

Research Needs for Uranium-Zirconium- Based Metallic Fuels

Assel Aitkaliyeva, Michael Tonks, Jacob Hirschhorn, Jeff Powers, Ian Greenquist, Benjamin Beeler

June 2020



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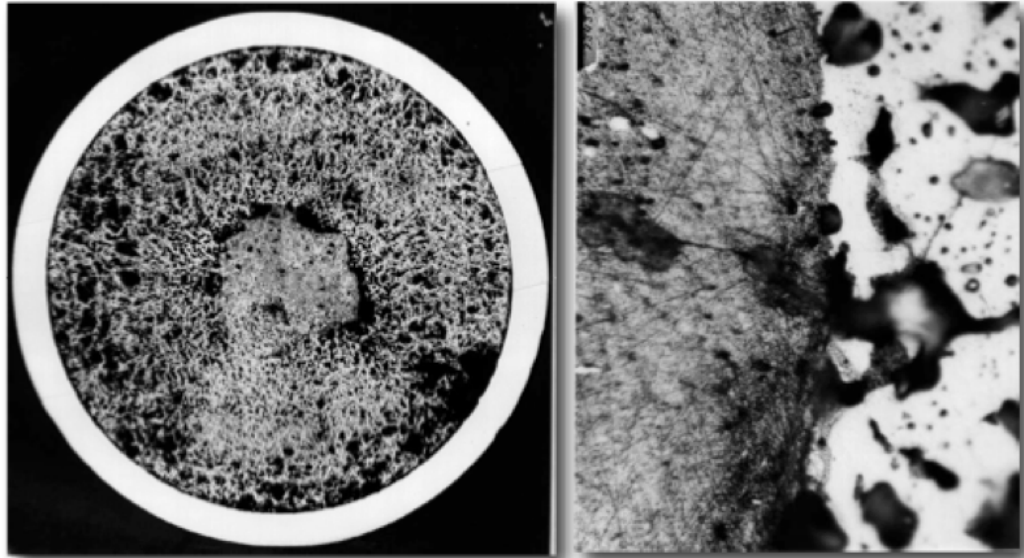
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**Prepared for the
U.S. Department of Energy**

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

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A technical report summarizing the outcomes from a workshop held at the University of Florida, in Gainesville, FL on November 14 and 15, 2019.

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2 List of Workshop Attendees

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- Ted Besmann, University of South Carolina
- Luca Capriotti, Idaho National Laboratory
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- Bruce Hilton, TerraPower LLC
- Jacob Hirschhorn, University of Florida
- Jianwei Hu, Oak Ridge National Laboratory
- Colby Jensen, Idaho National Laboratory
- Jie Lian, Rensselaer Polytechnic Institute
- Christopher Matthews, Los Alamos National Laboratory
- Mitch Meyer, Idaho National Laboratory
- Sophie Morrison, Oak Ridge National Laboratory
- Stephen Novascone, Idaho National Laboratory
- Aaron Oaks, Argonne National Laboratory
- Simon Phillpot, University of Florida
- Jeff Powers, Oak Ridge National Laboratory
- Thaddeus Rahn, University of Florida
- Michael Tonks, University of Florida
- Dan Wachs, Idaho National Laboratory
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- Yong Yang, University of Florida
- Jinsuo Zhang, Virginia Tech
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- Weiqian Zhuo, Virginia Tech

3 Synopsis

The purpose of this report is to summarize the needs and present recommendations related to the future direction for U-Zr-based metallic fuel research (including binary U-Zr and ternary U-Pu-Zr alloys). These needs and recommendations were determined by subject matter experts from various institutions during a two-day workshop held at the University of Florida in November, 2019. During open-floor discussions, the highest priority gaps in our understanding of U-Zr-based fuels were down-selected, and near- and long-term needs that directly impact the implementation of these metallic fuels were identified. The identified near-term needs include investigation of the following phenomena: i) swelling and fission gas release, ii) fuel-cladding chemical interaction, iii) phase evolution/constituent redistribution, and iv) thermal properties of the fuels. The long-term needs are: i) investigation of fuel creep and plasticity and ii) fission product (lanthanide) transport. In addition, there was general agreement that all institutions and subject matter experts would benefit from an open-source metallic fuels database with thermophysical property and microstructural data, along with fuel operation/irradiation history, which should be regularly updated with vetted information from new experimental and computational investigations and used to advance metallic fuels research and development. Finally, we recommend that metallic fuel research should be ongoing and that fuel qualification and fuel optimization should be equally prioritized; research combining experiments with modeling and simulation has the largest potential impact.

4 Introduction

4.1 Background on U-Zr-based metallic fuels

Early fast reactors in the US, such as Experimental Breeder Reactors EBR-I (1951-1963) and EBR-II (1965-1994), were fueled with metallic fuel, which consisted of unalloyed U, along with U-Zr and Pu-Al alloys [1]. The EBRs demonstrated the feasibility of a closed fuel cycle and commercial viability of fast reactors, in part through the Integral Fast Reactor (IFR) program, while allowing for down-selection of fuel composition/design and cladding material/geometry [2], [3]. Ternary U-Pu-Zr fuels with martensitic claddings such as HT-9 were determined to meet the essential requirements for the IFR program [4]. EBR-II irradiations showed that while fuel pin failures were initially caused by excessive fuel swelling, this limitation could be resolved by reducing fuel smear density (fraction of the cross-section of the cladding occupied by fuel) [5]. Later, interdiffusion between metallic fuel and cladding material was identified as a major source of failure for metallic fuel pins [6], [7].

The present-day metallic fuel stakeholders include the Advanced Fuel Campaign (AFC), Advanced Reactor Technologies (ART), Nuclear Energy Advanced Modeling and Simulation (NEAMS), Advanced Sensors and Instrumentation, and Nuclear Energy University Programs (NEUP) of the Department of Energy (DOE) and industry. AFC bears the primary burden of government programs to perform research, development, and demonstration activities for advanced fuel forms and considers U-Zr-based fuels to be the fuels of choice to power advanced fast reactor systems. AFC works closely with the Fuels Product Line of the NEAMS program to aid in the research and development of metallic fuels through a series of experiments that include separate effects testing, transient testing, advanced characterization, and post-irradiation examination (PIE). The research

will benefit designers and fuel vendors who also have a vested interest in the success of metallic fuels. The vendors considering metallic fuels are working with US-DOE and include TerraPower, GE Hitachi, ARC, OKLO, Toshiba, and Lightbridge [8]–[11]. In February 2019, DOE announced the plan to build a Versatile Test Reactor (VTR) to help accelerate the testing of advanced nuclear fuels, materials, instrumentation, and sensors, and they plan to complete the project within the next 7 years [12]. In response, AFC refined its vision for U-Pu-Zr fuels by setting new milestones that include establishing a baseline fuel performance code in BISON in 2021, compiling an NRC report in 2022, and establishing a sodium-free metallic fuel design option [13]. With these aggressive goals, the traditional route for fuel development and qualification should be revised to accelerate the process.

4.2 Summary of the workshop

The U-Zr-based Metallic Fuels Workshop was held in Gainesville, FL on November 14 and 15, 2019. It was hosted by the Nuclear Engineering program at the University of Florida. The goal of the workshop was to collocate as many subject matter experts on this type of metallic fuel as possible and to have an organized discussion focused on research needs for the fuel and how those needs can be addressed in the future.

The workshop started with a poster session in which sixteen attendees brought a poster summarizing their latest research on U-Zr-based fuels. We then started the main meeting with a presentation summarizing the AFC vision for metallic fuels. Following that, we had a series of presentations summarizing the current state-of-the-art in the areas of experiments and modeling and simulation applied to U-Zr-based fuels. The slides from these presentations can be found in Appendix II of this report.

After the talks, the attendees were broken into four groups with a range of expertise in each group. Each group brainstormed gaps in our current understanding of the fuel system with regards to its near-term use and then presented their list of gaps to the group. All attendees voted on which gaps were most important. The groups were then tasked to brainstorm solutions for the four gaps voted as most important.

After dealing with near-term gaps and solutions, the groups were assigned to brainstorm gaps for long-term improvement and optimization of the fuel. Again, the groups presented their gaps and they were voted on by all attendees. As a group, it was decided to change the approach for brainstorming solutions to long-term gaps, as it was felt that there had not been enough time to brainstorm solutions to four different gaps. Therefore, for the long-term gaps, the two with the highest number of votes were selected for brainstorming. Two groups were assigned the highest ranked gap and the other two groups were assigned the second highest ranked gap. The teams then developed an approach to overcome their assigned gap.

4.3 Purpose of this report

The purpose of this report is to provide a clear list of near- and long-term needs with regards to U-Zr-based fuel development that should be addressed. To fulfill this purpose, we present the outcomes from the workshop in a clear and concise manner. For both the near- and long-term, we first summarize the needs that were decided on by the group and then present the recommendations that were made on how the needs may be addressed. We also present other considerations that were discussed. We end with a set

of recommendations for funding agencies, program managers, and industry decision makers on areas where resources should be allocated to maximize the benefits of this important type of reactor fuel. Note that the full list of all outcomes from the workshop are available in Appendix I.

5 Gaps Related to Near-Term Use

In this section, we present four high priority gaps in the understanding of the Nuclear Fuels community with regards to the near-term use of U-Zr-based metallic fuels. We also present recommendations on how to overcome these gaps.

5.1 Swelling and Fission Gas Release

5.1.1 *Summary*

As a result of the fission process that takes place within metallic fuel, various fission products are produced, including the gaseous fission products Xe and Kr. These fission products have a very low solubility within the fuel and therefore they tend to cluster with vacancies and form fission gas bubbles. Fission gas bubbles nucleate within the material matrix and on phase boundaries. As these bubbles grow, they cause swelling in the material [14]. They also interconnect, eventually reaching the point where gas atoms can move from the interconnected bubbles to a free surface and release from the fuel slug into the gap and plenum [15]. This fission gas swelling and release in metallic fuel is quite distinct from the behavior observed in UO_2 , in which fission gas bubble percolation and release primarily occurs on grain boundaries.

Fission gas release in metallic fuel is complicated further by the multiphase nature of the fuel. Due to the temperature gradient, constituent redistribution occurs, causing the phase content of the fuel to vary radially across the fuel slug [16]. There is some axial variation as well, due to axial variation in the power and coolant temperature profiles. The fission gas behavior varies in the different phases, and therefore also varies across the radius of the slug. Larger and more developed bubbles are found in some regions compared to others. This radial heterogeneity in the bubble behavior contributes to anisotropic swelling of the fuel slug, with more swelling in the radial direction than in the axial [14]. Also, fission gas behavior will depend on the alloy content, including both the Zr and the Pu concentrations.

Due to the distinct nature of metallic fuel fission gas release, mechanistic fission gas release models developed for UO_2 , such as the fission gas release model in BISON developed by Giovanni Pastore, are not applicable [17]. For metallic fuels, an empirical fission gas release model and a simple swelling model has been available in BISON for some time, but it is not fully mechanistic, as it does not consider diffusion, the impact of phase, the impact of plasticity, the impact of temperature, or mechanistically predict anisotropic swelling. It also cannot accurately predict the impact of transients on fission gas release.

5.1.2 *Recommendations*

A fully mechanistic fission gas release model for metallic fuel for BISON is under development at Los Alamos National Laboratory. However, there is a significant amount of new data that is needed to inform the development of the model and to use for

validation, as well as improved access to existing data. The recommendations of the workshop attendees were:

- **Synthesize historic swelling/fission gas release data:** There is existing swelling and fission gas data from past metallic fuel experiments from EBR-II, FFTF, and other reactors. However, accessing these data can currently be difficult. These data need to be synthesized and compiled in an easy to access format.
- **Swelling and fission gas release of individual phases:** Experiments need to be designed to obtain swelling and fission gas release data on the individual phases present in the fuel alloys. We also need data characterizing the structure of the actual fission gas porosity within the fuel. This could be accomplished using small samples of various compositions with a carefully controlled temperature and as little temperature gradient as possible, e.g. mini-fuel experiments.
- **New integral test data:** Additional integral experiments focused on fission gas release and swelling are needed for a range of fuel compositions. These should include a significant number of low burnup experiments. They should include as much in-reactor instrumentation as possible. The microstructure of the samples (or similar samples) should be carefully characterized before and after the tests. The final characterization should capture the porosity structures that form.

5.2 Fuel-Cladding Chemical Interaction

5.2.1 *Summary*

Swelling-induced contact between the fuel and cladding enables fuel-cladding chemical interaction (FCCI). In FCCI, fuel constituents, impurities, lanthanide fission products, and cladding alloying elements interdiffuse and promote further phase formation, which includes formation of low melting point (U,Pu)/Fe eutectic phases and brittle lanthanide phases in the cladding [18]. FCCI is one of the most complex material behaviors affecting U-Zr-based fuels and is an important factor limiting its lifetime [19]. The interaction zone that develops during FCCI places both the fuel and cladding at risk through the reduction in cladding strength. FCCI can limit fuel burnup and thus mechanisms governing this process need to be well understood to make accurate predictions using fuel performance codes.

A robust and predictive FCCI model will provide fuel performance codes with the ability to predict cladding failure and fuel eutectic melting, which in turn can aid with FCCI reduction and extending fuel burnup beyond its current limits. The complexities of FCCI require separation of the phenomena for metallic fuel modeling efforts into three main modeling domains: lanthanide transport, fuel-cladding interdiffusion, and fuel cracking [20]. Lanthanide transport is discussed in section 6.2 and recommendations for studying this phenomenon are provided. Despite the work conducted to date, our ability to model FCCI needs improvement. Accurate modeling of FCCI will require a robust metallic fuel performance code backbone that captures material properties, creep, swelling, and constituent redistribution, all of which is currently lacking systematic experimental investigation.

Although many studies explored FCCI phenomena experimentally, physical behaviors for each separate model (lanthanide transport, interdiffusion, and fuel cracking) have not

been captured. The reported experiments have large discrepancies either due to different experimental techniques, impurities, or errors introduced by dated methods, all of which introduce uncertainties that cannot be fully accounted for during modeling and prevent development of the mechanistic understanding of FCCI in U-Zr-based fuels.

5.2.2 Recommendations

The primary recommendations of the workshop attendees included collection of new experimental data for both unirradiated and irradiated fuels in combination with modeling efforts to develop mechanistic understanding of FCCI. They also recommended additional research into engineered strategies to inhibit FCCI. These recommendations are listed below and will aid in development of a phenomenological model for FCCI in U-Zr-based fuels.

- **Conduct thermodynamic studies for unirradiated fuels:** New diffusion couple experiments should be conducted on unirradiated fuels and cladding materials with lanthanide content, with specific attention paid to consistency in fabrication techniques (including feedstock, processing history, etc.), impurity content, annealing parameters, and additives such as minor actinides and lanthanides. During new experiments, microstructure development should be closely monitored, and diffusion kinetics discerned for each observed phase. While past experiments provided baseline understanding, new experimental techniques should be utilized to fully capture the behavior of individual phases at the fuel-cladding interface.
- **Measure thermo-mechanical properties of FCCI phases:** The thermo-mechanical properties of the eutectic phases that form in the fuel and the lanthanide phases that form in the cladding are not well understood. These phases need to be created in unirradiated samples and then their thermo-mechanical properties need to be measured, including melting temperature, thermal expansion coefficients, elastic moduli, and fracture toughness.
- **Combine experimental data with modeling:** To ensure that mechanistic understanding of FCCI is developed, experimentalists are encouraged to closely work with modelers and ensure that the produced out-of-pile data can be combined and utilized in computational models.
- **Quantitatively study the impact of cladding liners:** Liners between the fuel and cladding could provide a diffusion barrier to prevent FCCI. Many studies have been performed with no clearly and reproducibly successful technology published. Additional studies would help to determine the optimal material and thickness for the liner.
- **Study the impact of additives:** Another strategy that has been suggested to reduce FCCI is to put additives (such as Sn, Pd, or Sb) in the fuel slug that inhibit the transport of lanthanides. Experimental results to date are mixed. Mechanistic studies of the impact of these additives should be carried out using both experimental and modeling approaches to better understand the fundamental process and guide development.

5.3 Phase Diagrams

5.3.1 *Summary*

The fuel's response to a given set of operational conditions is dominated by its structure, which is a complex function of composition, porosity, sodium content, texture, defect concentration, and crystalline phase. Of these features, the crystalline phase has a particularly strong influence on the fuel's thermal, mechanical, and chemical behaviors. Accurate fuel performance predictions will therefore require a detailed and complete understanding of the phases present in the fuel and the crystal structure and material properties of each.

Phase diagrams are a critical part of our understanding of a system's thermodynamic behavior, and several phase diagrams are available for U-Pu-Zr and its constituent binaries in the open literature. Sheldon and Peterson published an overview of the U-Zr system in 1989, complete with a phase diagram, the crystal structure of each phase, and various other thermodynamic data and observations [21]. Phase diagrams for the Pu-Zr and Pu-U systems were later published by Okamoto [22], [23]. The discussions of the latter two systems included much less detail, and the phase diagrams were drawn using fewer experimental data. Insufficient experimental data were available to precisely define the solvus lines and transition temperatures associated with intermetallic and high-solubility phases in each, particularly at low temperature.

