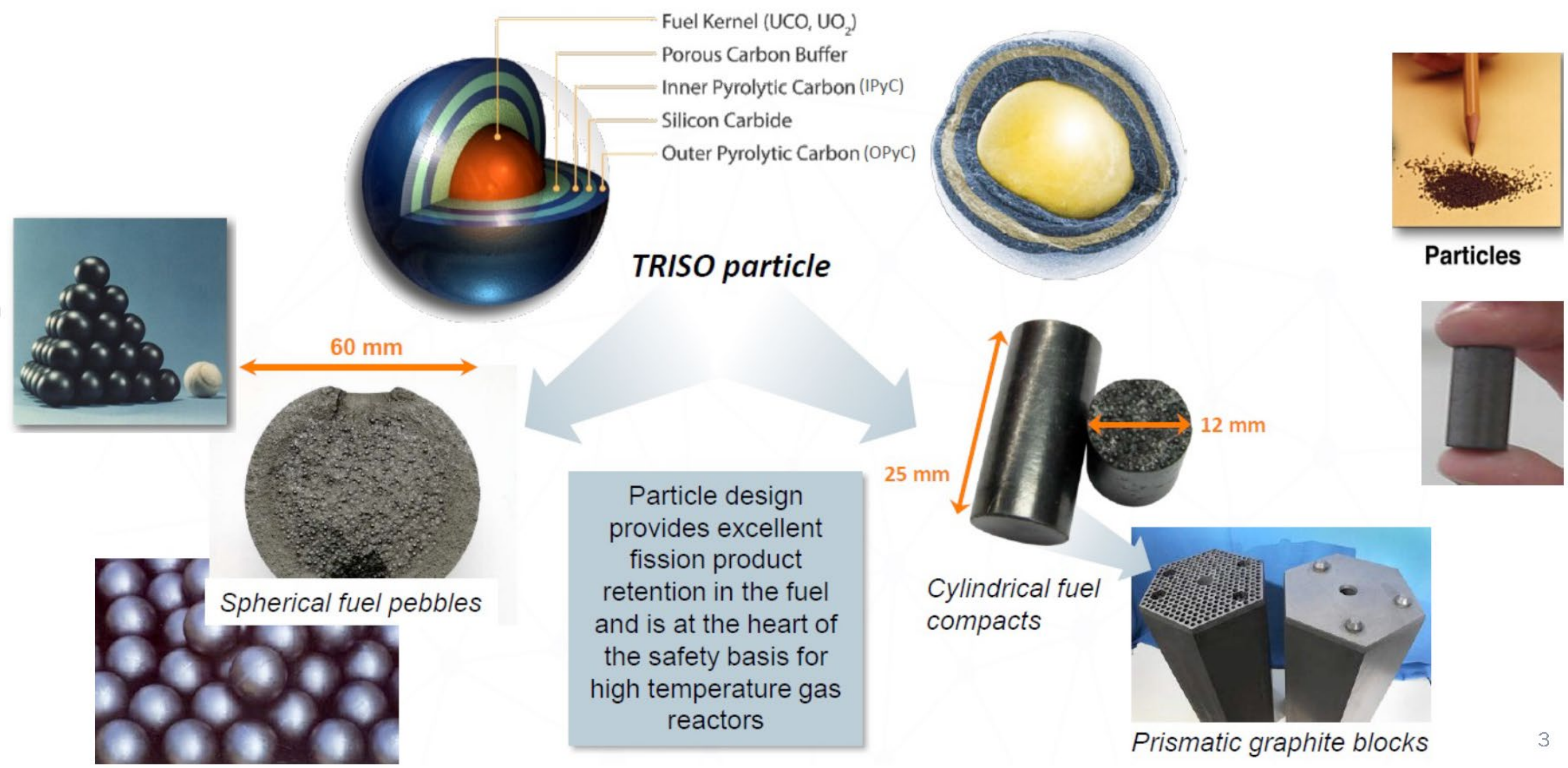
Overview

- Identify the material properties that have the largest impact on the failure probability of tristructural isotropic (TRISO)-coated fuel particles under irradiation.
- Most material constitutive properties were obtained from historical TRISO experimental data, some with large variability.
- The NE AGR TRISO Fuel program is evaluating the adequacy of the historical material properties data, and need to generate new data.
- The PARFUME TRISO fuel performance code was used to assess the importance of material properties on the probability of silicon carbide (SiC) layer failure.
- Although many (20+) material properties are used in PARFUME, only a few of them have a significant impact on the SiC failure probability.
- The most important properties are Pyrolytic Carbon (PyC) irradiation induced creep and strain (shrinkage, dimensional change).

References:
- Skerjank, W., B. Collin, INL/EXT-18-44631, Rev. 0, Aug. 2018.
- Skerjank, W. F., J. T. Maki, B. P. Collin, D. A. Petti, Evaluation of design parameters for TRISO-coated fuel particles to establish manufacturing critical limits using PARFUME, J. Nuclear Materials, vol. 469 (2016) pp. 99-105.

Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

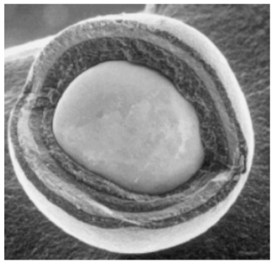
TRi-structural ISOtropic (TRISO) Coated Particle Fuel

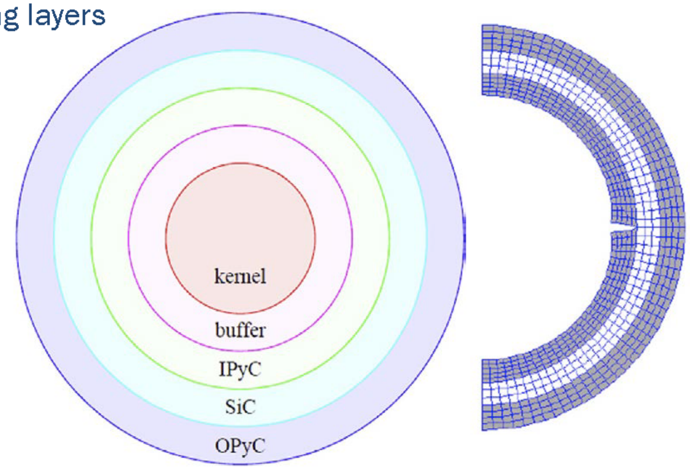


Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

PARFUME TRISO Fuel Performance Code

- Integrated mechanistic model of thermal, mechanical and physiochemical behavior of TRISO particles
- Calculates TRISO particle failure probability given the particle-to-particle statistical variation in physical dimensions and material properties under irradiation and postulated accident conditions
- Calculates fission product transport and diffusion through the coating layers into the fuel matrix and coolant
- Gaussian distribution for fuel design parameters
- Weibull statistical distribution for layer strengths and modulus
- PARFUME calculates inter-layer stresses and strains using:
  - Kernel diameter, 4 layer thicknesses
  - Pyrocarbon (PyC) layers and SiC densities
  - Degree of PyC anisotropy (Bacon Anisotropy Factor, BAF)
  - PyC creep coefficients
  - Poisson's ratio in PyC creep
  - Bond strength between IPyC and SiC layers
  - TRISO particle asphericity, measured by aspect ratio