While the U-Zr system has been characterized well, constructing phase diagrams for systems involving Pu is especially difficult due to its complex chemical behaviors, poorly-characterized kinetics, and high affinity for impurities [24]. These complications likely impacted the efforts of O'Boyle and Dwight, who used thirteen alloys to construct nine isothermal phase diagrams for the U-Pu-Zr system [25]. These are in good general agreement with the three binary phase diagrams but describe only a handful of temperatures in the detail necessary to accurately predict fuel performance.

The CALPHAD method has been applied to help supplement the sparse experimental data by filling in gaps in the published phase diagrams. CALPHAD thermodynamic assessments involve deriving semi-empirical functions that describe the thermodynamic behavior of each phase in a system over broad, continuous ranges of composition and temperature [26]. These functions can be used to inform predictive fuel performance models. However, their use can introduce additional uncertainties when applied to phases with poorly-characterized stability regions and crystal structures. Widely used thermodynamic assessments include those published by Kurata, and the Nuclear Energy Agency has an ongoing effort to aggregate this type of thermodynamic data within its Thermodynamics of Advanced Fuels – International Database (TAF-ID) [27], [28].

Unfortunately, even minor shifts in solvus lines and transition temperatures can drastically degrade our ability to model fuel behavior. The effects of irradiation increase the complexity of the problem further due to the accumulation of fission products and material defects. As such, accurate prediction of fuel performance will require improved phase diagrams for the unirradiated systems, representative thermodynamic assessments for those systems, and an understanding of how irradiation affects these thermodynamic descriptions. Further characterization of alloy kinetics, crystalline structure, and passivation may be necessary to meet these objectives.

5.3.2 Recommendations

The recommendations of the workshop attendees were:

- **Conduct thermodynamic studies and reassess unirradiated phase diagrams:** Thermodynamic studies will be necessary to advance our understanding of U-Zr-based alloys and accurately model the behavior of U-Zr-based fuels. Specifically, we recommend reassessment of the unirradiated U-Zr, Pu-Zr, Pu-U, and U-Pu-Zr phase diagrams to resolve discrepancies between the existing descriptions and to precisely define the stability regions of each phase. Emphasis should be placed on defining the transition temperatures and solvus lines associated with the α , β , γ , δ , and ζ phases (as defined in the ternary phase diagrams), which are frequently present in U-Zr and U-Pu-Zr fuels during normal operation. Current thermodynamic models need to be revised/replaced via CALPHAD optimizations to allow predictive calculation of phase equilibria and thermodynamics (chemical potentials).
- **Control passivation:** Experiments should be conducted using high-purity samples in inert atmospheres to control passivation, which has the potential to obscure characterization results. Long annealing times may be necessary to ensure that the collected data represent the equilibrium structures of the alloys.
- **Share the results from both successful and unsuccessful experiments:** We recommend that both successful and unsuccessful experimental efforts be published along with observations related to sample passivation and kinetics to expedite this process. These data will be useful for designing new studies, resolving discrepancies between datasets, and model development and validation.
- **Confirm crystallographic structure:** We further recommend a critical review of each phases' crystallographic structure so that thermodynamic assessments may be applied using the appropriate models. Thermodynamic assessments should then be performed.
- **Combine experimental data with modeling:** Supplementary studies should be conducted using Density Functional Theory to provide additional thermodynamic data for the assessments if necessary. Combined with existing behavioral models, these material property data will improve our ability to predict the performance of unirradiated U-Zr-based fuels.
- **Conduct thermodynamic studies on irradiated fuel:** Finally, experiments should be conducted to characterize the effects of irradiation on fuel thermodynamics. These studies could be conducted by irradiating fresh samples or by manufacturing samples from irradiated fuel rods. The results together with other information need to be used to generate thermodynamic models based on those for the unirradiated fuel. These can be created via CALPHAD optimizations to allow predictive calculation of phase equilibria and thermodynamics (chemical potentials) for the complex systems. These findings will help ensure that fuel performance predictions remain valid as burnup increases.

5.4 Thermal Conductivity

5.4.1 *Summary*

The thermal conductivity of metallic fuel substantially changes during reactor operation due to the microstructure evolution that occurs [29]. As the fuel constituents (primarily Zr and U) redistribute, resulting in phase transformations, the thermal conductivity will change since each phase has a different thermal conductivity and phase boundaries add additional thermal resistance [30]. More importantly, fission products decrease the thermal conductivity, with fission gas having the largest effect. Once the fission gas bubbles interconnect and contact the free surface, the fission gas is released and liquid sodium can enter the pores [31]. Sodium infiltration raises the effective thermal conductivity of the irradiated fuel. Thus, models of the thermal conductivity of metallic fuel during reactor operation need to include the impact of these various phenomena that take place.

While the existing literature documents substantial experimental data for thermal conductivity of unirradiated U-Zr and U-Pu-Zr metallic fuels, it only reports the effective thermal conductivity of the entire fuel sample and does not differentiate the thermal conductivity of the individual phases. Thus, it is only applicable to one specific fuel microstructure and will not necessarily be valid for all fuels at a given temperature and constituent distribution. In addition, only limited experimental data is available for irradiated U-Zr-based fuels. No published experimental data is known to exist for direct thermal conductivity determinations for irradiated U-Pu-Zr fuels, though a small amount of indirect data exists with high uncertainties requiring engineering judgment [32]. While the phenomena important to the effective thermal conductivity in irradiated U-Zr and U-Pu-Zr metallic fuels are generally agreed upon, models and correlations for the quantitative thermal conductivity in irradiated U-Zr and U-Pu-Zr metallic fuels differ greatly.

Stated uncertainties in the thermal conductivities also differ significantly, with little basis provided as to reasonable upper and lower bounds for applying uncertainties. No justification exists for treating the uncertainty using a normal distribution, though this is the dominant approach, and uncertainties often are given as error bars without a defined relationship to the standard deviation. Furthermore, the lack of definition in bounding absolute values or uncertainties leads to a situation where sampling from assumed distributions can result in negative effective thermal conductivity.

To summarize, a consensus on quantitative and mechanistic models of the thermal conductivity of metallic fuel during reactor operation are not available. Such models must account for the impact of constituent redistribution, fission product formation, and sodium infiltration. However, more experimental data and modeling and simulation effort are needed before such models can be developed.

5.4.2 *Recommendations*

The recommendations of the workshop attendees were:

- **Obtain new experimental data:** Significant improvements are needed in both experimental data and mechanistic models for thermal conductivity in U-Zr and U-Pu-Zr metallic fuels.
 1. **Phase-dependent unirradiated thermal conductivities:** New experimental measurements and atomic scale modeling and simulation are needed to determine

the intrinsic thermal conductivities as a function of temperature and composition of the various metallic fuel phases.

2. **Additional temperature-dependent data on unirradiated bulk thermal conductivity:** New bulk measurement data of the effective thermal conductivity of metallic fuel samples at various temperatures and compositions are also needed. However, detailed microstructure characterization on the same samples are also needed. Such samples would provide critical data for developing and validating models that predict the effective thermal conductivity of unirradiated metallic fuel as a function of temperature, composition, and *the specific microstructure* of the fuel.
3. **Direct experimental measurements of thermal conductivity of irradiated samples:** Direct experimental measurements of bulk thermal conductivity of the individual radial zones and integral center to periphery are recommended in both U-Zr and U-Pu-Zr fuels using samples extracted from binary and ternary alloys that were previously irradiated and remain in storage. Fuel alloys covering a range of possible compositions but focusing on U-10Zr and U-20Pu-10Zr (in wt%) are recommended, in conjunction with samples that cover a range of irradiation conditions (e.g., discharge burnups, temperatures, and active fuel heights).
4. **Quantitative determination of the impact of Sodium Infiltration:** The impact of sodium infiltration on the thermal conductivity of metallic fuel is still an open question that needs to be resolved. Thus, new experimental data on binary and ternary samples with sodium filled porosity is needed. These samples could be created using novel fabrication techniques with unirradiated fuel. Novel sample preparation techniques are needed that do not disrupt the sodium.
- **Develop and validate science-based mechanistic models:** Models are needed for the thermal conductivity in U-Zr and U-Pu-Zr metallic fuels that account for the impact of constituent redistribution, fission product formation (including fission gas bubbles), sodium infiltration, and cracking. If possible, these mechanistic models should account for local variations in parameters rather than rely on integral averages or maximum parameter values for the entire pin, and they should produce thermal conductivities that are valid for local calculations. Two examples of such an approach are presented in Chen et al. [33] and Zhou et al. [34] for U-alloys. Accurate and reasonable uncertainties would also be needed with this mechanistic approach.

6 Gaps Related to Long-Term Use

In this section, we present two high priority gaps in the understanding of the nuclear fuels community that will directly impact the long-term improvement and optimization of metallic fuels. We also present recommendations on approaches that could be taken to alleviate these gaps.

6.1 Fuel creep/plasticity

6.1.1 *Summary*

There are many internal and external sources of strain within metallic fuel. Internal sources include phase transformations, heterogeneous thermal expansion (either due to temperature gradients or anisotropic thermal expansion coefficients), fission gas bubble

pressures, and more. External sources include pressure inside the cladding and pellet/cladding mechanical interaction. These internal and external strains result in stress in the material. Since metals are typically ductile, large enough stresses can result in dislocation motion, causing permanent plastic deformation. In addition, thermal and radiation creep will occur over time causing additional permanent plastic deformation to reduce the internal stress [35]. These permanent deformation mechanisms can result in behaviors that significantly impact the fuel performance, including enlargement of fission gas bubbles, ductile tearing, and accelerated gap closure.

Metallic fuels are inherently multiphase and phase transformations can occur within the fuel during reactor operation. Each phase has a different crystal structure with different mechanical properties, including elastic constants, thermal expansion coefficients, dislocation slip systems, and dislocation critical resolved shear stresses. However, mechanical properties, fuel creep, and the plasticity behavior of the individual phases are not known. Some of these properties are known for the overall fuel slug, but these values are the effective macroscale properties of a multiphase material and are specific to a given composition, temperature, and microstructure. Our understanding of the mechanical behavior is especially poor for the Pu containing phases. Mechanistic modeling and simulation of metallic fuel is impossible until the mechanical properties, including those defining fuel creep and plasticity, are known as a function of temperature and radiation damage.

6.1.2 Recommendations

To overcome the significant gap in our understanding of the plasticity and creep behavior of metallic fuel, the workshop attendees suggested a multiscale approach involving tightly correlated experiments and simulation. This approach is summarized in the bullets, below:

- **Fresh fuel mechanical testing:** Carry out mechanical tests of fresh fuel to quantify the elastic and plastic behavior of the individual phases and how they vary with temperature and composition.
- **Fresh fuel creep tests:** Carry out creep tests on fresh fuel for various compositions at various temperatures. Characterize the microstructure of the samples before and after testing. Determine the behavior of the individual phases wherever possible.
- **Construct crystal plasticity model:** Construct a crystal plasticity model of both the plastic behavior and the creep of the various metallic fuel phases using values in the literature and using the new data from the previous two bullets.
- **Carry out creep and mechanical testing on irradiated fuel:** Collect experimental data for creep and plasticity on irradiated metallic fuel samples. This would require the construction of a load frame in a hot cell. Characterize microstructure before and after testing. Quantify dislocation density with TEM.
- **Defect behaviors under irradiation:** Use DFT and cluster dynamics to determine defect behaviors in irradiated metallic fuel
- **Quantify irradiation hardening using Discrete Dislocation Dynamics:** Carry out discrete dislocation dynamics simulations for various defect densities to quantify radiation hardening. Use the defect behaviors from the previous task. Inform the addition of radiation hardening to the crystal plasticity model.

6.2 Lanthanide transport

6.2.1 *Summary*

In this section, we present the key knowledge gaps in fission product transport, specifically lanthanide transport. Lanthanide transport provides the source term for FCCI, which is one of the primary contributing factors to cladding wastage, weakening, and ultimately failure [36]. An ability to describe, and predict, lanthanide transport through the fuel during reactor operation provides key insight into understanding the rate, location, and evolution of FCCI.

There are a number of primary lanthanides of interest, including Ce, Nd, La, and Pr, as well as the near lanthanides of Cs, Ba, and Xe [37]. The diffusive behavior of these individual species has been studied in UO_2 , most thoroughly for Xe diffusion, but there is not comprehensive understanding of the mechanism or rate of transport of lanthanides in metallic fuels. As the fuel evolves under operation, the microstructure changes into a multi-phase, variable composition, porous domain. Describing the stages from the generation of lanthanides, to bulk diffusion of lanthanides to bubbles, to surface diffusion along bubbles, to liquid or vapor diffusion of lanthanides through the sodium to the inner surface of the cladding is currently impossible, as there is limited data on any one of these individual stages. Currently, the state of the art is a single computational study on Ce, Pr, and Nd transport in liquid Na [38]. The primary method investigated for reducing transport of lanthanides to the fuel/cladding interface and prevent or mitigate FCCI is to utilize fuel dopants to hopefully capture and retain targeted fission products in intermetallic compounds within the fuel. These studies are primarily thermodynamic in nature, and the kinetic effects of radiation damage on these dopants and on the fission product behavior are still unknown. An improved understanding and quantification of the diffusive behavior of lanthanides in fuel, cladding and other structural materials would benefit development of fuel dopants, fuel/cladding barriers and other methods not yet identified. These should be used together with chemical potential-based transport relations from basic irreversible thermodynamics approaches and thus avoid needing to obtain Soret terms.

Currently, fuel performance models are being developed that will describe the fundamental thermophysical properties of the fuel and its evolution on a phase- and composition-dependent basis. Simplified models for Xe transport are currently utilized to describe fission gas swelling, which need to be improved upon, but models for lanthanide transport do not even exist. While there are several existing models in BISON for FCCI of metallic fuel, they are preliminary and need additional verification and validation. A refined model for FCCI will need to be generated that is spatially- and microstructurally-dependent that relies on an actual source of deleterious fission products being delivered to the cladding. In order to have any such mechanistic model to predict FCCI and its impact on cladding lifetime, a comprehensive model to describe lanthanide transport needs to be developed.

6.2.2 *Recommendations*

The recommendations regarding how to address the long-term knowledge gap regarding Ln transport in metallic fuel includes joint modeling and experimental efforts.

- **Atomistic modeling:** Computational studies on the atomistic level include density functional theory (DFT) and/or molecular dynamics (MD) studies of **individual Ln point defect transport** for each of the individual phases present in metallic fuel, for

each unique composition of the fuel, and over the compositional variations that present themselves under reactor operation. Additional suggested computational investigations include lanthanide transport in liquid sodium, lanthanide surface diffusion, and lanthanide irradiation enhanced diffusion. Any necessary molecular dynamics simulations would first require the development of interatomic potentials to describe the relevant interactions between all species of interest, including the fuel, the lanthanide of interest, and sodium.

- **Chemical Potential Driving Force:** The fundamental force for transport is a system moving toward the equilibrium state, which means uniform chemical potentials for components across a closed system. The use of this phenomenon in modeling solid state transport is well established within irreversible thermodynamics, and allows the relatively easy computing of thermal and concentration driven transport utilizing mobilities that provide the time-dependent behavior. Obtaining the thermochemical representations of the lanthanides in the fuel phases together with experimental/computational determination of mobilities would allow accurate prediction of movement of the lanthanide components.
- **Multiscale modeling:** Subsequently, multiscale modeling efforts are suggested that utilize this fundamental computational data to incorporate the effects of the evolving microstructure in the fuel on lanthanide transport. This would include the development of interconnected porosity and lanthanide diffusion to and through porosity to the periphery of the fuel to the regions of FCCI. These mesoscale modeling efforts will leverage ongoing research to improve thermophysical property descriptions of each of the individual phases that present in metallic fuels under operation. Combining atomistic and mesoscale simulations along with empirical diffusion formulations can provide an encompassing computationally-based description of lanthanide diffusion in metallic fuel systems.
- **Experimental investigation and validation:** A number of experimental investigations would be needed to elucidate the lanthanide transport behavior and to provide validation data for the modeling and simulation efforts:
 1. Experimental investigations are needed on diffusion couples of metallic fuels with lanthanides, with and without sodium, as well as on fuel that is unirradiated and irradiated.
 2. Experiments are needed to analyze the fundamental microstructural evolution of the fuel, such that an actual model describing porosity interconnection and thus sodium infiltration can be described and predicted. Relatedly, experiments explicitly targeting the extent of Na infiltration into the fuel (e.g. using radioactive tracer isotopes) are critical such that a macroscale evaluation of the role of Na on lanthanide transport can be obtained.
 3. A series of separate effects experiments on individual diffusion mechanisms of lanthanides in fuel are proposed to both corroborate computational investigations and to further elucidate potential diffusion mechanisms that are potentially being overlooked.

This comprehensive set of coordinated and synergistic computational and experimental investigations can provide key insights to describe lanthanide transport, such that fuel performance models can incorporate a descriptive and predictive source term for lanthanides at the fuel periphery and inform the FCCI development models that are simultaneously being constructed.

7 Other Considerations

Many of the recommendations made here require access to experimental data. Some integral test data already exist based on metallic fuel experiments performed from the 1970s to the 1990s. In order to simplify the use of these data as much as possible, they should be stored in a metallic fuel experimental database.