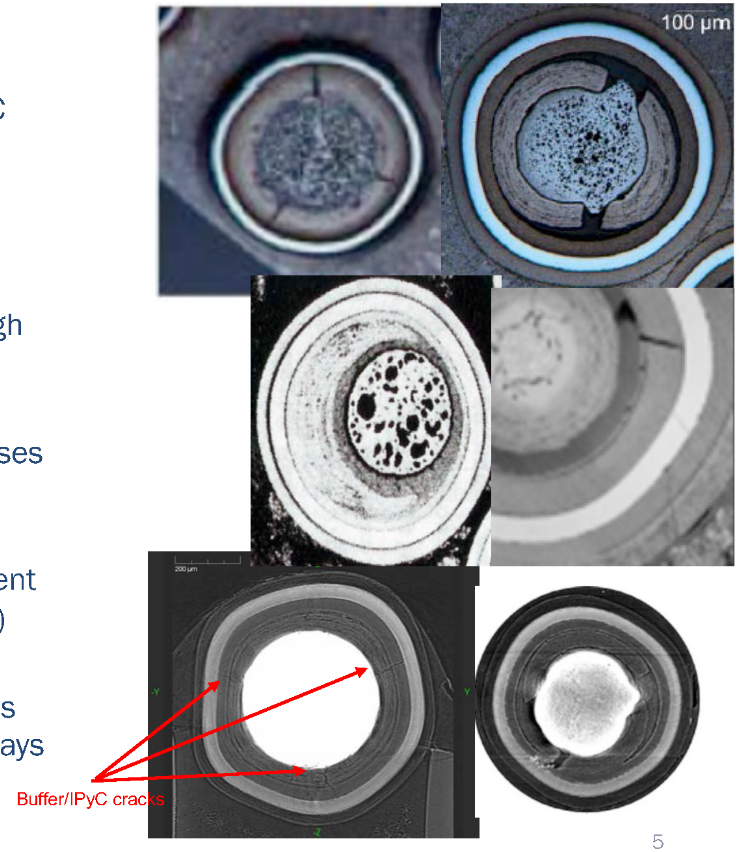
Typical TRISO-coated particle geometry model.

4

Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

TRISO Fuel Particle Failure Mechanisms

- Irradiation-induced shrinkage of IPyC and OPyC layers put the SiC layer into compression.
- Shrinkage/swelling response of PyC layers is highly anisotropic, depends on irradiation temperature, degree of anisotropy (BAF)
- Irradiation-induced shrinkage of IPyC layer can cause partial debonding of IPyC from SiC layer and IPyC cracking caused by high tensile stress,
- Increasing internal gaseous fission product pressure produces tensile component to the hoop stress in the SiC layer, and increases tangential stress in SiC beyond SiC fracture strength. Uranium Oxycarbide (UCO) fuel limits CO production seen in UO_2 fuel.
- Kernel migration (amoeba effect) where large temperature gradient causes equilibrium CO gas imbalance. Uranium Oxycarbide (UCO) fuel limits CO production seen in UO_2 fuel
- Mechanical interaction between kernel/buffer with PyC, SiC layers (rarely observed in irradiations, since gap stays open as buffer stays bonded to kernel during densification)



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Sensitivity, Importance Evaluation Methodology

- Use parametric variations of each material property to calculate stress levels in each particle layer
- Calculate resultant failure probability under various irradiation temperature conditions
- Determine importance of each material property by using sensitivity multiplication factors (SMF) varied around nominal property value and by comparing calculated failure probabilities
- Use AGR-5/6/7 fuel specification values and average irradiation conditions

Table 1. Irradiation conditions. AGR-5/6/7 qualification experiment average values

Condition	EFPD	Burnup (%FIMA)	Fast fluence ($\times 10^{25}$ n/m^2, E > 0.18 MeV)	Irradiation Temperature (°C)
1	500	13.5	5	700
2	500	13.5	5	1000
3	500	13.5	5	1300

Skerjank, W., B. Collin, INL/EXT-18-44631, Rev. 0, Aug. 2018

Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

Table 2. Fuel parameters used in PARFUME modeling.

Category	Parameter	Nominal Value ± Standard Deviation
Fuel characteristics	^{235}U enrichment (wt%)	15.5
	Carbon/uranium (atomic ratio)	0.4
	Oxygen/uranium (atomic ratio)	1.5
	Uranium contamination fraction	0
Particle geometry	Kernel diameter (μm)	425 ± 10
	Buffer thickness (μm)	100 ± 10
	IPyC / OPyC thickness (μm)	40 ± 3
	SiC thickness (μm)	35 ± 2
	Particle asphericity (SiC aspect ratio)	1.040
Fuel properties	Kernel density (g/cm^3)	11.0
	Kernel theoretical density (g/cm^3)	11.4
	Buffer density (g/cm^3)	1.05
	Buffer theoretical density (g/cm^3)	2.25
	IPyC density (g/cm^3)	1.90 ± 0.02
	OPyC density (g/cm^3)	1.90 ± 0.02
	IPyC/OPyC (post compact anneal) BAF	1.05 ± 0.005

AGR-5/6/7 fuel specification parameter average values

Skerjank, W., B. Collin, INL/EXT-18-44631, Rev. 0, Aug. 2018.

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Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

PARFUME uses these SiC layer material properties:

- Weibull characteristic strength σ_o
- Weibull modulus m variability in measured strength.
- Elastic moduli, Poisson's ratio
- Thermal conductivity and expansion

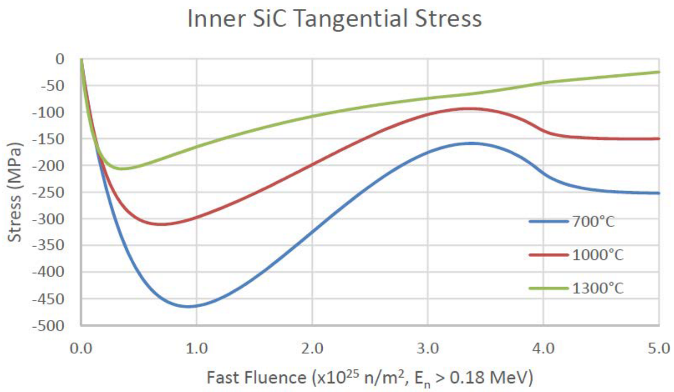

Table 3. Failure probability in the nominal conditions.

Condition	Probability of SiC failure			Probability of IPyC cracking
	Total	Contribution from IPyC Cracking	Contribution from Pressure	
1	4.03×10^{-4}	4.03×10^{-4}	0 *	8.94×10^{-1}
2	2.52×10^{-6}	2.52×10^{-6}	0	5.48×10^{-2}
3	2.21×10^{-9}	2.21×10^{-9}	2.82×10^{-13}	1.16×10^{-3}

* UCO fuel internal gas pressure too low to cause fuel failure

Weibull theory, coating layer failure probability:

$$P_f = 1 - \int_V \left(\frac{\sigma}{\sigma_o}\right)^m dV$$

using tensile stress (σ)

Skerjank, W., B. Collin INL/EXT-18-44631, Rev. 0, Aug. 2018.

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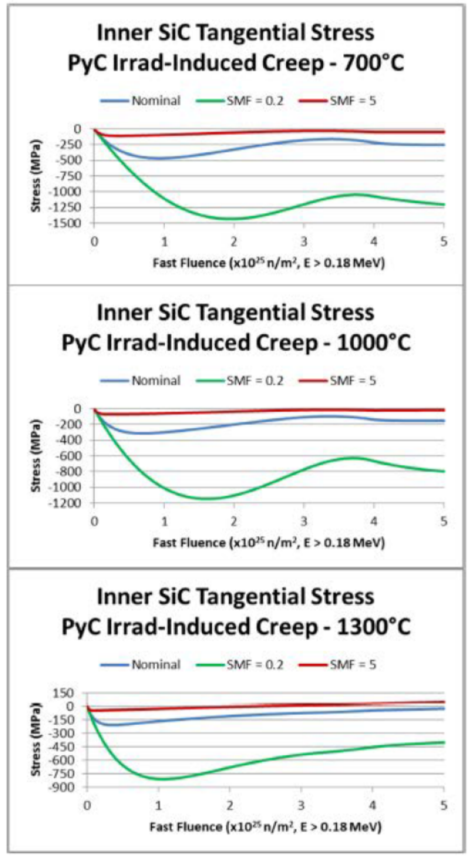
Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

Table 15. Failure probability: PyC irradiation-induced creep.

Condition	Sensitivity Multiplication Factor	Probability of SiC failure	Probability of IPyC cracking
1	0.2	2.48×10^{-1}	9.99×10^{-1}
	0.33	5.07×10^{-2}	9.99×10^{-1}
	0.5	1.01×10^{-2}	9.99×10^{-1}
	1 (nominal)	4.03×10^{-4}	8.94×10^{-1}
	2	1.49×10^{-7}	1.06×10^{-2}
	3	5.35×10^{-10}	3.50×10^{-4}
	5	3.35×10^{-13}	3.99×10^{-6}
2	0.2	5.57×10^{-2}	9.99×10^{-1}
	0.33	7.80×10^{-3}	9.99×10^{-1}
	0.5	1.24×10^{-3}	9.99×10^{-1}
	1 (nominal)	2.52×10^{-6}	5.48×10^{-2}
	2	1.76×10^{-10}	1.57×10^{-4}
	3	4.96×10^{-13}	4.32×10^{-6}
	5	2.52×10^{-16}	4.22×10^{-8}
3	0.2	7.50×10^{-3}	9.99×10^{-1}
	0.33	7.00×10^{-4}	9.98×10^{-1}
	0.5	2.43×10^{-5}	2.73×10^{-1}
	1 (nominal)	2.21×10^{-9}	1.16×10^{-3}
	2	2.88×10^{-8}	3.04×10^{-6}
	3	2.98×10^{-7}	8.34×10^{-8}
	5	1.30×10^{-6}	8.12×10^{-10}



PARFUME Results for PyC Irradiation-induced creep

PARFUME uses these PyC layer material properties:

- Elastic moduli
- Poisson's ratio
- Thermal conductivity and expansion
- *Irradiation-induced creep* *
- *Poisson's ratio in creep* *
- *Strain rates* *
- *Weibull strength and modulus* *

* These parameters have significant impact on SiC failure probability

Skerjank, W., B. Collin, INL/EXT-18-44631, Rev. 0, Aug. 2018.

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Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

Summary of maximum impact of material properties on SiC failure probability

Material Property	Sensitivity Multiplication Factor or Material Property Value	Irradiation Temperature (°C)	Increase in SiC failure probability	SiC failure probability
PyC elastic moduli	× 3	700	1.6	6.54×10^{-4}
		1000	2.7	6.84×10^{-6}
		1300	2.0	4.47×10^{-9}
PyC Poisson's ratio	0.5	700	1.3	5.04×10^{-4}
		1000	1.6	3.96×10^{-6}
		1300	1.4	3.03×10^{-9}
PyC irradiation-induced creep	× 0.2	700	1.1	2.48×10^{-1}
		1000	2.2×10^{4}	5.57×10^{-2}
		1300	3.4×10^{6}	7.50×10^{-3}
PyC Poisson's ratio in creep	Failure probability is maximum at nominal Poisson's ratio in creep			

Skerjank, W., B. Collin, INL/EXT-18-44631, Rev. 0, Aug. 2018. 10

Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

Summary of maximum impact of material properties on SiC failure probability (cont.)

Material Property	Sensitivity Multiplication Factor or Material Property Value	Irradiation Temperature (°C)	Increase in SiC failure probability	SiC failure probability
PyC irradiation-induced dimensional change	× 5	700	2.4×10^{3}	9.68×10^{-1}
		1000	1.7×10^{5}	4.21×10^{-1}
		1300	1.1×10^{7}	2.48×10^{-2}
PyC Weibull parameters (m / σ_0)	8/10.0	700	1.04	4.20×10^{-4}
		1000	2.1	5.37×10^{-5}
		1300	4.1	9.02×10^{-9}
SiC elastic modulus	× 5	700	1.6	6.45×10^{-4}
		1000	1.7	4.21×10^{-6}
		1300	1.4	3.01×10^{-9}
SiC Poisson's ratio	0.5	700	2.6	1.03×10^{-3}
		1000	2.7	6.79×10^{-6}
		1300	2.6	5.67×10^{-9}
SiC Weibull parameters	4 / 0.76	700	12.4	4.99×10^{-3}
		1000	26.5	4.03×10^{-4}
		1300	76.3	1.01×10^{-5}

Skerjank, W., B. Collin, INL/EXT-18-44631, Rev. 0, Aug. 2018.

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Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

TRISO PyC Materials Properties with Significant Impact on SiC Layer Failure Probability:

- PyC irradiation-induced creep
- PyC irradiation-induced strain (dimensional change)

TRISO SiC Properties with Major Impact on SiC Layer Failure Probability:

- SiC Weibull modulus, m
- SiC Weibull characteristic strength, σ_o

Shrinkage (strain) of the PyC layers puts them into tension and the SiC layer into compression but the irradiation creep relieves that tensile stress and reduces SiC layer compression.

An increase of the irradiation-induced PyC strain or a decrease of the irradiation-induced PyC creep creates additional tensile stress in the SiC layer, increasing the SiC layer probability of failure.

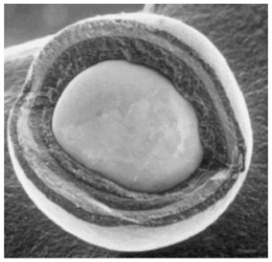
TRISO Materials Properties with No Significant Impact:

- Kernel swelling rate
- Kernel thermal conductivity
- Buffer elastic modulus
- Buffer Poisson's ratio
- Buffer irradiation-induced creep
- Buffer Poisson's ratio in creep
- Buffer irradiation-induced dimensional change
- Buffer thermal conductivity
- Buffer thermal expansion
- PyC thermal conductivity
- PyC thermal expansion
- SiC thermal conductivity
- SiC thermal expansion.

Skerjank, W., B. Collin, INL/EXT-18-44631, Rev. 0, Aug. 2018.

Importance of TRISO Fuel Materials Properties for Irradiated Fuel Performance Analysis

Summary and Conclusions



- PARFUME TRISO particle modeling involves ~ 20+ materials properties.
- Parameter sensitivity studies combined with the use of sensitivity multiplication factors (SMF) varied around nominal property values can identify which parameters are most important.
- TRISO material properties exhibit a large variability according to published historical data.
- Determining which properties are most important can help prioritize the generation of new properties data when historical materials property data is not available or deemed adequate.
- Determining TRISO materials properties as a function of temperature, neutron irradiation fluence or damage (dpa) is difficult, involves thin coating layer samples, and requires spherical geometry samples, vs. flat thin plates.
- Parameter importance ranking studies can also be used to improve modeling details when code predictions differ from well-planned experimental results.