The three most important test reactors for metallic fuels in the US were EBR-II, FFTF, and TREAT. Currently, data on metallic fuel experiments from these reactors are either disparately published in a number of journals, stored onsite in file cabinets or local computers, or, in select cases, stored in distinct individual databases. There are currently two databases for EBR-II: one (referred to as FIPD) maintained by ANL, and another maintained by INL that also exists in a parallel form inside an INL GitLab repository. Both are export controlled and are under active development. There is also a database for FFTF data maintained by PNNL. Like the EBR-II databases, it is under development and export-controlled. Both ANL and INL maintain databases for TREAT data. Additionally, the IAEA hosts the International Nuclear Information System (INIS) which contains bibliographic references and full-text documents including scientific and technical reports, conference proceedings, patents, and theses.

In order to increase usability and accessibility of the experimental data while also reducing duplicative efforts, it would be highly recommended and advantageous to combine all relevant metallic fuels experimental data into a single database. Once the database is complete, it will facilitate model development, model validation, experiment design, and other important aspects of metallic fuels development.

In addition, as research on metallic fuels is accelerating and new data is being generated, there is the need for a centralized, accessible database of metallic fuels properties and irradiation behavior such that researchers from distinct groups are able to utilize the same data and validate their findings. A model database exists in the NIST inorganic crystal structure database (ICSD), which evaluates and disseminates chemical, physical and crystallographic information of nonorganic compounds, containing over 210,000 entries and covering the literature from 1913. While this database is well established, it provides a guiding system for the construction of a controlled database on metallic nuclear fuel properties, from computational, experimental, and irradiation studies.

Extensive effort has been put forward in the generation of the metallic fuels handbooks, which contain some fundamental property data such as crystal structures, thermal expansion, phase diagrams, thermal conductivities and heat capacities on unirradiated fuels [39], [40]. This is incredibly valuable information, but is insufficient for the goal of developing improved, qualified metallic nuclear fuel for advanced reactors. As such, a database including unirradiated thermophysical property data as well as metallic fuel operational history data, that can be updated with vetted information from new experimental and computational investigations is a key step in advanced metallic fuel research and development.

8 Broader Recommendations

To end this report, we make a number of broader recommendations regarding metallic fuel:

- **Metallic fuel research is essential to near term deployment and should be ongoing:** Metallic fuel for fast reactors has the unique and powerful potential to improve uranium utilization and economics, facilitate breed and burn fuel management, and increase safety, which is essential for the future of nuclear energy. The new focus on reactors using metallic fuel, including TerraPower, OKLO and the VTR, demonstrates that the interest in these fuels is only increasing. Thus, it is critical that funding for research on metallic fuels also continue and even increase. This funding should include programmatic funding through DOE programs such as AFC, but also metallic fuel scope in NEUP and small business grant calls.
- **Research regarding fuel qualification and fuel optimization should be equally prioritized:** A major push right now is to ready metallic fuel for use in near term reactors. Thus, research that supports this readiness and the near-term qualification of metallic fuel is very important. However, it is critical that such near-term research not become the only focus, such that longer term research is neglected. Once reactors using metallic fuel begin operating, a desire will quickly arise to optimize the fuel performance making the reactors safer and more efficient. Such optimization will benefit from more fundamental understanding of metallic fuel behavior and if no long-term research has been underway, the optimization efforts will be significantly slowed. Thus, it is essential that research for fuel qualification and fuel optimization both be prioritized by funding agencies and researchers.
- **Multidisciplinary research that combines new experiments with modeling and simulation has the largest potential impact:** During the discussions by the participants of the metallic fuel meeting, experts in both experiments as well as modeling and simulation worked together to determine how to overcome existing gaps in our understanding of the fuel performance. Due to the diverse expertise of the participants, unique approaches were discussed that combined experiments with modeling and simulation in unique ways to obtain knowledge that would not be possible by either approach by itself. Thus, it is critical that future research on metallic fuels take a multidisciplinary approach that takes advantages of the strengths of both experiments and modeling and simulation.
- **Enhancement of atomic scale simulation capability for metallic fuels is important and should be encouraged:** There are many material properties that are required for mechanistic models of metallic fuel behavior, but are difficult and expensive to measure experimentally. Atomic scale simulations such as DFT and MD provide a viable and effective means of obtaining preliminary values for such properties. However, both methods have limitations with regards to metallic fuel. A general consensus on the best approach for applying DFT analysis to U-Zr alloys is still needed. In the literature, the magnitude of the Hubbard U term in the

DFT+U approach and the incorporation of spin orbit coupling vary by the properties of interest, and the general accuracy of actinide pseudopotentials is not wholly accepted. Interatomic potentials for these alloys (required for MD simulations) are usually developed for individual phases, making it difficult to compare the properties of different phases given by different potentials. Potentials that are capable of describing the existence and coexistence of multiple U-Zr phases are needed. Finally, the addition of Pu complicates things even more for both DFT, due to localized f-electrons, and MD, where there is a total lack of suitable interatomic potentials.

9 References

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10 Appendix I: Full list of workshop outcomes

10.1 Group membership

10.1.1 *Group 1*

- Nicholas Woolstenhulme
- Luca Capriotti
- Benjamin Beeler
- Kaylee Cunningham
- Ted Besmann
- Ian Greenquist

10.1.2 *Group 2*

- Jeffrey Powers
- Cynthia Adkins
- Thaddeus Rahn
- Jie Lian
- Michael Benson
- Bruce Hilton

10.1.3 *Group 3*

- Mitch Meyer
- Sophie Morrison
- Jinsuo Zhang
- Stephen Novascone
- Daniel Wachs
- Xianming Bai

10.1.4 *Group 4*

- Steven Hayes
- Geoffrey Beausoleil
- Jacob Hirschhorn
- Larry Agesen
- Christopher Matthews
- Aaron Oaks

10.2 Near-term Gaps

10.2.1 *Group 1*

- High burnup structure beyond 20 at% burnup
- Ferritic/martensitic cladding swelling and properties beyond 200 dpa
- U-Fe eutectic melting behavior in over-heat conditions
- D9 cladding model
- Solubility of FP in Na liquid – plus model of the thermal solution
- Lanthanide transport in Na free designs
- Fully mechanistic fission gas release model
- Swelling model in BISON

- Thermal conductivity degradation: plasticity, defects, different phases
- Safety performance of fuel in pump coast-down and loss-of-flow scenarios
- Degree of Na infiltration with effect on thermal conductivity
- Phase formation and composition
- Radiation effects quantification for modern structural materials
- Low burnup microstructure
- Fuel creep thermal irradiation
- Fuel/cladding friction and interaction
- Thermodynamic database for U-Pu-Zr and clad and fission product phases
- FCCI thermodynamics
- Diffusion in different phases
- Quantification of radiation effects

10.2.2 Group 2

- How much does Na impact understanding?
- Transient furnace capability for engineering scale
- Irradiation experiment database that includes all EBR-II/FFTF, new PIE data and is accessible by the public and contains specifications and operating conditions
- Metal fuels handbook for microstructure
- Determine amount of Na intrusion into pores
- Phases and phase diagrams under irradiation
- Transient furnace
- FCCI (temperature, burnup, time)
- Anisotropic swelling as a function of burnup (no data and no BISON models are available)
- Fission gas release (T, burnup, Pu); retained fission gas axial and radial; porosity including radial and axial distribution
- Lack of phase ID pre and post irradiation
- Thermal conductivity as a function of composition, temperature, and burnup
- Mechanical properties
- Usable historical databases that are easy to populate and locate
- FCCI mechanisms
- Fuel pin temperatures (radial and axial) and operational history
- Na infiltration
- Fuel column axial growth (burnup, t)
- Fundamental properties (thermodynamic, mechanical, thermal, diffusivity, interfacial, properties)
- Mechanistic fission gas release model
- Mechanistic swelling model
- Thermal conductivity of U-Zr, U-Pu-Zr as a function of irradiation, T, burnup
- Clearly define the types of data that are needed to develop and validate multiphysics models
- Thermal benefits and drawbacks
- Fabrication limitations
- FCCI (additives, plating, effects under irradiation)

- Fuel swelling data and models during transients
- High dose cladding performance (>200 dpa)
- Fuel thermal transport (burnup, T evolution)
- Robust modeling approach for fuel-cladding contact
- Transient experimental data
- Licensing approach, commercialization what is our strategy and how do designers/vendors license in NRC and how does AFC/NEAMS minimize risk?
- Communicate issues across DOE campaigns, industry, NRC, etc.
- Materials handbook should be linked (AFC/exp) to modeling and should include correlations
- Na free fuel behavior: thermal transport, Ln/FP behavior

10.2.3 Group 3

- Properties: thermal conductivity, Na infiltration, rad effects on thermal conductivity, base thermal conductivity for UPuZr
- Baseline for existing models what are the actual gaps in M&S tools?
- FCCI: redistribution (La, Zr, Fe,...); transient eutectic; liner
- Swelling models: need improvement, low burnup data, phase dependent properties such as thermal and mechanical, creep, etc.
- Cladding properties such as in-situ creep data (strains from integral tests)
- Source term
- Transient fission gas release (axial expansion, framing)
- Coupling to other tools (MARMOT/BISON, BISON as system code; non expert user of BISON should be able to do work)

10.2.4 Group 4

- Thermal conductivity
- Phase diagrams both in-pile and non-equilibrium
- Mechanical properties of the fuel
- Ln transport mechanism
- Na infiltration
- Porosity development/morphology
- Power history
- FCCI
- Fission gas release/swelling

10.2.5 Down-selected gaps

- FCCI – 20 votes
- Thermal conductivity – 18 votes
- Swelling and fission gas release - 0 votes
- Phase diagrams – 9 votes

10.3 Near-term solutions

10.3.1 Group 1

- FCCI

- Kinetic studies of fission production/cladding interactions
 - Implementation of the new kinetic data in a model
- Thermal conductivity
 - Conduct integrated radial thermal conductivity experiments
- Swelling and fission gas release
 - Synthesize historic swelling/fission gas release data
- Phase diagram
 - Conduct experiments in and out of pile to mature phase diagrams

10.3.2 Group 2

- FCCI
 - Evaluation of additive effects (Sn, Pd, Sb)
 - Transport properties determination for Ln in U-Zr, U-Pu-Zr, cladding
 - Eutectic phase properties of fuel elements and cladding elements
 - Characterize residual strength of cladding
- Thermal conductivity
 - Measure conductivity of individual phases vs bulk
 - Measure properties of irradiated U-Zr and U-Pu-Zr
 - Na logging impact
 - Porosity effects on PSD and pore shape
 - Integral measurements (power to melt, thermocouple in fuel)
- Swelling and fission gas release
 - Measurement of burnup dependent anisotropic swelling
 - Swelling contribution from individual phases
 - Gas bubble nucleation in each phase
- Phase diagram
 - Assessment of radiation effect on phase equilibrium
 - Phase boundaries on strain mismatch

10.3.3 Group 3

- FCCI
 - Liner additives
 - Better understanding separate effects testing
- Thermal conductivity
 - Measure properties LFA
 - Simulation model (predictions)
 - Integral TREAT measurements
- Swelling and fission gas release
 - Low burnup measurements
 - Phase dependent measurements
 - Merge Topher's model and evaluate
- Phase diagram
 - Resonance ultrasound spectroscopy test in TREAT
 - Models and simulations

10.3.4 Group 4

- FCCI
 - Model informed experiment design to identify mechanism
- Thermal conductivity
 - Measurement of phase and composition dependence for fresh and irradiated fuels
- Swelling and fission gas release
 - Swelling and fission gas release behaviors of individual phases (perhaps via mini-fuel experiments)
- Phase diagram
 - Phase stabilities in fresh and irradiated fuels (particularly ternary)

10.4 Long-term Gaps

10.4.1 Group 1

- Phase specific mechanical properties as a function of temperature and composition
- Interatomic properties for U-Pu-Zr system
- Free energy models for U-Pu-Zr
- Specific diffusion in different phases (Zr+FP; surface+bulk; Na)
- A robust model to infer fuel microstructure from power history to replace burnup as your x-axis (burnup is not a unique history for a microstructure of the material and should be replaced so that models are not correlated to burnup alone since it does not affect properties)
- Initial phase interaction/composition
- Pre-irradiation microstructure data
- Systematic characterization of U-Zr/U-Pu-Zr system for both as-cast and irradiated fuels that includes all techniques

Selected for presentation:

- Systematic characterization of U-Zr/U-Pu-Zr system as cast and PIE
- A robust model for fuel that doesn't depend on just burnup alone
- Zr and FP diffusion in different phases and in Na

10.4.2 Group 2

- FCCI
 - Rate limiting transport of lanthanides
 - Alloying elements in cladding and in the fuel
- Phase diagram under irradiation
 - Enthalpy of formation (phases)
 - Individual phase properties (conductivity, fission gas, solubility, diffusion)
- Porosity distribution and evolution
- Availability of feedstock materials for experiment design
- Measurement of light elements (C, O, N)
 - Control of impurities during fabrication

Selected for presentation:

- Porosity distribution/evolution

- Impact of light elements
- Irradiation effects on phase diagrams

10.4.3 Group 3

- Fission gas nucleation, diffusion, surface energy, and resolution
- Radiation effects: microstructure, phase array, point defect population, thermal conductivity experimental data
- Ln transport: radiation enhanced and Na infiltration

10.4.4 Group 4

- Fission product diffusion coefficients
- Na infiltration
- Phase specific conductivity
- Fuel creep/plasticity
- Bulk anisotropic swelling
- Transient foaming
- Cladding microstructure and irradiation resistance

Selected for presentation

- Fuel creep/plasticity
- Cladding microstructure

10.4.5 Down-selected gaps (top two, shown in bold, were selected for solution discussion)

- **Fuel creep/plasticity – 10 votes**
- **Ln transport – 10 votes**
- Radiation effects on microstructure and properties – 5 votes
- Irradiation effects on phase diagrams – 7 votes
- Porosity distribution/evolution – 6 votes

10.5 Solutions to long-term gaps

Note: Each group was assigned one to discuss

10.5.1 Group 1 (Ln transport)

- DFT simulation: calculate transport behavior of Ln in solids and defect contributions; simulate Ln transport in liquid Na;
- MD-solid state transport that considers microstructural evolution during irradiation
- Set of experiments – diffusion couples (Na evaporates based on the experiments conducted by Jinsuo and identified pathways to containing Na) and evaluate microstructural evolution with irradiation
- Modeling – liquid Na transport out of the fuel into interface

10.5.2 Group 2 (fuel creep/plasticity)

- Start with fresh fuel creep tests (experiments)
- Construct crystal plasticity model (like VPSC) and link it to the creep test data
- Irradiation experiments on samples under load
- Variation between polycrystalline and single crystal data

- TEM on post irradiated, post stress testing for dislocation density
- DFT-formation and migration energy of dislocations
- Ion irradiated in-situ TEM on fuel
- Dislocation dynamics and crystal plasticity with irradiation

10.5.3 Group 3 (*Ln transport*)

- Ln U-Zr diffusion in different phases
- Conduct in pile and out of pile experiments on diffusion couple type specimens with and without Na, synthesize data and mature model
- Micro- and macro-scale investigation of the mechanisms through out of pile and PIE studies
- Ln surface diffusion MD and AIMD
- Na infiltration experimentally

10.5.4 Group 4 (*fuel creep/plasticity*)

- Build Pu load frame in hot cell
- Defect behaviors under irradiation (DFT/CD)
- In-pile strain measurements (for irradiation creep)
- VPSC model
- Carbon tax and policy reform

10.6 Additional discussions

There was significant discussion related to databases of U-Zr-based fuel data:

- Material design databases are available in the industry that has established standards that we can emulate.
- Vetting data is important – referee
- AGR example = PI's load data, data is evaluated, and vetted data is available
- Assign DOI to data and allow putting all data into the database
- Metadata – processes, instruments, in addition to .cvs file
 - E.g.: NIST is developing SCEMA – structured data entry protocols. Talk to them and to materials genome
- Argonne is hosting EBR-II data
- Talk to GAIN about it (they want to do it)
- NMDQI – targeting data as low hanging fruit too (NSUF driven)
- Need to connect all databases to make them efficient – how do we integrate them? This effort has to be funded programmatically but it has to be useful and publicly available (supported top down). You can't use it if you can't see it.
- FFTF (PNNL), ANL (FIPD), INL (EBR-II) – need to integrate their databases (GAIN is facilitating the process)
- New data – NIST model type for new database
- Old data – legacy database

11 Appendix II: Slides from individual talks

11.1 Advanced Fuels Campaign: Vision for U.S. Metallic Fuel R&D

Colby Jensen, Idaho National Laboratory

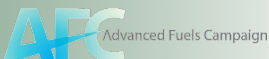
Nicolas Woolstenhulme, Idaho National Laboratory

Nuclear Technology Research and Development

Advanced Fuels Campaign Vision for U.S. Metallic Fuel R&D

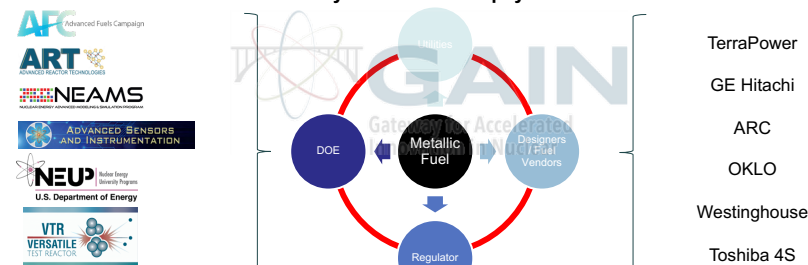
Colby Jensen
Deputy Lead for Advanced Reactor Fuels
Nicolas Woolstenhulme
Irradiation Testing Lead for Advanced Reactor Fuels

Metallic Fuels Meeting
University of Florida, Gainesville, FL
November 14, 2019



A Tall Order... and Promising Opportunity

- Metallic fuel is a mature and key strategic U.S.-developed and owned technology
- Who are the stakeholders? ... beyond the U.S. taxpayer!