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APPENDIX I - Energy Multiplier Module (EM^2) Accelerated Fuel Qualification Strategy

Energy Multiplier Module (EM^2) Accelerated Fuel Qualification Strategy

By
John Bolin

Nuclear Technologies and Materials
General Atomics

January 16, 2020

GENERAL ATOMICS

EM² AFQ Strategy White Paper
NRC Pre-Application License Review

Contents include:

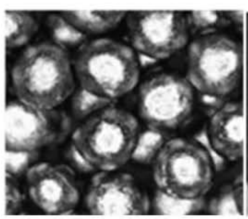
- Description of EM²
- Fuel design bases and criteria
- Analysis methods and material properties
- Performance evaluation
- Legacy approach to fuel qualification
- Strategy for accelerated qualification

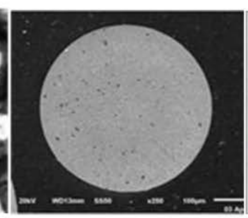
GENERAL ATOMICS

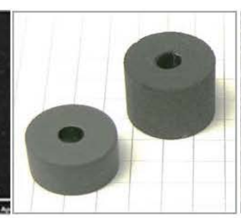
EM^2 Fuel Design Driven by Top Level Goals

Innovative EM^2 fuel design driven by:

- **Lower generation cost**
- **Fuel cycle flexibility**
- **Improved safety performance**
- **Higher net efficiency**
- **Higher fuel utilization**
- **Much less high-level waste**
- **Proliferation-resistant fuel cycle features**


UC kernel via sol-gel


200 μm diameter high density kernel


Annular pellet via hot pressing


Porous UC pellet

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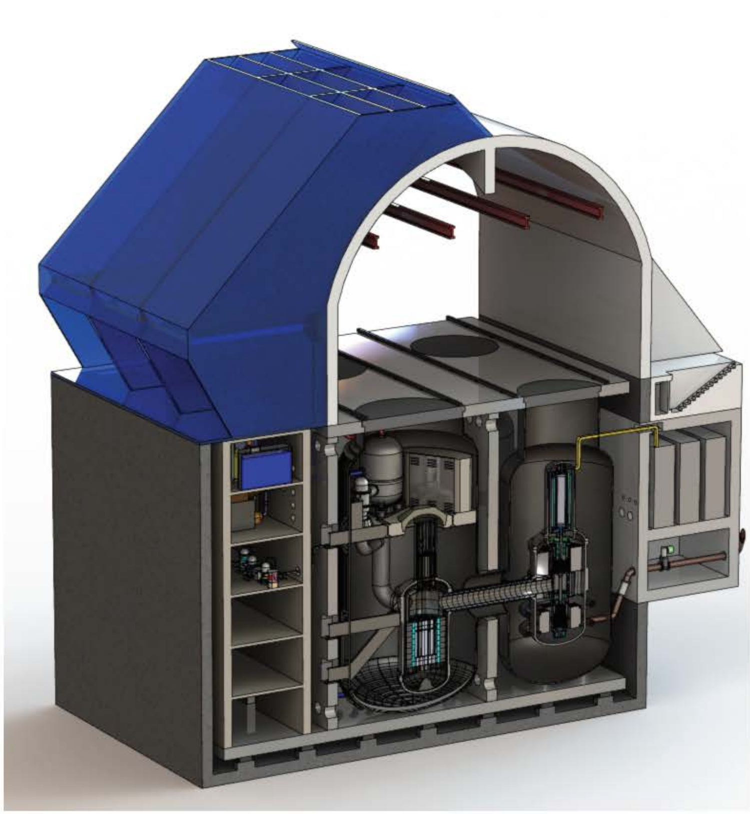
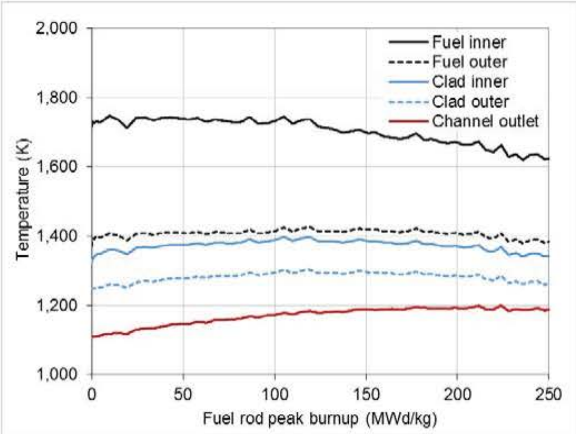
EM² is a Modular, Gas-Cooled, Convert-and-Burn, Fast Reactor

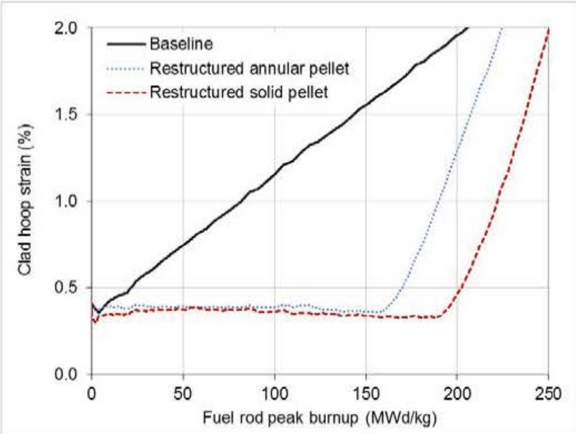


- 265/240 MWe per reactor for water/dry cooling
- 500 MW_t reactor power
- 4 modules per standard plant
- 60 year plant life; 30 year core life
- 60 year dry fuel storage
- 14% average fuel burnup
- Multi-fuel capable

Performance Evaluation
Normal Operation

- FRAPCON-4.0GA modified for UC fuel and SiGA SiC composite cladding
- Baseline calculation uses restrained swelling model
- Restructured annular pellet includes fuel swelling into open pores
- Restructured solid pellet has increased pellet porosity (17% increasing to 26.8%)

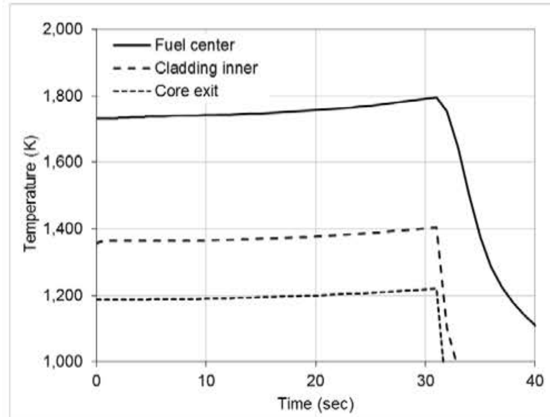




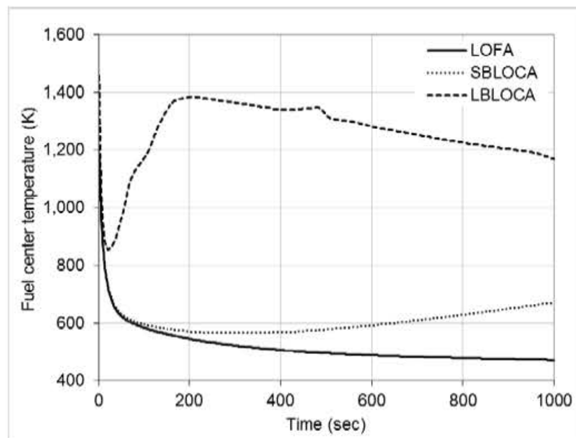
GENERAL ATOMICS

Performance Evaluation
Accident Conditions

- Uncontrolled control rod withdrawal at middle-of-life conditions
- Reactor trips at 109% at 31 s
- Peak fuel temperature of 1789K well below melting point of 2705K
- Cladding circumferential strain 0.59% close to design limit of 0.62%

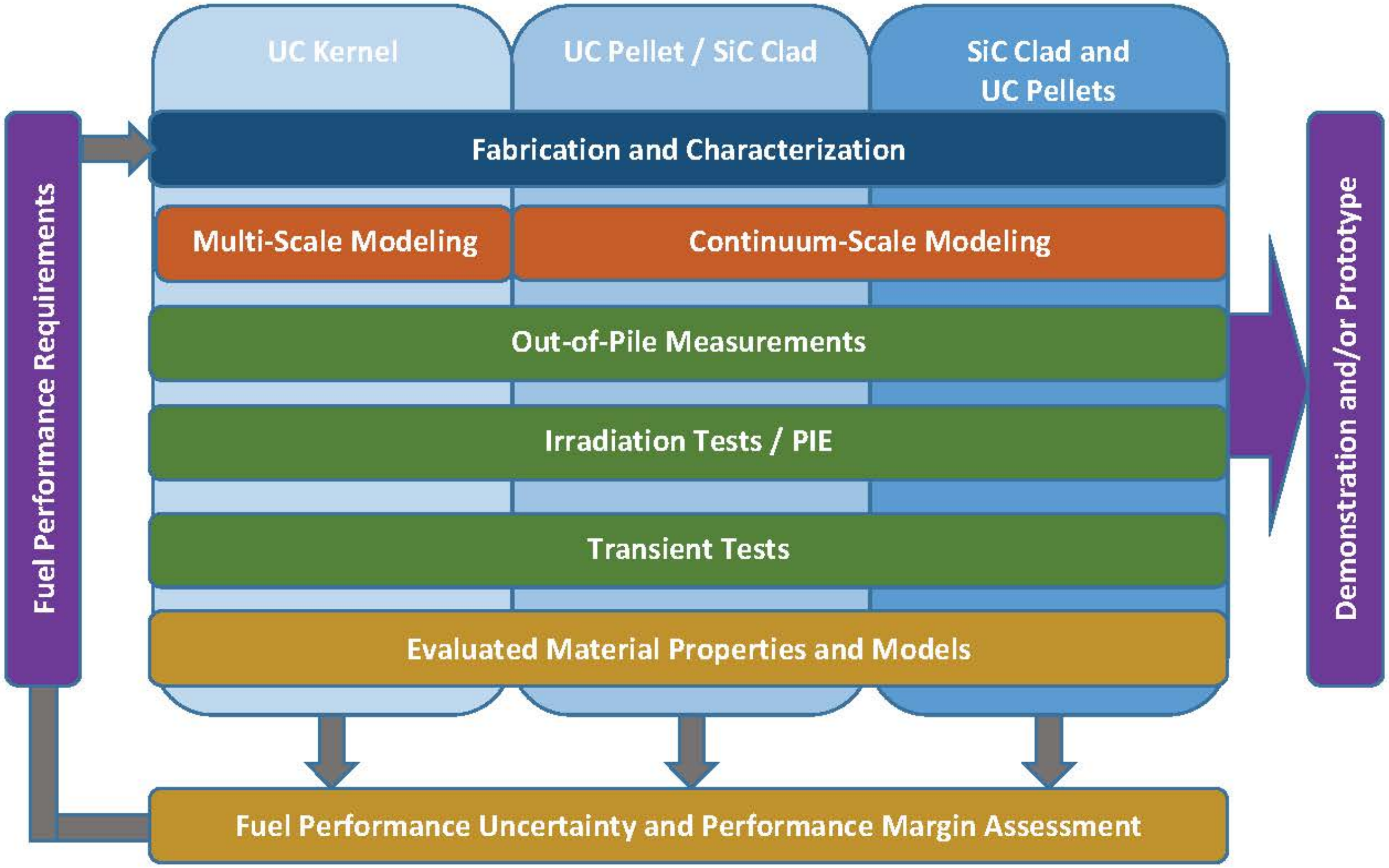


- Loss of Flow Accident (LOFA) with trip of Power Conversion System
- Small Break LOCA of 10 cm^2
- Large Break LOCA of 400 cm^2
- All transients assume only one of two passive cooling trains are operational



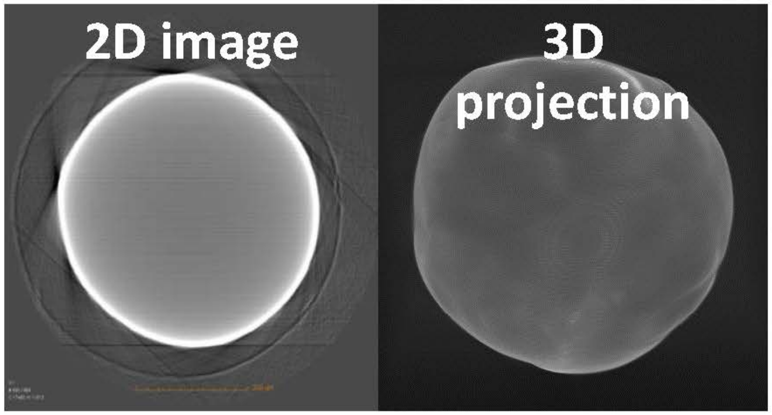
GENERAL ATOMICS

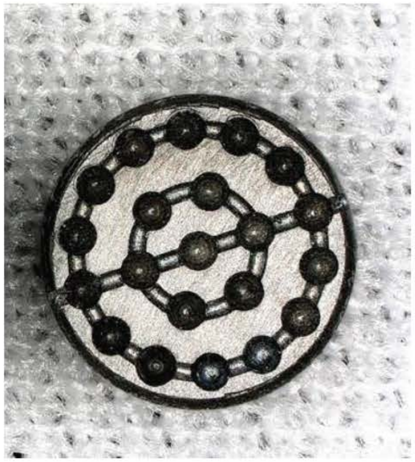
Step-Wise AFQ Methodology
Advanced M&S Reduces Design Iterations



Mini-Fuel Irradiation of UC Kernels at HFIR

- **HFIR irradiation delayed due to shutdown in 2019**
- **XCT of kernels before and after to determine fuel swelling**
- **Capsules will be assembled and inserted into HFIR in first quarter of 2020**



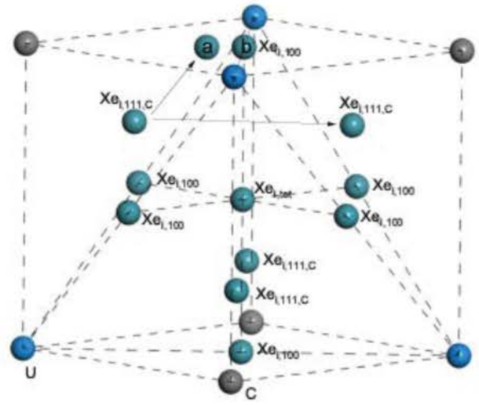


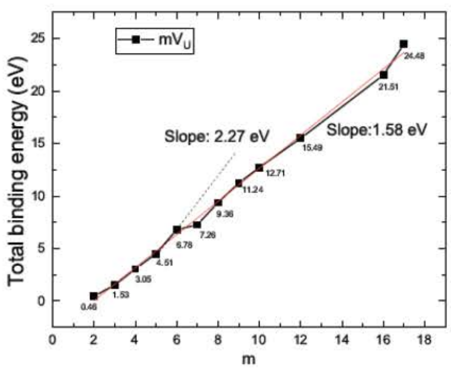
OAK RIDGE National Laboratory

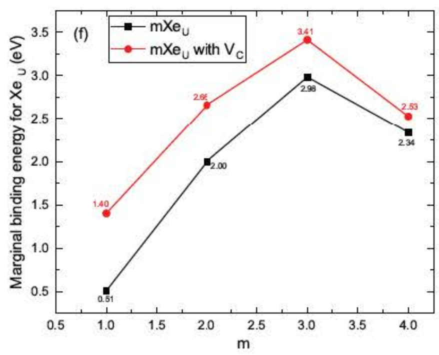
GENERAL ATOMICS

Multi-Scale Modeling Progress

- **Ab-initio electronic structure modeling of Xe behavior, diffusion and clustering in UC**
- **Density functional theory calculations of vacancy and Xe clustering**
- **Preparing parameterization of Xolotl calculations of bubble populations**