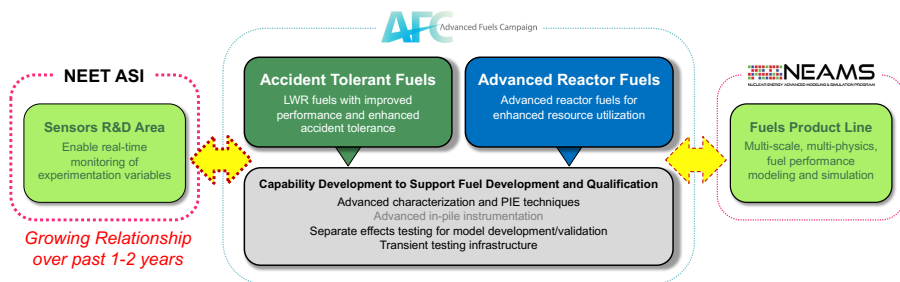
- Remaining presentation is from the perspective of the fuel R&D lead in this context

"In preparing for battle I have always found that plans are useless, but planning is indispensable." D. Eisenhower 2

Advanced Fuels Campaign: Structure and Mission

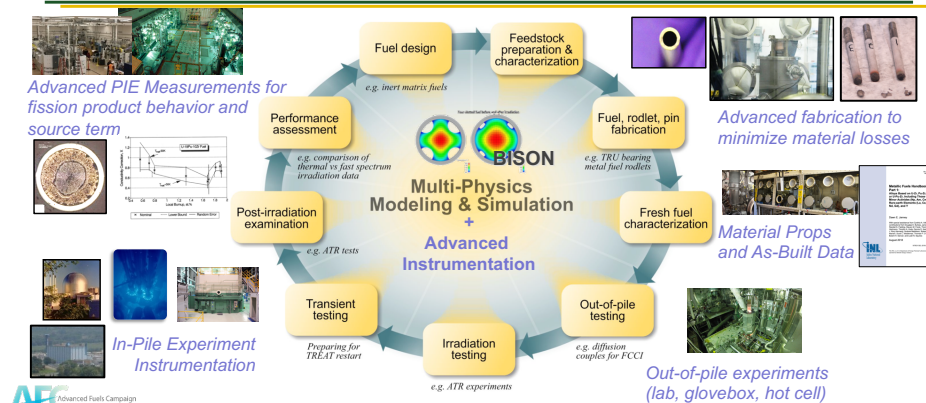
■ Mission:

- 1) Support development of **near-term Accident Tolerant Fuel (LWR)** technologies
- 2) Perform research and development on **longer-term Advanced Reactor Fuel** technologies



3

AFC Embodies All Needed Elements of Fuel R&D



4

Industry-Led Development of ATF Concepts

Laboratory roles

- Develop and maintain fuel testing/qualification infrastructure
- Perform uniform and independent testing of ATF concepts
- Support individual industry FOA teams as requested and approved.

Great success on many fronts!

- Reinvigorated industry, laboratory/university, regulator relationships!

Framatome

- Cr-coated M5 cladding
- Doped UO_2 for improved thermal conductivity and performance
- SiC cladding.



ATF Industry FOA Awards

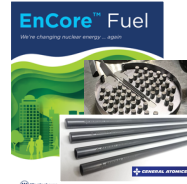
General Electric

- Coated Zr cladding
- Iron-based cladding (FeCrAl)
- ODS variants for improved strength.



Westinghouse

- Cr-coated Zirlo cladding
- SiC cladding
- Alternative fuels with improved thermal conductivity and high density.

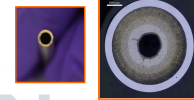


5

Advanced Reactor Fuel Development Thrusts

Fuels for Once-through Fast Spectrum Reactors

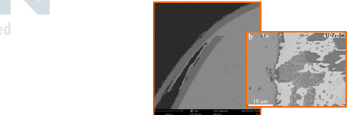
- Na-free (e.g. annular) metallic fuel concepts (VTR, TerraPower, Westinghouse)
- Ultra-high burnup for enhanced resource utilization (TerraPower)
- Non-traditional applications such as microreactors (Oklo, Westinghouse)



TerraPower

Fuels for High Temperature, Fast Spectrum Reactors

- Higher cladding temperature/performance (ODS alloys)
- Metallic fuels with additives and/or cladding coatings/liners
- UN, UO_2 for LFR (Westinghouse)
- UC for GFR (General Atomics)
- TRISO... currently under other DOE programs



KAERI
한국원자력연구원
Korea Atomic Energy Research Institute

Metallic Fuels for Closed Fuel Cycles and Actinide Transmutation

- Historic mission for SFRs, not ending but decreasing in priority

6

GAIN Advanced Fuels Workshop March 2019

Recommendations for Fast Reactor Fuels

- Expand efforts to collect, archive, organize, and preserve legacy data
- Focused physical characterization of fuels (mat props)
- Appropriately scaled and targeted irradiation campaigns
- Modeling and simulation development, including tools that may support licensing
- Development of an advanced fuel cycle including front-end considerations

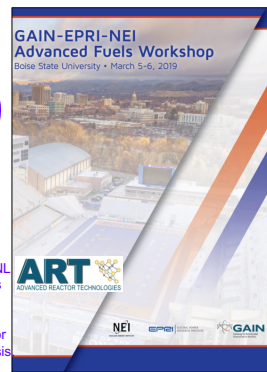
BISON
MARMOT

HALEU
(not discussed further here)

See next by N. Woolstenhulme



- GAIN ANL/INL metallic fuels databases
- Provide framework for licensing basis NRC Topical Report?

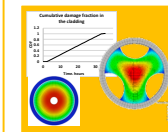


INL/EXT-19-55476

7

AFC Vision for ~5 years

2021



Establish baseline fuel performance code in BISON for U-xPu-10Zr.

(while continuing advanced model development)

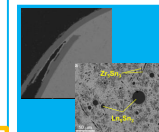
2022



Compose "NRC Topical Report on Metallic Fuel" for U-10Zr, U-20Pu-10Zr alloys.

Wrap up key historic metallic fuel R&D program R&D gaps (e.g. legacy PIE, TREAT metal experiments)

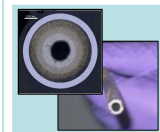
2023-24



Intermediate R&D objectives:
High temperature fuel design for up to ~700°C (stretch goal!)

Power-to-melt and thermal conductivity focused R&D

2025



Establish Na-free metallic fuel design option.

Prepare for lead test rod/assembly. Demonstrate accelerated fuel development model.

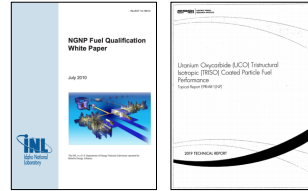
Challenges

- High-dose cladding R&D
- Prototypic fast reactor testing option
- Multi-length scale model development and validation
- Improving industry/DOE engagement

8

Importance of Consolidated Data and Licensing Basis

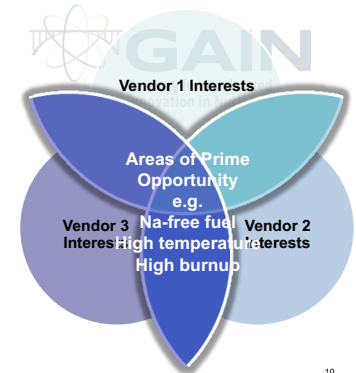
- **AGR program provides an interesting study case**
- **Modern success for fuel qualification of TRISO fuel for HTGR**
 - Successful multi-irradiation campaign for ~20 years
 - Focused qualification plan expressly connected to regulatory requirements
- **Noteworthy outcomes**
 - Recent submittal of NRC Topical Report by EPRI
 - Wide interest from industry
 - Many applications planned extending from established performance envelope
- **Implication**
 - Established technology continues to attract potential commercial adopters
 - Reduce risk for market entry!
- **Metallic fuel experience is vast and already proven**
 - Is there a similar metallic fuel technology package available today? If not, should there be?



9

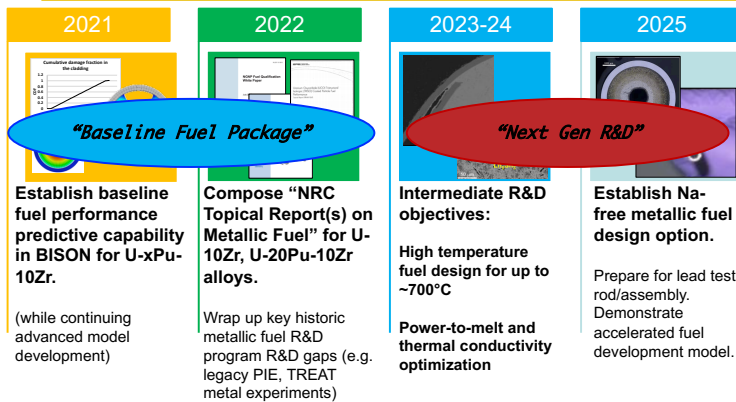
How to Improve Industry/Laboratory Engagement?

- **Are there aspects of the ATF program that can benefit metallic fuel success?**
- **Propose annual advanced reactor fuels workshop with industry and laboratories and universities**
 - Hosted by GAIN?
 - Technical meeting focused on R&D developments and plans (plans contingent on yearly funding approval)
 - Opportunity for industry expression of interests and needs
 - Some similarities to Halden joint project program meetings
 - Regular communication and interaction
- **Potential benefits**
 - Networking and collaboration building opportunities
 - Technical feedback and effort toward unity in goals – “community R&D” effort
 - Creates environment conducive to meaningful deployment!



10

AFC Vision for ~5 years



Challenges

- High-dose cladding R&D
- Prototypic fast reactor testing option
- Multi-length scale model development and validation
- Improving industry/DOE engagement

11

Feedback and Questions

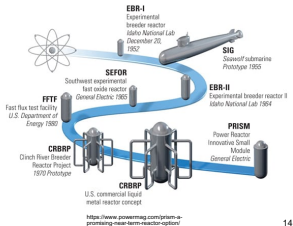
12

Irradiation Testing Strategy N. Woolstenhulme

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The Backdrop for a New Era

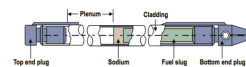
- **AFC irradiations have made remarkable contributions to date**
 - Demonstrated viability of metallic fuels to burn actinides and reduce repository radiotoxicity
 - Successful international collaborations on electrorefining recycle technology
 - Numerous scientific successes with various fuel types, additives, etc.
 - Confirmation that the same old problems (e.g. FCCI) are still the battle ground for some of the most valuable innovations
- **What has changed since AFC was born**
 - Dissolution of GNEP and the birth of GAIN → Emphasis on domestic nuclear energy
 - Natural gas fracking → Focus on economics of advanced reactors as first barrier to entry
 - Fukushima → Increased emphasis on passive safety
 - Vogtle budget overrun → emphasis on smaller reactor platforms and supply chains
 - Increased political attractiveness for grid integration with renewables
 - Resumption of operations at TREAT and increasing momentum for VTR
- **This is the backdrop in which we must reframe our vision for irradiation testing and maturation of advanced reactor fuels**



14

Focus Areas → Closure Points

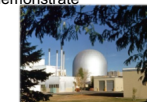
- **R&D for R&D's sake has its benefits in terms of discovery potential**
 - But the time has come for advanced fuels to rally around some concrete mission closure points (case study: TRISO qual effort presently spinning off into micro-reactor applications)
- **Putting a capstone on the metallic fuel state of the art**
 - QA-archiving, collation, and completion of a formal metallic fuels performance basis
 - Underpinned by maturation of fuel performance modeling
 - Expand baseline package with addenda (complete IFR M-series tests at TREAT, metallic fuel MA addition data)
- **Develop advanced metallic fuels design**
 - Preparing for VTR MkII driver fuel LTAs (history of SFR metallic fuels development is a big story of incremental improvements to driver fuel designs in EBR-II, FFTF, etc.)
 - Sodium free design offers benefits for disposition complexity, LFRs coolant interaction, and very high burnup physics effects
 - FCCI-mitigating design(s) offer economic gains via increased temperature outlet and burnup
 - Pilot program for accelerated fuel development approach
- **MOX-SFR closure points → Working with international partners to develop**
- **Closure points for advanced ceramics, advanced SFRs, and non-SFR applications → Working with US industry to develop**



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Purpose of Irradiation Testing & PIE

- **Groups of hard-working people can do amazing things when they work together for a common goal (closure point)**
- **Building reactors were these goals for nuclear R&D in the early days (as it ought to be today)**
 - Nexus of nearly all disciplines in science, engineering, and construction
- **An irradiation campaign does the same thing for fuel developers**
 - Like a mini-reactor design/build project - combines most of the nuclear disciplines into one goal
 - Depending on the details, can be time/cost intensive - forces prioritization of most viable fuel systems and sharpens R&D focus
 - Reveals phenomena and connectivity that would otherwise be unknown or misrepresented - maximizes the performance potential of fuel
 - Overarched from cradle to grave by model maturation - key to demonstrate understanding and enable licensing



Various photos of awesome things designed with slide rules

16

DOE's 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 capsule, lead out, and loop irradiations

HFIR:

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

TREAT:

- Graphite-based transient reactor started in 1959
- Unparalleled transient shaping capability
- Rich history of SFR fuel safety research
- Restarted 2018 with fuels safety testing

VTR:

- Sodium-cooled fast spectrum material test reactor
- Planned construction* for test availability by 2025
- 30 dpa/yr capability
- Drop-in sodium-cooled test capabilities
- Liquid-metal, molten salt, and gas environment isolated loop capabilities

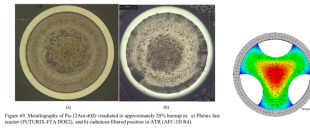
*413.3B Pre-decisional project status

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ATR Irradiation Testing Capabilities

■ AFC

- Full SFR-diameter rodlet testing in high flux ATR position using Cd-lined basket
- Rodlet-capsule gas gap thermal resistance for SFR temperatures
- Several tests executed on metallic fuel (and some on MOX, UN, & UC)
 - Results compare well to true SFR performance
- Burnup accumulation is slow process
- Ongoing and future metallic fuel irradiations addressing:
 - Na-free fuel designs, FCCI-mitigating liners/additives for high temperature performance, and recycled fuel effects



■ FAST

- Reduced diameter rodlets in "sodium bath" inner capsule, gas gap to outer capsule
- Innovative approach to managing thermal aspects for boosted enrichment and acceleration at representative SFR temperatures
- To be demonstrated starting 2020 on ~50 U-Zr based rodlets
- Currently being assessed for geometry-scaled features and ceramic fuels. LANL can supply advanced ceramics (e.g. UN)
- Likely somewhat limited for:
 - Rate effects and time-at-temperature phenomena
 - Synchronizing cladding damage fuel burnup behavior
 - Predominantly-fertile breeder fuel compositions



18

Advanced Reactor fuels in Thermal Spectrum Irradiation Capability (ARTIC)

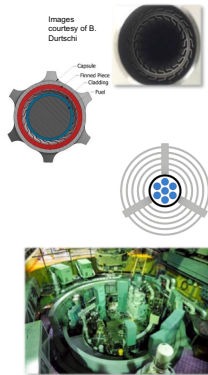
■ A great deal of good work has been done in Cd-lined baskets AFC capsules in ATR, primary design limitations include:

- Success story has been more incremental than monumental
- Fast neutron population too low for cladding dpa
- Gas gap yields high uncertainties in fuel temperature control
- Specimen size inadequate to evaluate at-scale fabrication effects or fuel relocation safety performance

■ Gathering input for near future design of enhanced testing approach in existing thermal spectrum reactor

- Longer rodlet and fueled section
- Intrinsic metal fins or similar to reduce gas gap sensitivity
- Spectral refinement/boosting schemes
- Passive and live-lead instrumentation strategies
- Finish truncated irradiations of abandoned IFR-era structural materials
- Optimization for various acceleration schemes (enrichment-boosting à la FAST vs flux boosting for predominantly breeder fuels)
- Other needs???