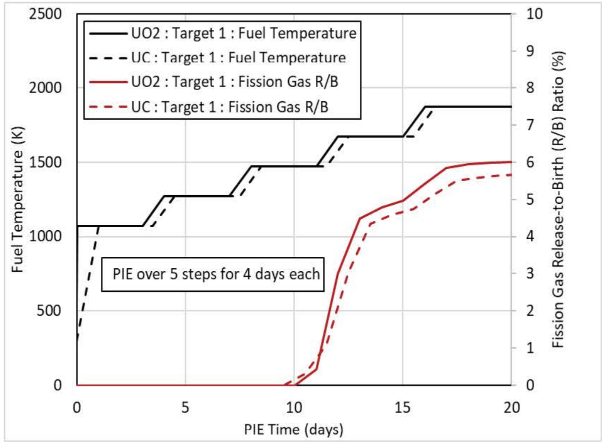


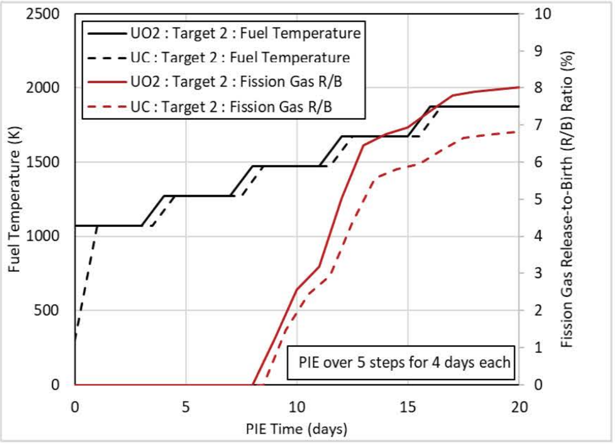
THE UNIVERSITY OF TENNESSEE KNOXVILLE
DEPARTMENT OF NUCLEAR ENGINEERING

GENERAL ATOMICS

Pre- and Post-Irradiation Analysis and Testing Planned and Proposed

- **XCT to quantify kernel swelling**
- **Fission gas release from capsules**
- **Preliminary fuel performance analysis using BISON**
- **Post-irradiation heating tests proposed to measure fission gas release at elevated temperature**

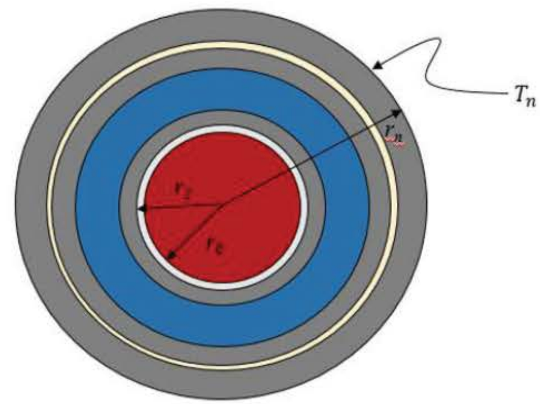




GENERAL ATOMICS

Accelerated Irradiation at INL Advanced Test Reactor

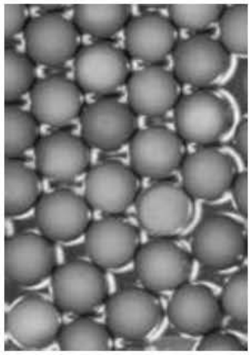
- **Accelerated irradiation of UC pellets using INL Fission Accelerated Steady-state Testing (FAST) capsule design and approach**
- **Reduction in pellet diameter and increase in enrichment result in higher fission density and accelerated burnup with similar peak fuel temperatures**
- **Initial capsule design, scaling relationships, and fabrication for EM^2 UC pellets is supported by GA under a recent three-year INL Laboratory-Directed Research and Development project**



Reduced Size UC Pellet Irradiation

Key objectives

- Fission gas release
- Fuel swelling
- Creep
- PIE and post-irradiation testing
- Validate science-based models

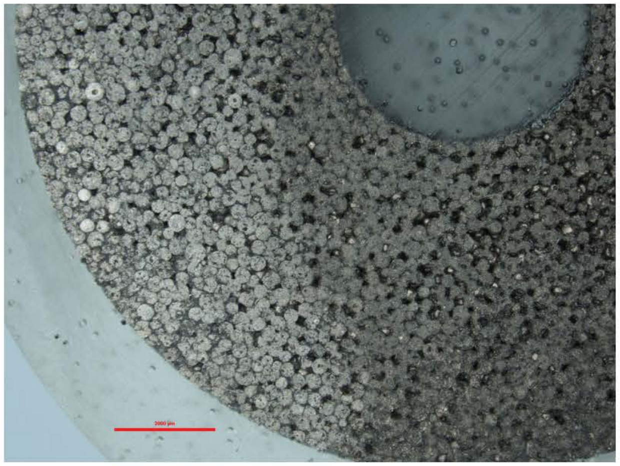


Proposed irradiation facilities

- Mini-pellet discs in HFIR
- Reduced-size pellets in ATR using FAST approach

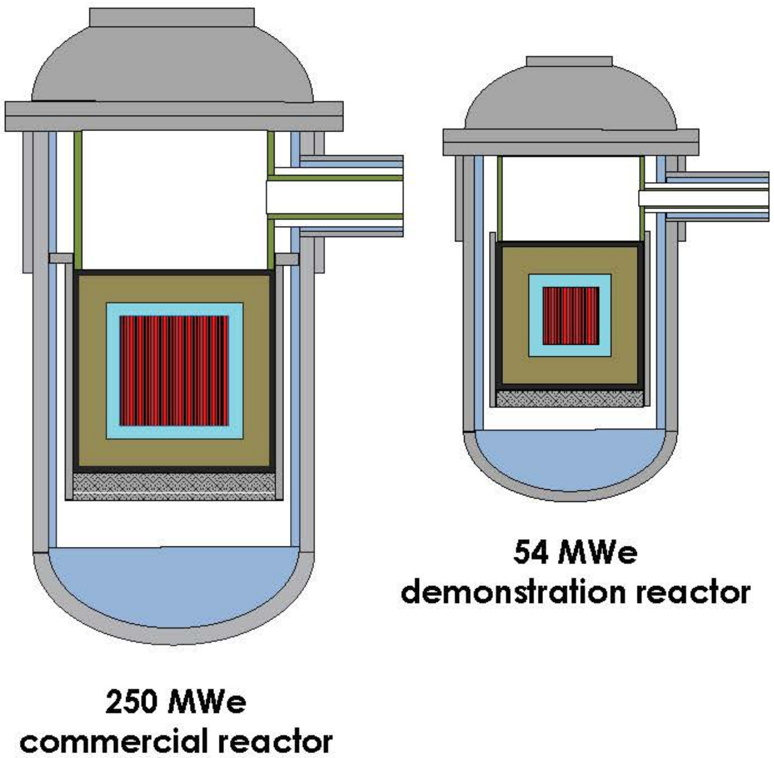
Pellet-Clad Interaction Integral Fuel Testing

- Swelling, creep and fission gas release interrelationships
- Validate advanced modeling and simulation
- Initial testing in ATR using on-line FGR monitoring used in AGR Fuel testing of TRISO compacts
- Prototypical testing in gas cartridge loop in Versatile Test Reactor



Demonstration / Prototype Reactor Fuel Surveillance and Operating License Conditions

- **Safety case established from science-based modeling validated by testing**
- **Fuel qualification for full burnup conditional on periodic fuel surveillance and testing to reduce performance uncertainties and risk**
- **Fuel qualification risk reduction similar to reactor vessel material surveillance and life extension measures in current fleet**



Key Objectives of EM^2 AFQ Strategy

- **Science-based approach to predictive performance of nuclear fuel can fulfill some integral test requirements**
- **Accelerated fuel irradiations as part of science-based approach can be substituted for integral fuel irradiations**
- **Fuel surveillance and conditional operating license is appropriate for EM^2 long life core as substitute for full burnup fuel testing under prototypical conditions**

GENERAL ATOMICS

Thank You

ACKNOWLEDGEMENT

This material is based upon work supported by the Department of Energy under Award Number DE-NE0008831.