■ Potential ~2023 restart of JOYO opens collaborative opportunities while awaiting the commissioning of VTR

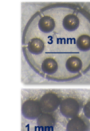


19

HFIR Irradiation Testing Capabilities

■ Structural Irradiations

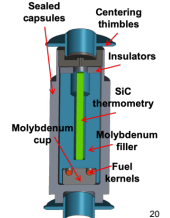
- High neutron flux in HFIR leveraged to accumulate dpa in structural materials



Consult Chris Petrie, the "MiniFuel Master," for more details

■ MiniFuel

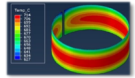
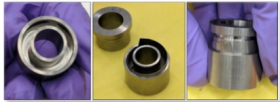
- Rapid burnup accumulation under controlled conditions to support accelerated fuel evaluation
- Small fuel volume reduces temperature gradients & decouples fuel temperature from fission rate
- Capsule recently commissioned with UN fuels
- AFC currently developing future U-Zr metallic fuel test to evaluate swelling of specific metallurgical phases



20

BR2: DISECT Experiment

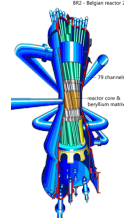
- **Near future irradiation in BR2 reactor, sponsored by NSUF**
 - metallic fuel foil and disc type specimens
- **Systematic exploration fission rates and temperature of U-Zr and U-Mo for SFR and MTR application, respectively**
 - Live instruments for temperature monitoring
 - PIE targeted toward fundamental fuel microstructure evolution and performance phenomena



W. Williams et al, "Thermal-Hydraulic and Neutronics Overview of the DISECT Experiment," Proceedings ANS Meeting, June 2019.

Alloy (Wt%)	Target Temperature [°C]	Target Power [W]
U-30Zr	250	3192
U-30Zr	640	3154
U-10Zr	750	4088
U-10Zr	750	5240
U-10Zr	640	5364
U-30Zr	550	3918
U-30Zr	678	3965
U-30Zr	750	5572
U-30Zr	750	5983
U-10Zr	678	5364
U-10Zr	710	5178
U-30Zr	710	5563
U-30Zr	678	3377
U-30Zr	640	2914

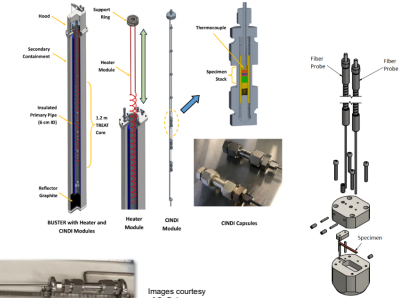
Alloy (Wt%)	Target Temperature [°C]	Target Power [W]
U-7Mo	150	3500
U-10Mo	150	4000
U-7Mo	300	4250
U-7Mo	250	6000
U-10Mo	250	8000
U-7Mo	300	7500
U-7Mo	300	11500
U-10Mo	300	14000
U-12Mo	300	13000
U-12Mo	150	11750
U-10Mo	250	11000
U-10Mo	150	10000
U-10Mo	150	7750
U-12Mo	300	7750
U-12Mo	150	5000



21

TREAT: Low-Dose Microstructure Evolution Experiments

- **Two microstructure metallic fuel experiments under preparation for TREAT**
 - Temperature monitored and controlled by electric heater (tube furnace surrounded by a reactor)
- **CINDI: Small microstructure and thermophysical properties characterization specimens**
 - Very low dose (1day irradiation: 1E15 fis/g) for fundamental damage mechanisms and lower length scale model development
 - Matrix includes various alloys of U & Pu with Zr at 550 and 700 °C, irradiation with a few months
- **Resonant Ultra-Sound Laser (RUSL) method measures real time phase transitions in pile**
 - Develop in-pile phase diagrams as function of fission rate
 - U-Mo, and perhaps other alloys, to be addressed under aLEU project within 1 year from now

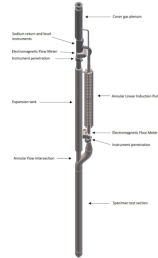
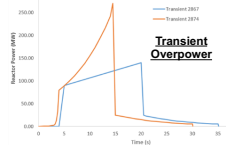
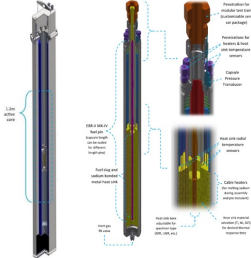


Images courtesy of C. Baker

22

TREAT Safety Testing Capabilities

- **THOR Capsule**
 - Single SFR pin in solid metal heat sink combined with transient power shaping
 - Cost effective method for studying nuclear heated transient temperature histories
 - First tests in 2020 (including fresh Na-free designs)
- **Sodium Loop**
 - Historic sodium loop 3 year modernization project w/ TerraPower, first tests in FY22
 - Individual pins in flow tubes or 7 pin bundle
 - Western world's largest selection of pre-irradiated SFR fuel at INL (EBR-II, FFTF) specimen supply

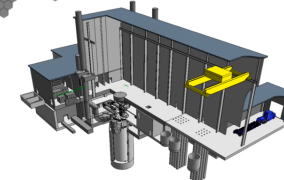
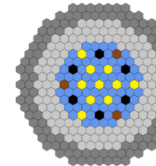


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VTR Irradiation Testing Capabilities



- Startup core Na-bonded U-Pu-Zr fuel
- Logo tells the story (Pu fission = 2.89 neutrons)
- VTR is a dpa machine (30 dpa/yr)



- **2026 experiment capability, sodium-cooled drop-in driver fuel positions:**
 - Sodium free Mk-II driver core (Pu bearing, high dpa:burnup ratio)
 - Pu-free advanced fuels for commercial SFR plants (lower dpa:burnup ratio)
- **Closed loops available a couple years later**
 - Different coolant (lead, gas, salt)
 - Enhanced Instrumentation
 - Vented & deliberately breached fuel

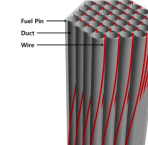


Image from: SFR Design Study, under the Energy Policy Act of 2005. The SFR Design Study is a report by the U.S. Department of Energy, Office of Nuclear Energy, Office of Advanced Reactors and Technology, Volume 1, Issue 1, 2010. Pages 80-81.

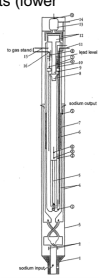
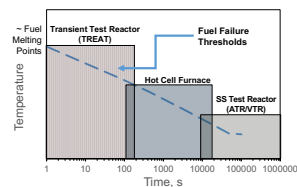


Image from: SFR Design Study, under the Energy Policy Act of 2005. The SFR Design Study is a report by the U.S. Department of Energy, Office of Nuclear Energy, Office of Advanced Reactors and Technology, Volume 1, Issue 1, 2010. Pages 80-81.

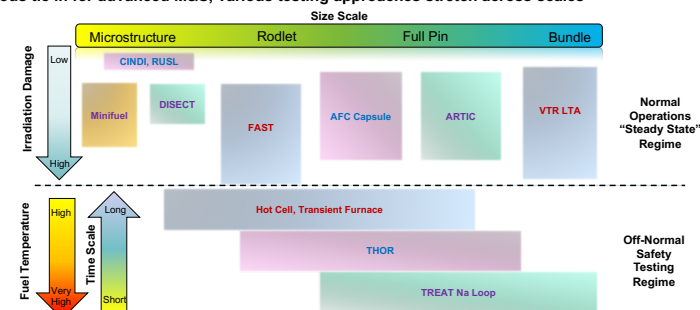
24

- **Hot cell capabilities bridge gaps and capstone the data**
- **Full PIE capabilities**
 - Neutron radiography
 - Metrology (profilometry)
 - Precision gamma spectroscopy scanning
 - Fission gas puncture and analysis
 - Metallography, electron microscopy
 - Mechanical and thermal properties measurement
- **New transient furnace development planned, will bridge gap between transient test reactors and material test reactors**
- **Electrorefining demo capability well underway**
- **Assembly of TREAT experiments**

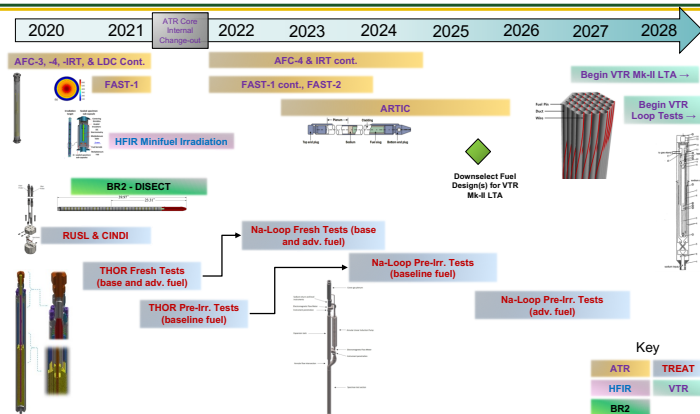


Testing Across Scales


- **Accelerate fuel development and qualification is our ultimate enterprise**
 - Going faster in some processes certainly helps (e.g. fission rate boost for burnup accumulation)
 - But ultimately can only succeed if the strategy connects multiple scales and physics domains
- **Obvious tie in for advanced M&S, various testing approaches stretch across scales**



A notional roadmap for He-Bonded Advanced SFR Fuel as Mk-II VTR driver core



Summary

- **The situation has changed a little, and AFC's metallic fuels plan is being realigned for “the dawn of a new era” (corny phrase, but true)**
 - R&D program has ~5 years to shift the spectrum a little from “R” to “D” using a multi-reactor and hot cell test platform
 - Structured engineering approach to balance risk/reward decisions and sharpen research focus
 - Fostering industry partnerships during this period crucial to develop optimal test capabilities and grow advanced fuels efforts
 - **Closure points crucial to community success**
 - Capstone package for baseline metallic fuel performance state of the art
 - Development of advanced sodium free fuel with FCCL-mitigating features crosscuts many industry and DOE needs
 - Commensurate with model maturation, advanced M&S aided by multi-scale irradiation testing strategy
- 



<https://www.forbes.com/sites/rodamma/2017/02/28/fast-spectrum-reader-developer-will-be-more-entrepreneurial-and-more-recognized-for-it/#18787731ab7d7>

11.2 State of the Art for Engineering-Scale PIE
Steven Hayes, Idaho National Laboratory

State of the Art for Engineering-Scale PIE

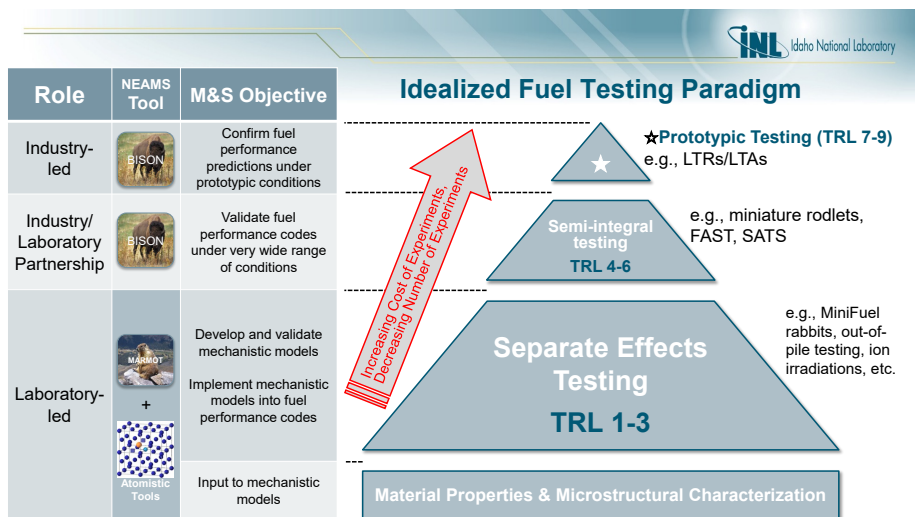
Metallic Fuels Meeting University of Florida

Steven L. Hayes, PhD
Director, Nuclear Fuels and Materials Division

November 14, 2019

Outline of Presentation

- Idealized Fuel Testing Paradigm
- Engineering-Scale Postirradiation Examinations
 - Non-Destructive Examinations
 - Destructive Examinations
- Assessment of Existing vs. Needed PIE Data
- Need for Micro-Scale Characterization of Irradiated Fuels
- PIE Needs: Conclusions



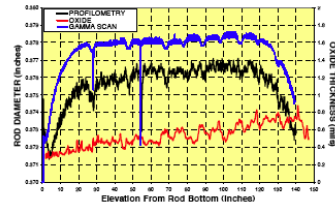
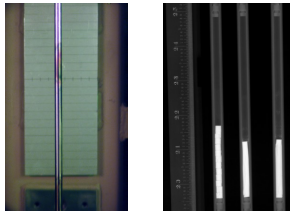
Overview

- Non-Destructive Examinations
- Destructive Examinations



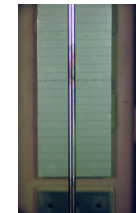
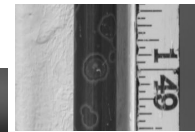
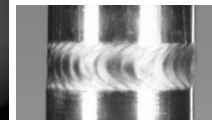
Non-Destructive Examinations

- Visual Inspection
- Neutron Radiography
- Dimensional Inspection
- Gamma Ray Spectroscopy
- Eddy current Oxide Layer Tester
- Eddy current Cladding Integrity Tester



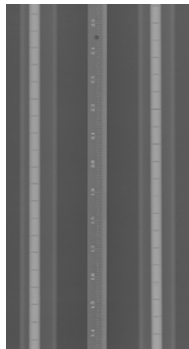
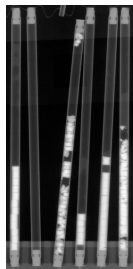
Visual Inspection

- Detailed Visual Inspection
 - Thru-cell wall periscope 2X, 10X, 25X
 - Digital Still Camera Photography
- Macro Photography Inspection
 - Thru Hot Cell window
 - Digital Video Camera Photography
 - Digital Still Camera Photography
 - Full color with grey balance



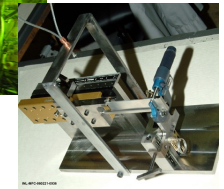
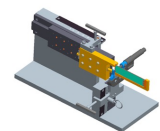
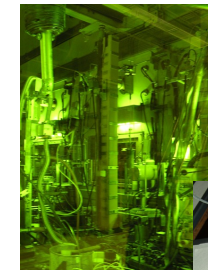
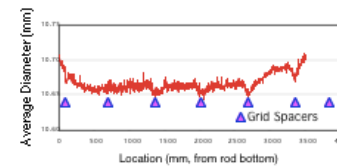
Neutron Radiography

- **Purpose:** Non-destructively interrogate internals
- **Application:**
 - Evaluate fuel integrity and movement
 - Hydriding in LWR cladding
 - Tomography



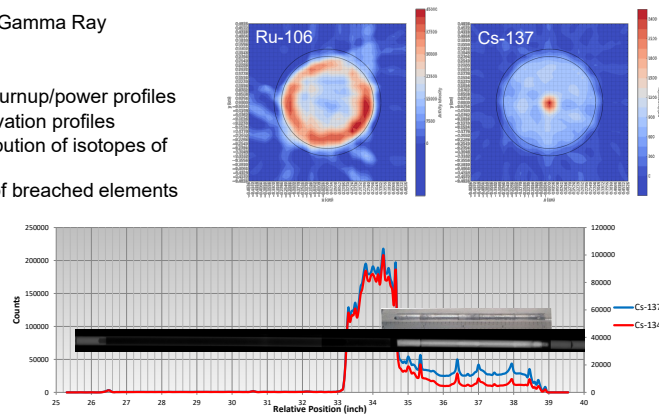
Dimensional Inspection

- **Purpose:** Measure diameter / plate thickness and bow and length
- **Application:**
 - Cladding creep down in-reactor service and creep out during dry storage
 - Irradiation induced swelling
 - Fuel rod growth
- **Description:**
 - Element contact profilometer: diam. ± 0.0002 in. (± 0.0051 mm)
 - Bow and Length: ± 0.02 in. (± 0.51 mm)



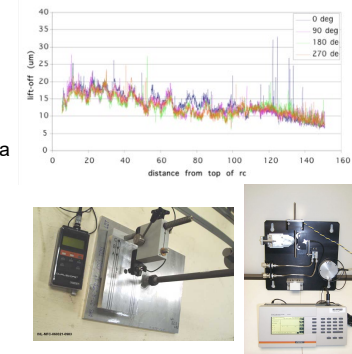
Gamma Ray Spectroscopy

- Gross and Isotopic Gamma Ray Spectroscopy
- Uses
 - Relative fuel burnup/power profiles
 - Structural activation profiles
 - Relative distribution of isotopes of interest
 - Identification of breached elements
 - Tomography



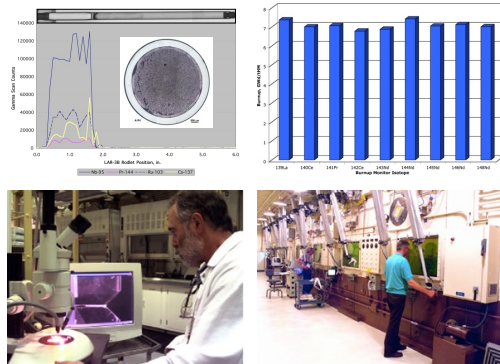
Eddy current measurement system

- Purpose:** Non-destructively evaluate the structural performance of nuclear fuel cladding
- Application:**
 - Detect and characterize material defects
 - Non-destructively measure oxide layer thickness
 - Measures electrical current induced when a conductor is placed in a region of shifting magnetic flux
- Description:**
 - Max. sample size: 1 in. D x 154 in. L
 - Oxide thickness uncertainty: $\pm 5 \mu\text{m}$