APPENDIX J - Advanced Fuel Qualification Methodology Report

TerraPower

Advanced Fuel Qualification Methodology Report

Pete Gaillard

January 16, 2020

Overview

- TerraPower was notified in September 2019 of an award to develop the *Advanced Fuel Qualification Methodology Report* for metallic fuel in a sodium fast reactor environment
- The Report will provide a methodology addressing the qualification of advanced reactor fuel
- The Report will describe a process to evaluate regulatory deficiencies or gaps faced by advanced reactor designs for fuel qualification

TerraPower

Goals

Implementing the methodology will result in:

- Development of a process to identify and develop regulatory requirements and design criteria for advanced reactor fuel
- Identification and development of specific regulatory requirements applicable for metallic fuel – but the process may be used for other advanced reactor developers)
- A method for development of Regulatory Acceptance Criteria (RAC) to ensure compliance with regulatory requirements and design criteria

TerraPower

Initial Steps

- Identify and describe the aspects of the fuel system design to be addressed
- Identify applicable regulatory requirements
  - The regulatory requirements are expected to be similar to requirements described in NUREG-0800, Section 4.2, *Fuel System Design*
- Modify or remove requirements that are not applicable

TerraPower

Regulatory Acceptance Criteria (RAC)

- The RAC will be analogous to SRP AC but are expected to differ due to inherent differences between SFR and LWR technology
  - SRP - Stress, strain, or loading limits for spacer grids, guide tubes, thimbles, fuel rods, control rods, channel boxes and other fuel system structural members should be provided
  - RAC - Stress, strain, or loading limits for all fuel system components shall be established
- The RAC will be used to establish functional and performance design requirements

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Additional Information

- Additional information included in the report may specify design, analysis, programmatic, testing, documentation, or other types of requirements necessary to ensure the plant design complies with applicable regulatory requirements and expectations
- The Report will describe approaches (acceptance criteria and compliance methods) that may be used to demonstrate compliance with the regulatory requirements addressed in a specific SAR section.

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Other Information

Additional information to demonstrate compliance may include:

- Specification of design requirements (directly or by reference to codes and standards)
- Identification of required design and safety analyses
- Identification of design, construction, or operation procedural control programs

TerraPower

Expected Results

- Expected results after the process is developed and implemented are descriptions of requirements for fuel system design necessary to ensure:
  - The fuel system is not damaged during any condition of normal operation, including the effects of anticipated operational occurrences (AOOs)
  - The number of fuel pin failures predicted for postulated accidents is not underestimated
  - Fuel coolability will be maintained during postulated accidents
  - Fuel system damage during postulated accidents will not prevent reactivity control/standby rod insertion when required

Summary

The Advanced Fuel Qualification Methodology Report will describe a method which when implemented will result in:

- Identification of specific regulatory requirements applicable for metallic fuel that will need to be addressed in the Safety Analysis Report (SAR)
- Descriptions of requirements for fuel system design including acceptance criteria and compliance approaches

The NRC will review and evaluate the report

TerraPower

APPENDIX K - Fuel Qualification, NRC Perspectives

U.S.NRC
United States Nuclear Regulatory Commission
Protecting People and the Environment

Fuel Qualification
NRC Perspectives

Accelerated Fuel Qualification Workshop
January 16, 2020

Topics

- NRC fuel qualification obligations under NEIMA
- Advanced reactor fuel qualification strategy options
- Open discussion for path forward

NRC Fuel Qualification Obligations Under NEIMA

U.S.NRC
UNITED STATES NUCLEAR REGULATORY COMMISSION
Protecting People and the Environment

The Nuclear Energy Innovation and Modernization Act (NEIMA) directs the NRC to modernize its approach to nuclear energy regulation.

https://www.congress.gov/bill/115th-congress/senate-bill/512/text

SEC. 103. of NEIMA covers “Advanced nuclear reactor program” and addresses fuel qualification in three subparts:

(b) Report To Establish Stages in the Commercial Advanced Nuclear Reactor Licensing Process.--
(4) Required evaluations. --Consistent with the role of the Commission in protecting public health and safety and common defense and security, the report shall evaluate--
(A)(ii) strategies for the qualification of advanced nuclear reactor fuel, including the use of computer modeling and simulation and experimental validation...

U.S.NRC
UNITED STATES NUCLEAR REGULATORY COMMISSION
Protecting People and the Environment

NRC Fuel Qualification Obligations Under NEIMA (cont.)

(c) Report to Increase the Use of Risk-Informed and Performance-Based Evaluation Techniques and Regulatory Guidance --

(4) Required evaluations. --Consistent with the role of the Commission in protecting public health and safety and common defense and security, the report shall evaluate--

(A) the ability of the Commission to develop and implement, where appropriate, risk-informed and performance-based licensing evaluation techniques and guidance for commercial advanced nuclear reactors within existing regulatory frameworks not later than 2 years after the date of enactment of this Act, including policies and guidance for the resolution of—

(i)(V) issues relating to the qualification of advanced nuclear reactor fuel; and...

(e) Report To Complete a Rulemaking To Establish a Technology-Inclusive Regulatory Framework for Optional Use by Commercial Advanced Nuclear Reactor Technologies in New Reactor License Applications and To Enhance Commission Expertise Relating to Advanced Nuclear Reactor Technologies.--

(1) Report required. –Not later than 30 months after the date of enactment of this Act, the Commission shall submit to the appropriate congressional committees a report... for--

(B) ensuring that the Commission has adequate expertise, modeling, and simulation capabilities, or access to those capabilities, to support the evaluation of commercial advanced reactor license applications, including the qualification of advanced nuclear reactor fuel.

May 31, 2019 4

Strategies to Meet Fuel Qualification Obligations Under NEIMA

Internally, the staff has developed a strategy regarding the qualification of advanced nuclear reactor fuel as required by NEIMA Sec. 103(c)(4)(A)(i)(V):

(1) Staff will issue technology-neutral guidance as white paper, which will turn into RG.

(2) Staff to complete review of TRISO fuel performance topical report.

(3) Staff to complete review of topical report for metal fuels legacy data QA program.

(4) Contract with ORNL to produce a draft letter report describing regulatory policy guidance on the acceptability of an MSR fuel property measurement approach to fuel salt qualification and the technical basis for MSR fuel qualification and regulatory guidance documentation, which may be used to produce a formal NRC guidance document.

(5) Several vendors/designers have indicated plans to submit a topical report requesting NRC review and approval of its proposed fuel qualification methodology.

Options for Technology-Neutral Guidance

The staff has committed to identifying (and beginning to implement) a technology-neutral guidance document by January 2021. This could take various forms:

1. White paper or NUREG, which leads to a future Regulatory Guide
2. Approval of a generic industry topical report
3. NRC participation in an industry-led report which leads to a future Regulatory Guide endorsing (in part or whole) the industry-led report

Thoughts/comments?

Content Ideas for Advanced Reactor Fuel Qualification Guidance

- Provide definition of fuel qualification
  - Explain the design role within fuel qualification vs. licensing role
- Description of various license options (e.g. Part 52, prototype, etc) and impacts on licensing basis requirements
- Introduce the concept of graduated fuel qualification for license applications
  - Licensing oversight would be tied to the safety significance of the fuel for a given reactor design
- Fuel code verification and validation discussion
- Other topics?