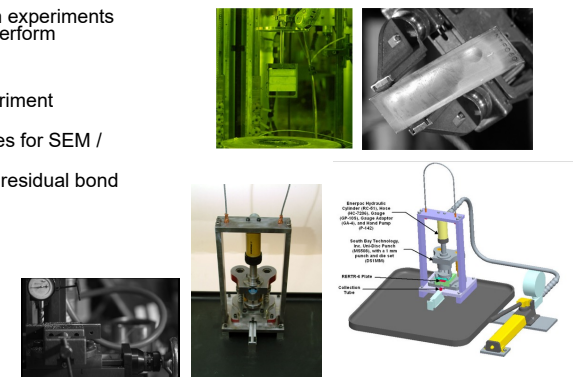
Destructive Examinations

- Fission Gas Puncture & Analysis
- Fuel annealing Furnace
- Isotopic & Burnup Analysis
- Metallography / Ceramography



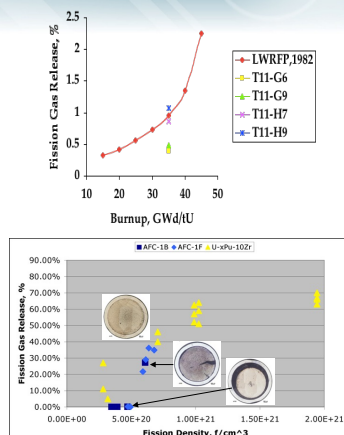
Test disassembly, sample retrieval and furnace testing

- Purpose:** Disassemble irradiation experiments and retrieve samples for testing. Perform furnace annealing tests.
- Application:**
 - Disassemble irradiation experiment capsules
 - Retrieve reduced size samples for SEM / TEM analyses in EML
 - Evaluate irradiated plate fuel residual bond strength
- Description:**
 - Table top Mill
 - SEM Punch
 - Furnace temp: 1200°C
 - Furnace cavity: 6" D x 24" H



Fission Gas Puncture & Analysis

- **Purpose:** Puncture fuel rod and analyze fission gas pressure/internal void volume and chemical/isotopics
- **Application:**
 - Determine fission gas and helium release
- **Description:**
 - Laser puncture system
 - Fuel rod internal void volume and gas pressure, $\pm 5\%$
 - Plenum gas batch sample chemical analysis



Fuel annealing furnace for fission gas release studies

- **Purpose:** Measure temperature-driven release of condensable fission products and fission gases from irradiated fuel
- **Application:**
 - Heat irradiated fuel in helium sweep gas ($T \leq 2000^\circ\text{C}$)
 - Condense fission products during annealing on water-cooled cold plate for subsequent measurement
 - Collect and measure released fission gases (Kr, Xe) in cryo traps
- **Description:**
 - Max temp: 2000°C
 - Graphite heating element
 - Helium atmosphere (@ ambient pressure)
 - Hot zone: $\sim 3.25''$ diameter x $\sim 6''$ high
 - Computer controlled operation
 - Automated cold plate exchange



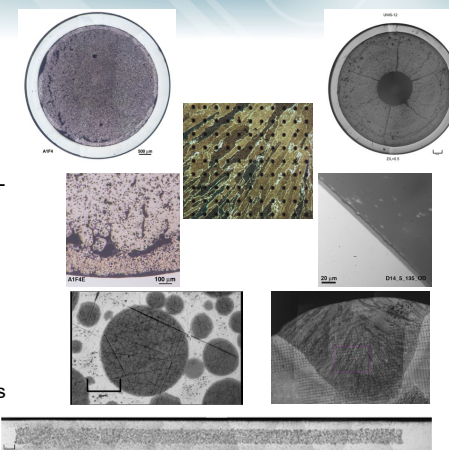
Isotopic and Burnup Analysis

- **Purpose:** Measure bulk isotopic and chemical composition of actinide fuel samples as-fabricated and postirradiation.
- **Application:**
 - Perform nuclear material accountability measurements by Thermal Ionization Mass Spectrometry (TIMS) isotope dilution
 - Inductively Coupled Plasma Mass Spectrometry-Dynamic Reaction Cell (ICPMS-DRC) to mitigate isobaric interferences and obviate chemical separation
 - ICP-Optical Emission Spectrometry
 - Derive burnup of metallic, oxide, nitride, carbide and dispersion fuel forms.
- **Description:**
 - U, Pu isotopics: $< \pm 1.0\%$
 - Fission product isotopes: $\pm 2\%$
 - Elemental analysis: $\pm 2-5\%$
 - NIST traceable standards



Metallography / Ceramography

- **Purpose:** Characterize microstructure and micromechanical properties of irradiated fuels and materials
- **Application:**
 - Characterize irradiated fuel grain size and morphology, porosity, phase, fuel-cladding interaction
 - Measure cladding oxide thickness, hydride distribution
- **Description:**
 - Leitz MM5 RT Metallograph (80X to 800X)
 - Microindenter Hardness Tester
 - Automatic stage control
 - Integrated data collection and analysis
 - Digital Still Photographic Image



Assessment of Experimental Data: Existing vs. Needed for Validation

- Historical Data on Metallic Fuels Comes Mostly from Integral Experiments
 - Quantitative data mostly from macroscopic PIE (engineering-scale)
 - What microscopic PIE data is available is mostly non-quantitative
 - Detailed characterization of fuels needed as input for modern simulations was not performed (i.e., grain size/pore distributions, phase fractions, etc.)
 - Irradiation experiments not instrumented, so considerable uncertainty on fuel power (~10%), which influences and dominates all other uncertainties
- Data Needed to Inform/Validate Multiscale Models
 - Instrumented irradiation experiments to reduce uncertainties
 - Shorter-term irradiation experiments to elucidate time/path-dependencies
 - Microscopic characterization:**
 - of as-fabricated fuels for input to simulations
 - of irradiated fuels during PIE

Since multiscale modeling effort for fuels is focused on microstructure evolution under irradiation as the key to accurate predictions at the engineering-scale, microstructural characterization is the key to validating modeling efforts.

Microscale Characterization of Irradiated Fuels and Materials

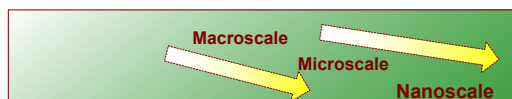
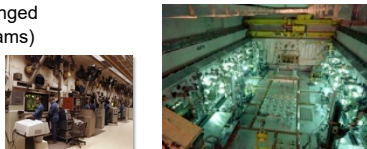


Microstructure-based mechanistic fuel modeling requires characterization of irradiated fuels and materials at level of microstructure for validation.

- IMCL was established to meet this need; gloveboxes provide containment inside shielded enclosures, which house an array of characterization capabilities:
 - Shielded cell for sample preparation
 - Dual beam FIB for preparing TEM lamella, Plasma FIB for preparing block samples for microscale characterization
 - Micro X-Ray Diffraction (μ XRD), Electron Probe Micro-Analyzer (EPMA)
 - Laser flash diffusivity, differential scanning calorimetry (DSC), Thermal Conductivity Microscope (TCM)
 - Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM)

PIE Needs to Support Advanced Modeling & Simulation Activities

- Need for Macroscopic Characterization will Remain Unchanged
 - i.e., Standard suite (non-destructive & destructive exams)
 - Assess feasibility of innovative fuel concepts
 - Characterize integral effects
- Also Need Micro-scale Characterization of Irradiated Fuels and Materials
 - Detailed PIE of integral and "separate effects tests" to inform/validate M&S effort
 - Characterization of:
 - Microstructure
 - Chemistry
 - Crystal structure
 - Properties



11.3 Metallic Fuel Macroscale Modeling Overview

Topher Mathews, Los Alamos National Laboratory



Metallic fuel macroscale modeling overview



Topher Matthews

Cetin Unal, Jack Galloway, LANL
Steve Novascone, Al Casagrande, Pavel Medvedev, INL

November 14th, 2019



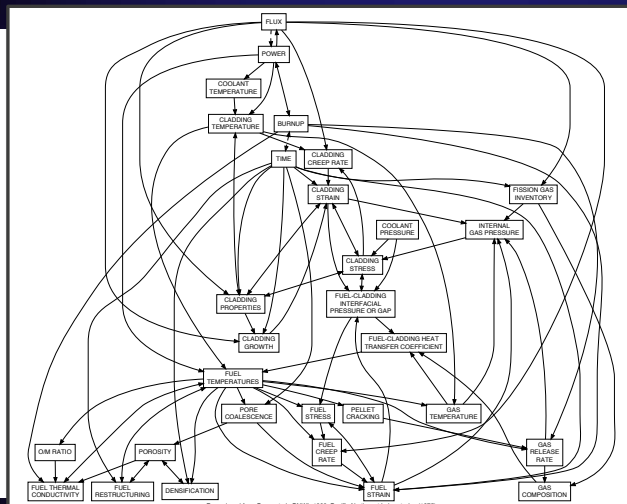
Managed by Triad National Security, LLC for the U.S. Department of Energy & NNSA

Why is modeling nuclear fuel so interesting...?

Los Alamos National Laboratory

11/13/19 | 2

Why is modeling nuclear fuel so interesting...?



...because it depends on everything!

Fission gas impacts (almost) everything!

Fission gas is natively multi-scale

Los Alamos National Laboratory

11/13/19 | 3

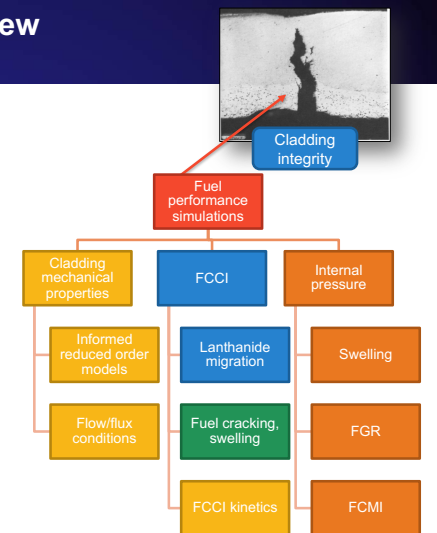
Metallic Fuel Modeling Overview

Goal: Develop advanced mechanistic tools to grow BISON metallic fuel capabilities

- 1) Fuel integrity
- 2) Fuel cladding chemical interaction (FCCI)
- 3) Fission gas release
- 3) Cladding properties

- Entering a new regime for support *for* VTR and industry...
 - Checking boxes is not enough, models need to be mechanistic to extend usefulness
- ...and support *from* NEAMS
 - Lower length scale information
 - Part of larger suite of coupled codes

Collaboration has led to rapid improvements...but much more work to do!



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11/14/19 | 4

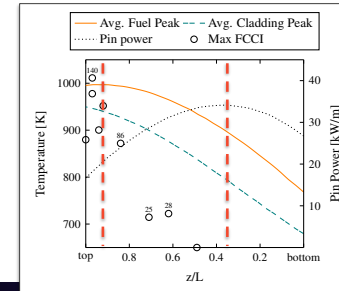
Presentation overview

- What do we know?
- Data comparison example 1: Zirconium redistribution
- Data comparison example 2: Pin design parametric experiment X441
- Where are we now?
- Where to next?

What do we actually know: Operating data

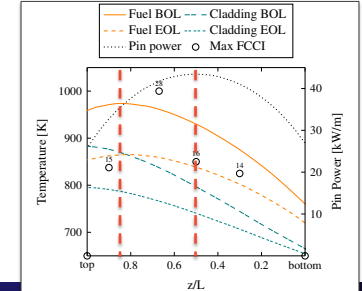
EBR-II

- IMIS database
 - As built geometry
 - Calculated rod power, mass flow rate, burnup
 - Measured FGR, axial swelling
- FIPD under development by ANL

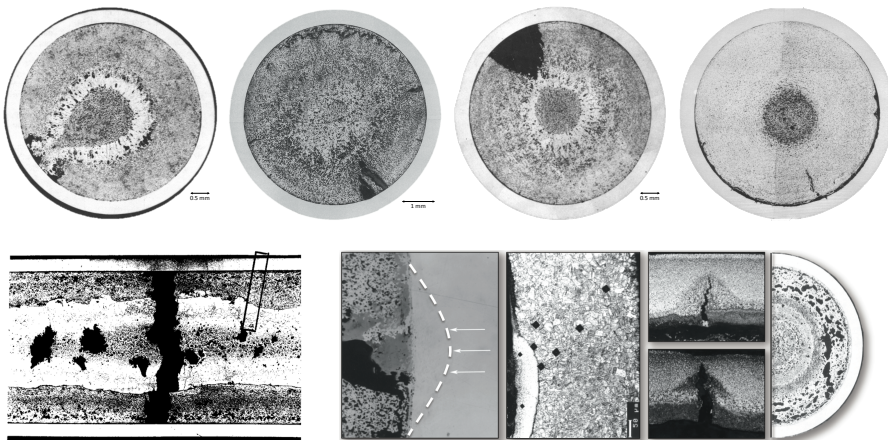


FFTF

- Limited metallic fuel experiments
- Essential for validation of models
- Database under development by PNNL

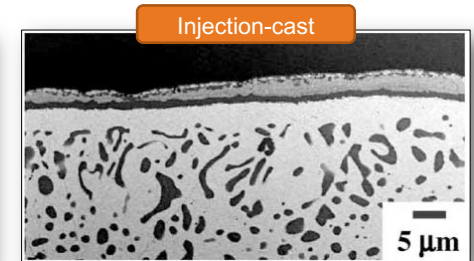
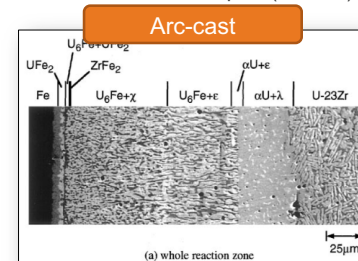


What do we actually know: PIE Micrographs



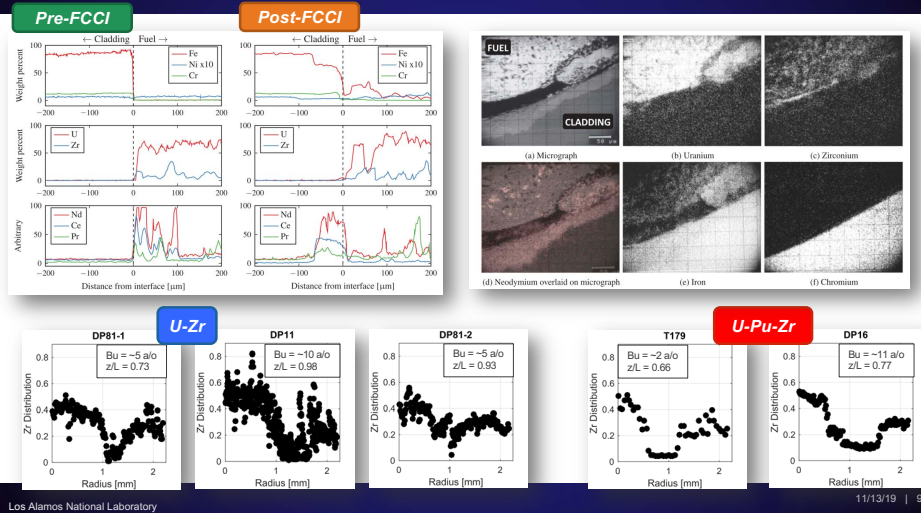
What do we actually know: Diffusion couple micrographs

- Many diffusion couple studies in literature, etc. U-Pu-Zr-Ce/Fe-Ni-Cr ... and more
- Some great characterizations, others are more dated
- Rind develops on injection-cast samples, stops diffusion (historic EBR-II)
- No rind in arc-cast samples (CREIPI)

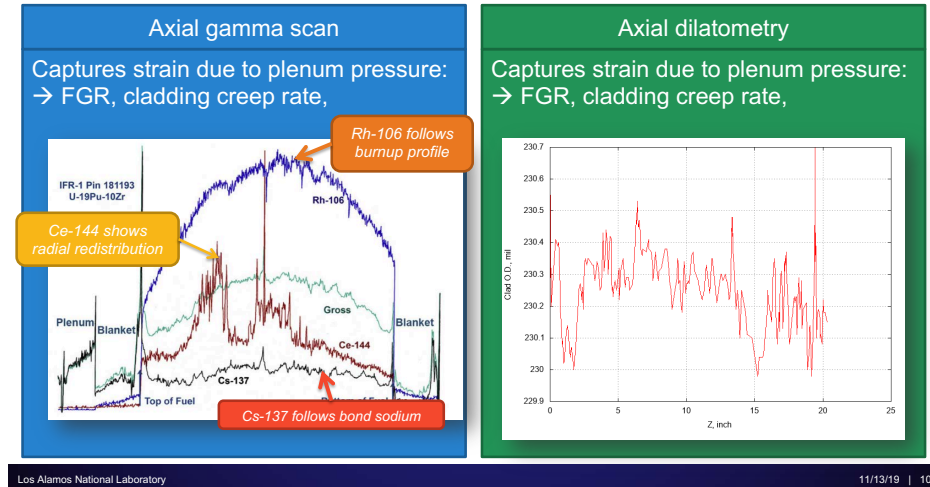


Not all materials are created equal

What do we actually know: EPMA compositions



What do we actually know: Axial scans



➤What do we know?

➤Data comparison example 1: Zirconium redistribution

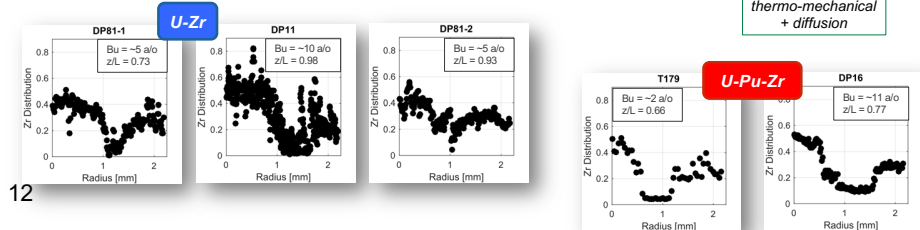
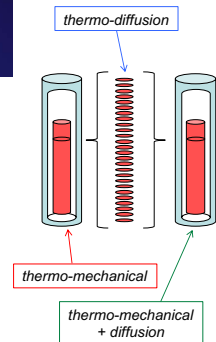
➤Data comparison example 2: Pin design parametric experiment X441

➤Where are we now?

➤Where to next?

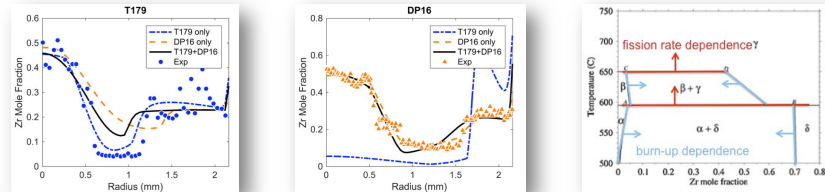
Zirconium Redistribution EBR-II comparison

- Due to lack of separate effects testing, calibration to integral data is necessary
- Utilized local experts on calibration techniques to avoid “re-learning” the science
- Requirements on calibration setup to help developers while minimizing time
 - Model needs takes thousands of 1D perturbed runs to match data to model
 - Calibration needs to be consistent and repeatable as models are updated
 - Calibration needs to predict across data sets to ensure applicability
 - Calibration cannot make up for failure of models to capture the physics



Zirconium Redistribution EBR-II comparison

- Single case calibration → Results look reasonable
- Multiple case calibration → Results look poor for U-Pu-Zr, and completely unusable for U-Zr
- Three things can be occurring
 - BISON usage or input is incorrect
 - Mitigated by mining best available parameters from database
 - Redistribution model is incorrect and needs to add missing physics
 - Fission rate dependence on the phase diagram is already known, but not calibrated
 - This can be approached by changing the phase diagram or changing the physics
 - Underlying BISON models are providing poor state variables and need to be updated
 - This is a known issue already for swelling (i.e. calculated swelling does not match observed PIE results)



Pin Geometry EBR-II Comparison

- Initial characterizations using the X441 EBR-II assembly
- Varies plenum size, composition, smear density, and cladding thickness
- U-19Pu-xZr with HT9
- Compared against cladding strain

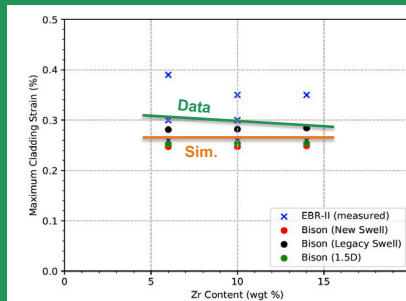
X441 Experimental Parameters

Group	Plenum/Fuel (Vol. Ratio)	Zr content (wt%)	Smear Density (% TD)	Clad Material	Clad Thickness (mils)
A	1.5	10	75	HT9	15
B	2.1	10	75	HT9	15
C	1.1	10	75	HT9	15
D	1.5	6	75	HT9	15
E	1.5	14	75	HT9	15
F	1.5	10	85	HT9	15
G	1.5	10	70	HT9	15
H	1.5	10	75	HT9	18

Pin Geometry EBR-II Comparison

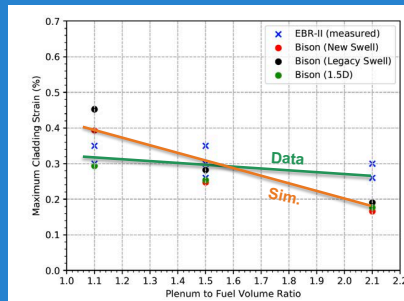
Zirconium Content

Captures strain due to fuel composition:
→ FGR, swelling



Plenum Volume

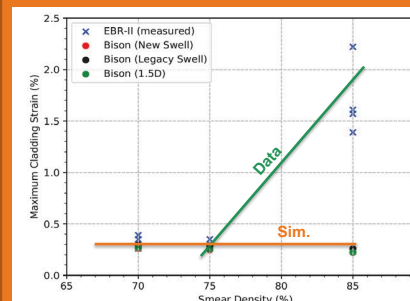
Captures strain due to plenum pressure:
→ FGR, cladding creep rate,



Pin Geometry EBR-II Comparison

Smear Density

Captures strain due to FCMI:
→ Swelling, mechanical properties



Conclusions

- Comparison to parametric X441 experiment is missing physics
 - FCMI is difficult to capture
 - Composition dependence is probably not captured here
 - Cladding creep behavior is not accurately captured
 - FGR/swelling shows up *everywhere*


Why is modeling nuclear fuel so interesting...?

Why is modeling nuclear fuel so interesting...?



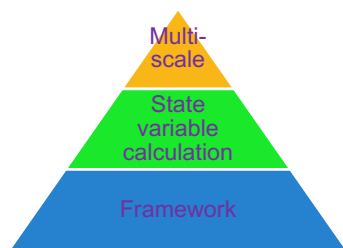
...because it depends on everything!

Fission gas impacts (almost) everything!

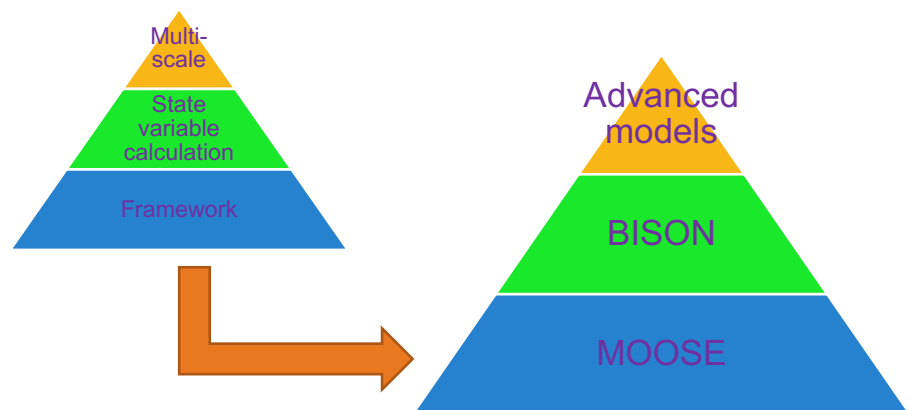


Fission gas is natively multi-scale

Context is important!



Context is important!



Where to from here?

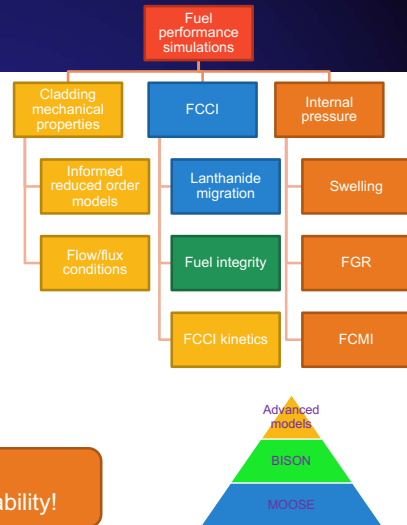
Metallic fuel is fundamentally different than UO_2 ...

- High swelling
- Extensive contact
- Tightly-coupled non-linear material behavior

...requiring different ways to attack the problem

- Near-term updates
 - Framework level updates
 - Mechanistic swelling model
 - ROM cladding model
 - Zirconium redistribution advancements

Robustness is paramount...
... but *mechanistic* is essential for applicability!



(incomplete) Model overview

Phenomenon	Imp.	Current	In progress	Long-term
Swelling, FGR	++	Simplified eigenstrain	Viscoplastic model	Multi-scale informed
Zirconium redistribution	o	Calibrated Fickian/Soret	Thermo-dynamically informed Fickian/Soret	Thermo-dynamically informed free-energy calculation
Thermal conductivity	+	Model that combines all data for all U-Pu-Zr concentrations	Empirical sodium/burnup, new data	Multi-scale sodium/burnup
Assessments	++	Hand full of scattered cases, initial organization	Organized assessment cases, linked to database, add FFTF	Automatic calibration
FCCI	+	N/A	Empirical fit	"Follow-the-lanthanides" multi-physics
Cladding	+	Empirical J2 creep rate	ROM HT9 modeling	New irradiated PIE data
Phase	+	Thermo-dynamic database lookup	Improved database	Fission rate and burnup
Radial power	+	Zr, fission rate MCNP fit	N/A	N/A
Contact	O	Shaky Frictionless	Robust Frictionless, Frictional	Robust Frictional
Code robustness	+	Automatic differentiation/scaling	Geometric scaling	TBD
Transient	O	?	?	?
BCs	++	Historical calculations	?	?
Properties	+	Fresh fuel, composition/temperature	New data	Phase+Burnup dependent

Swelling

Phenomenon	Imp.	Current	In progress	Long-term
Gamma swelling	+	Simplified eigenstrain	Viscoplastic model	Multi-scale informed
Alpha tearing	+	N/A	Simplified eigenstrain	ROM viscoplastic model
Beta fracturing	o	N/A	?	?
Interconnectivity	+	Smoothed polynomial	Phase-field informed interconnection	N/A

FCCI

Phenomenon	Imp.	Current	In progress	Long-term
Lanthanide diffusion	O	Proof-of-concept migration phenomenon	Lower-length scale informed diffusion	Multi-scale informed
Fuel fracturing	+	Basic peridynamics	?	?
Fuel/cladding inter-diffusion	+	?	?	?
Fuel eutectic melting	O	Basic thermo-dynamics	?	?

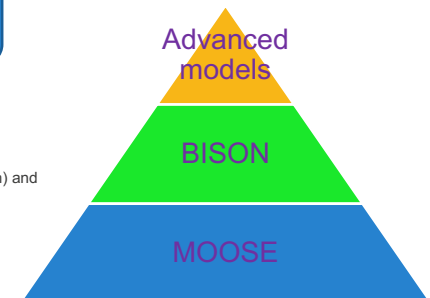
Framework development

Metallic fuel is fundamentally different than UO_2 ...

- High swelling
- Extensive contact
- Tightly-coupled non-linear material behavior

...requiring different ways to attack the problem

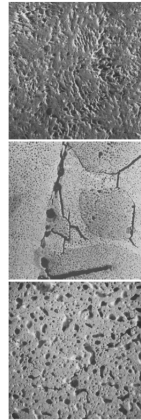
- Many framework-level features that have been implemented and are being put through the paces
- **Automatic differentiation** (AD) implementation complete for metallic fuel
 - Heavy lifting by Alex Lindsay (framework implementation) and Daniel Schwen (tensor mechanics)
 - Recall: AD requires only the residual (ie physics) only
 - Analytical Jacobians are faster, but error prone, and not possible in highly distorted geometry not possible
- **Automatic scaling**
 - No more "scaling" parameter
- **Mortar method for contact**
 - Robust method for mechanical and thermal contact



Collaboration with the MOOSE team led to success in advanced MOOSE features

Mechanistic fission gas model

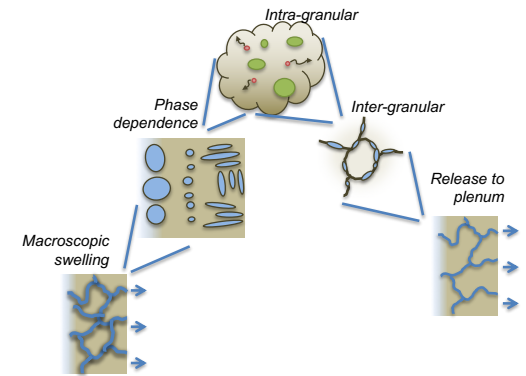
- The historical fission gas model has long been identified for update
 - Inconsistencies with reproducing observable swelling
 - Potential cross-contamination with calibration
 - Empirically based = Limited application
- Swelling, not release, is the primary metric of comparison for fission gas behavior in metallic fuels
- Inter-twined behavior of fission gas required to produce correct fuel state for many other models
 - Porosity leads to accurate thermal behavior of the fuel → Temperature
 - Stress-state needed for eventual cracking studies → Stress, creep, FCCI
 - Interconnection is an integral piece for lanthanide migration → FCCI
 - Interconnection is needed to estimate sodium infiltration → Temperature
 - Interconnection leads to fission gas release and lanthanide migration → Stress, creep, FCCI
- Model requirements lead to phase dependent bubble size coupled to temperature and stress



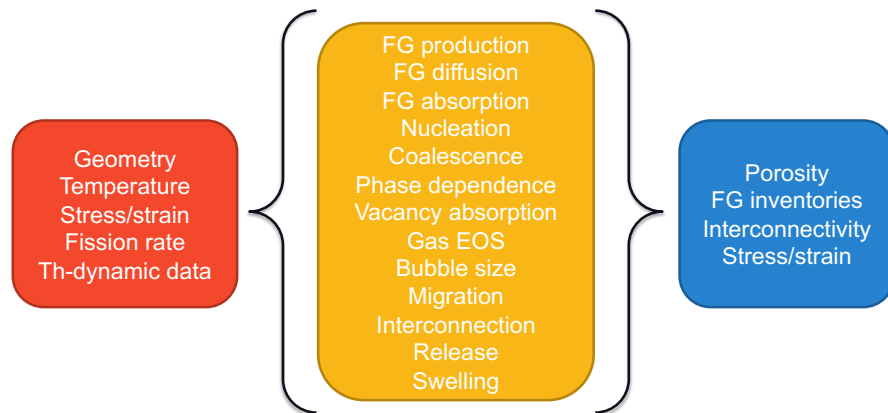
A robust, mechanistic swelling model is required by all other models

Fission gas behavior depends on fuel type

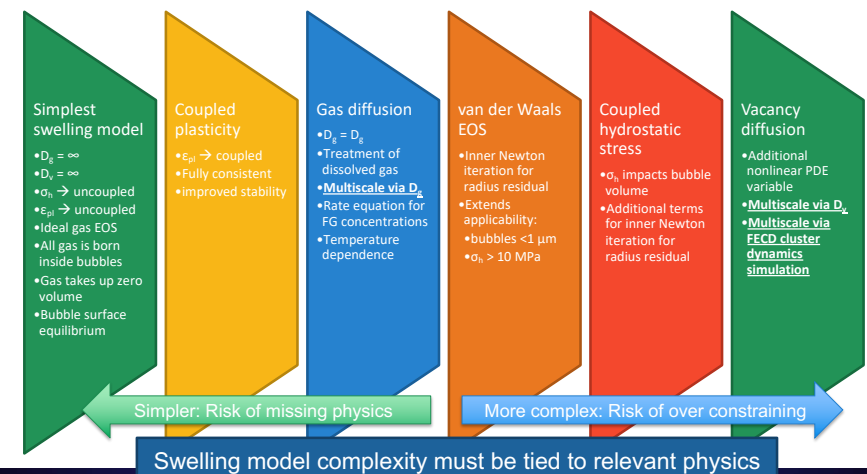
- Ceramic fuel (e.g. UO_2)
 - Inter-granular lenticular bubble interconnection
 - Grain perforation
 - Small gas release fraction
 - Primary impact: Fission gas release and plenum pressure
 - Generally bottom-up modelling approach
- Metallic fuel (e.g. U-Pu-Zr)
 - Large bubbles
 - No clear grain structure
 - Phase dependence in bubble size
 - Tightly coupled with mechanical state of fuel
 - Primary impact: large swelling
 - Generally top-down modelling approach



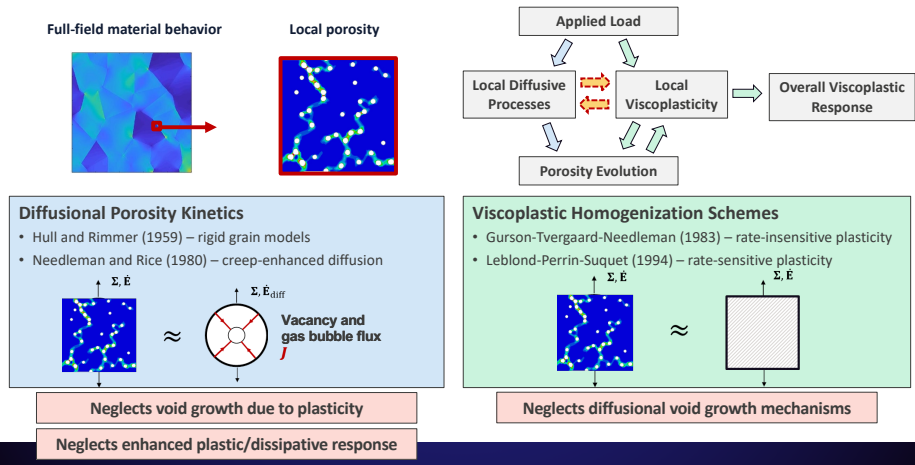
What does a (metallic) fuel swelling model look like?