APPENDIX L - Lower Length Scale Modeling Examples

Lower Length Scale Modeling Examples

Antoine Claisse, Denise Adorno Lopes, Kallie Metzger

January 16, 2020

Westinghouse

Advanced Modeling Applications

- Assist in understanding experimental results
  - Interpolation and extrapolation of experimental data points
  - Help to derive FRD models (to be validated on experiments)
- Materials screening and development
  - Prediction of material behavior
  - Rare or not yet commercially available materials accessible
  - Combining with experiments to get deeper understanding
- Design of experiments
  - Ensure selected conditions will highlight phenomena of interest
  - Evaluate behaviors in extreme conditions (i.e. high burn up)

Accelerate deployment of safe designs

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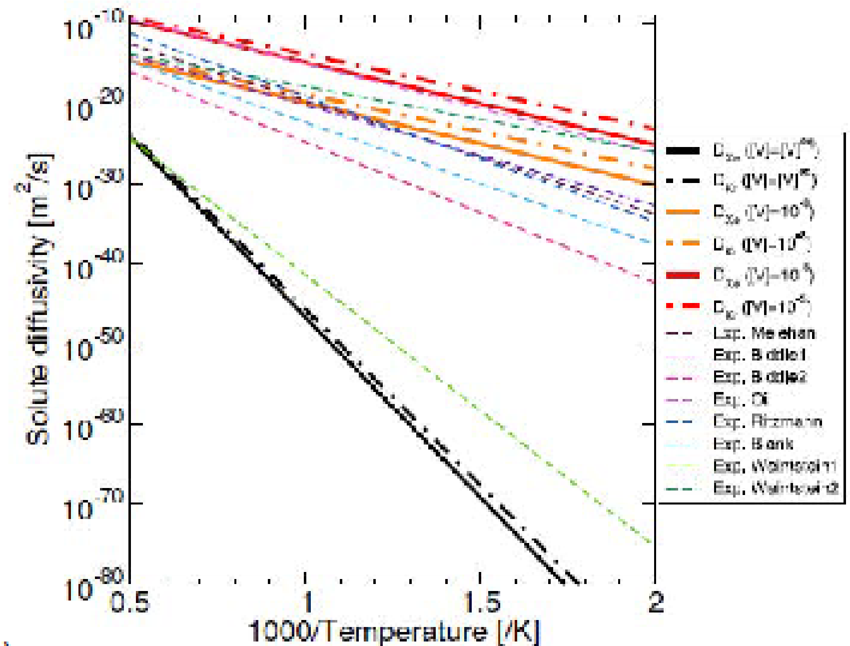
Example of application: understanding experimental results

- Xe diffusion in UN
- Large experimental discrepencies
- Modeling shows that a probable cause is the amount of vacancies in the material, varying too much and making comparison hard



Claisse, A., Schuler, T., Lopes, D. A., & Olsson, P. (2016). Transport properties in dilute UN (X) solid solutions (X= Xe, Kr). *Physical Review B*, *94*(17), 174302.

Atomistic modeling offers an explanation for apparently inconsistent experimental results

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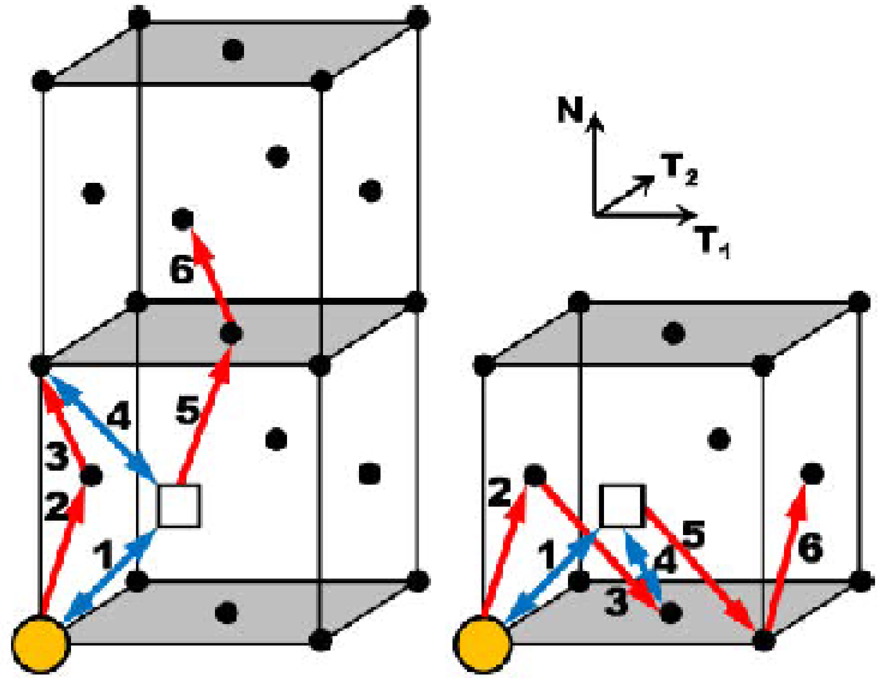
Example of application: extrapolation/cliff behaviors

- Xe diffusion in UN
- By understanding the diffusion mechanisms, we can
  - Know the diffusion path
  - Estimate if it will change with temperature
  - Predict if there will be a sudden behavior change



Claisse, A., Schuler, T., Lopes, D. A., & Olsson, P. (2016). Transport properties in dilute UN (X) solid solutions (X= Xe, Kr). *Physical Review B*, *94*(17), 174302.

Atomistic modeling can allow to predict changes of physical behavior, or possibility of extrapolation

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Example of application: support to find equilibrium phases

- Work mostly carried out by our partners at USC
- Combining SERPENT results (Fp concentration at a given BU), CALPHAD modeling and small-scale modeling allowed to predict the phase of FPs in U_3Si_2

Element	Phase	ΔH_f (ev/atom)
Cerium	CeSi	-0.631
	Ce_5Si_4	-0.598
	Ce_5Si_3	-0.550
Barium	$BaSi_2$	-0.359
	Ba_3Si_4	-0.406
	BaSi	0.422
	Ba_5Si_3	0.331
	Ba_2Si	-0.310
Gadolinium	Gd_5Si_3	-0.657
	Gd_5Si_4	-0.739
	GdSi	0.825
Plutonium	Pu_3Si_2	-0.297
	Pu_5Si_3	-0.510
	PuSi	-0.633
Yttrium	YSi	-0.851
	Y_5Si_4 (P21/c)	0.773
	Y_5Si_4 (Pnma)	-0.776
	Y_5Si_3	-0.720

Element	25°C	200°C	400°C	600°C	800°C	1000°C	1250°C
U	U_3Si	U_3Si	U_3Si	U_3Si	Liquid*	Liquid	Liquid
Ba	BaSi	BaSi	BaSi	BaSi			
Ce	-	-	-	-	-	-	-
Gd	GdSi	GdSi	GdSi	Gd_5Si_4	Gd_5Si_4	Gd_5Si_3	Gd_5Si_3
Mo	U_4MoSi_6	U_4MoSi_6	U_4MoSi_6	U_4MoSi_6	U_4MoSi_6	U_4MoSi_6	U_4MoSi_6
Pu	-	-	-	-	-	-	-
Se	Se (s)	Se (s)	Se (l)	Se (l)	Se (g)	Se (g)	Se (g)
Y	YSi	Y_5Si_4	Y_5Si_4	Y_5Si_3	Y_5Si_3	Y_5Si_3	Y_5Si_3
Zr							

Thermomechanical properties depend on the state of the fuel, which is really complicated to assess in real-time

APPENDIX M - Participants

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