Swelling model evolution

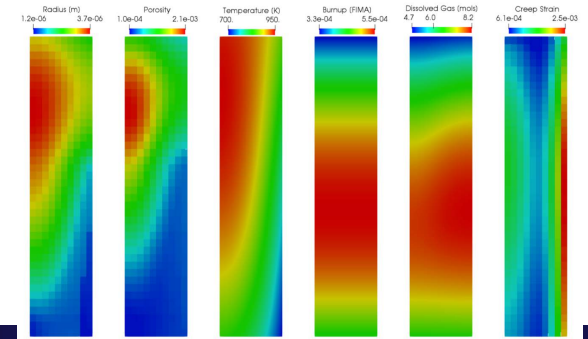


Plasticity and Porosity Evolution are Highly Coupled



Mechanistic fission gas model: Preliminary results

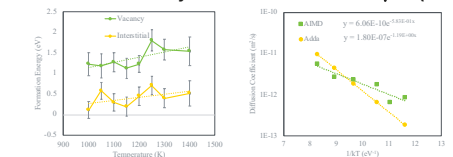
- Preliminary results show good behavior at high tensile stresses
- Assessment in EBR-II pins underway to determine best set of realistic parameters (e.g. diffusivities, bubble densities, etc)



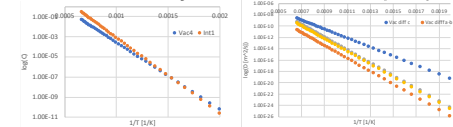
Calculating properties for uranium metal fuels from atomic scale simulations (Beeler, Andersson, et al.)

- Meso- and engineering scale models of metal fuel performance, e.g. swelling, require phase dependent properties of point defects, fission gas atoms and gas bubbles.
- Several of these are poorly characterized from experiments and atomic scale simulations based on empirical potentials and density functional theory may be used as complement to improve model fidelity.

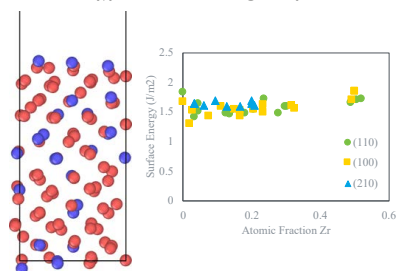
Point defect thermodynamics and diffusion in γ -U (DFT)



Point defect thermodynamics and diffusion in β -U (DFT)

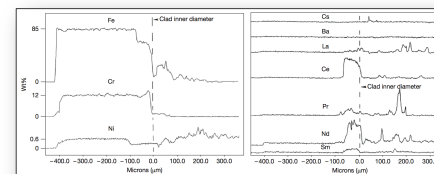


UZr (γ) surface energies (DFT, AIMD)

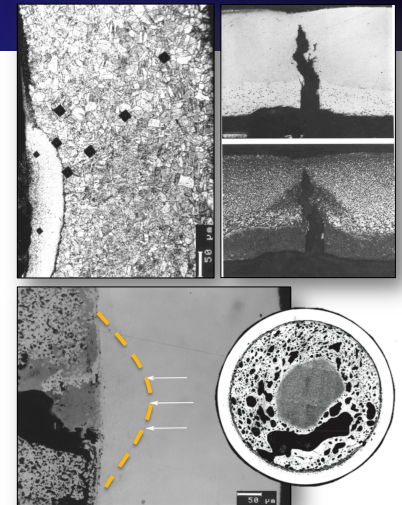


Fuel-Clad Chemical Interaction: Big Picture

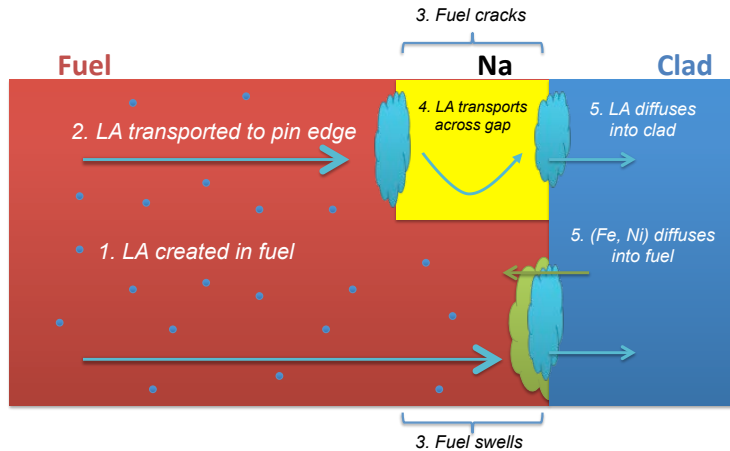
- FCCI described by inter-diffusion of lanthanides & iron
- Fe + U/Pu = Low temperature eutectic
 - Fuel melting = BAD!**
- SS + LA = brittle clad → creep failure
 - Cladding failure = BAD!**
- Life limiting parameter
- Modeling limited to empirical fits
- Limited methods of control: liners, microstructure/chemical tailoring



If you know where the lanthanides are, you know where FCCI is

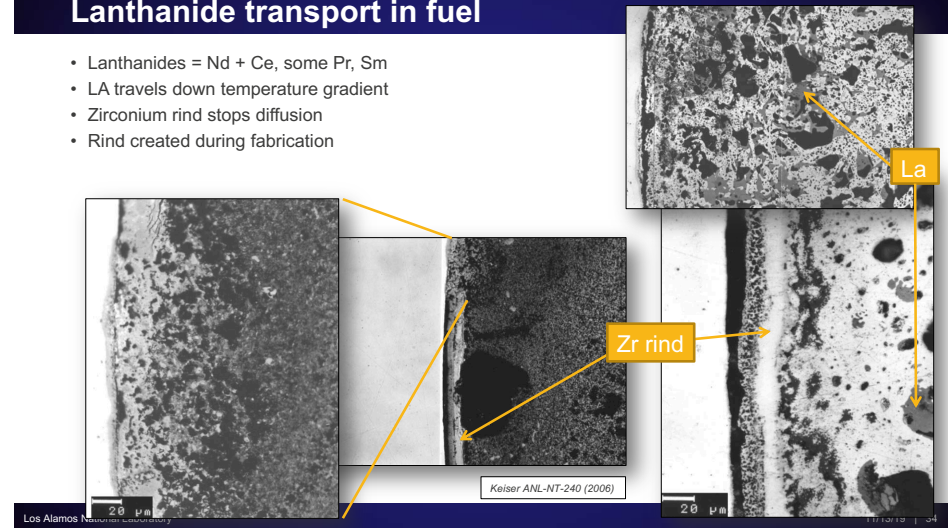


Conceptual model: Follow the Lanthanides



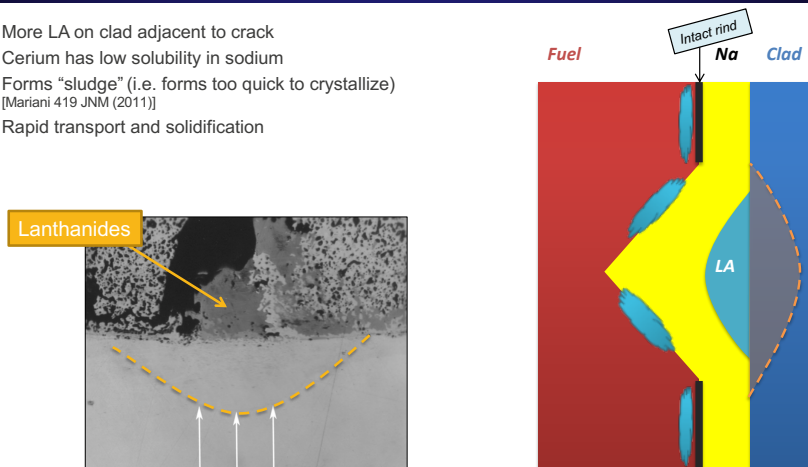
2. FCCI Observations: Lanthanide transport in fuel

- Lanthanides = Nd + Ce, some Pr, Sm
- LA travels down temperature gradient
- Zirconium rind stops diffusion
- Rind created during fabrication



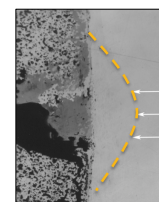
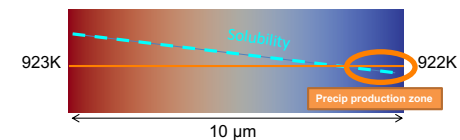
4. FCCI Observations: Lanthanide transport through Sodium

- More LA on clad adjacent to crack
- Cerium has low solubility in sodium
- Forms "sludge" (i.e. forms too quick to crystallize) [Mariani 419 JNM (2011)]
- Rapid transport and solidification



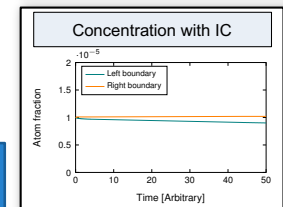
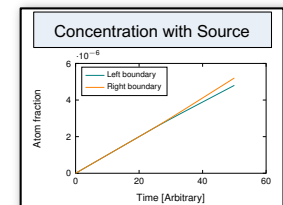
How do lanthanides move then?

- Using simple precipitation model, *interconnected* bubbles act like a pump
 - Result of rapid diffusivity and temperature dependent solubility



Conclusion:
Interconnectivity drives lanthanide migration

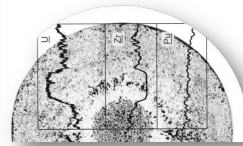
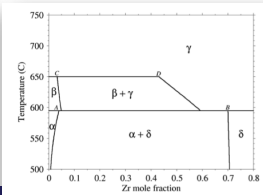
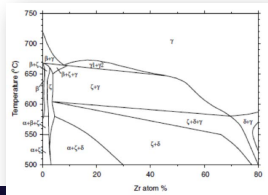
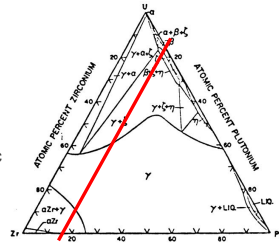
Next step: Capture microstructure
1) Interconnectivity
2) Swelling/cracking



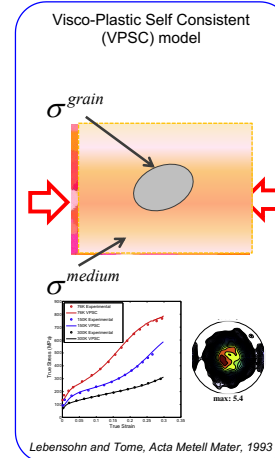
Redistribution Advancements: Model corrections

In BISON
UF collaboration

- Model Evolution:** Historical phase diagram is too simple to capture complex behavior:
 - Zeta phase absent
 - Off-normal plutonium concentrations unavailable
 - Ternary-lever rule incorrect
- Model Revolution:** Zirconium redistribution is really a thermodynamic process:
 - Soret/Fickian diffusion are bulk approximations of the underlying phase stability and behavior
 - Difficult to solve because of *data* and *computational expense*



Reduced order modeling of cladding Laurent Capolugo, LANL



Example: FCC polycrystal with 50 grains (Number of slip systems is 12)

VPSC

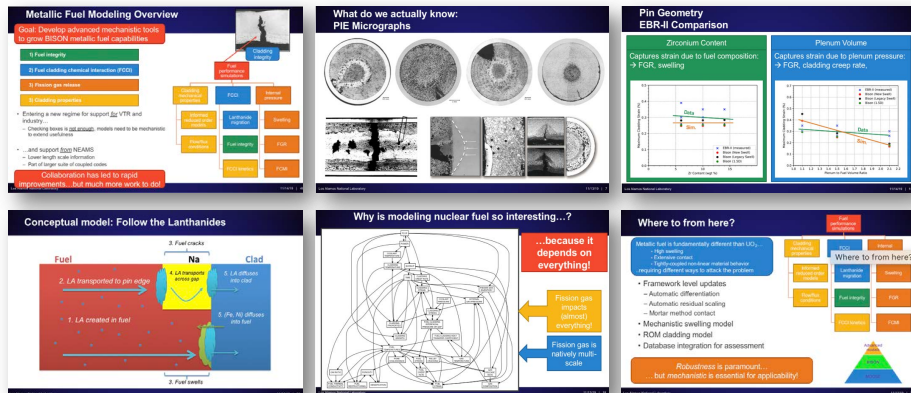
$\rho_{cell}^{s,g}$: 600 DoF
 $\rho_W^{s,g}$: 600 DoF
 ϵ_{medium} : 6 DoF
 σ_{medium} : 6 DoF
 T : 1 DoF

Model Reduction

ROM

$\bar{\rho}_{cell}$: 1 DoF
 $\bar{\rho}_W$: 1 DoF
 ϵ_{vm} : 1 DoF
 σ_{vm} : 1 DoF
 T : 1 DoF

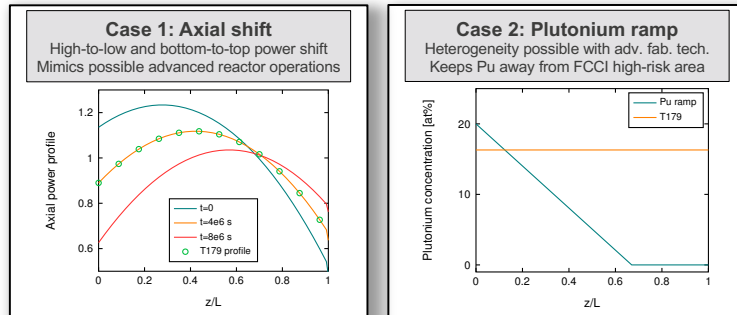
Collaboration has led to rapid improvements...but much more work to do!



Backup slides

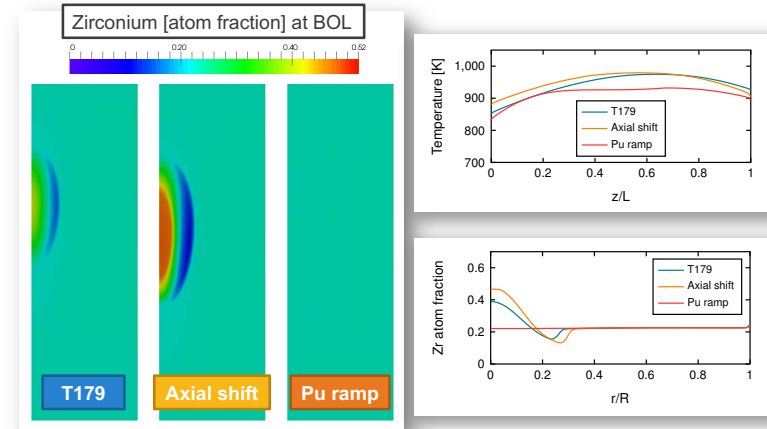
Advanced Simulation Aided Fuel Design

- Use BISON to explore design space
- Broad assumptions still in place
 - Assumes U-Pu-Zr zirconium diffusivities, inadequate historical swelling, etc.

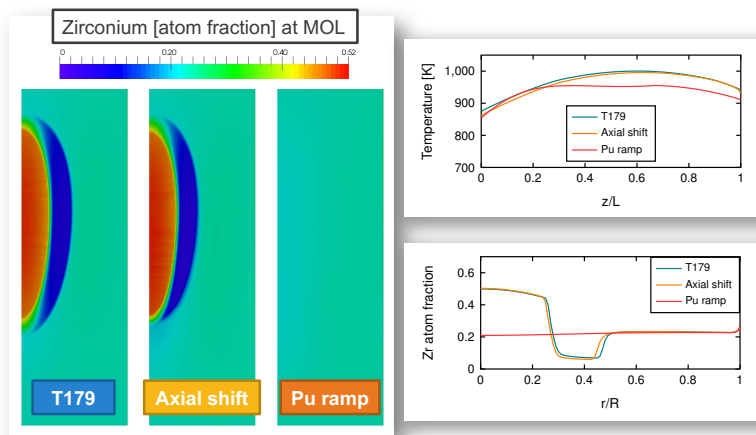


41

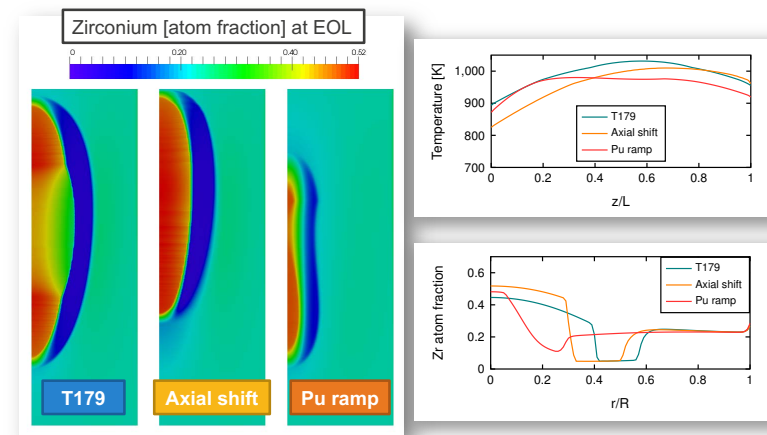
Advanced Simulation Aided Fuel Design



Advanced Simulation Aided Fuel Design

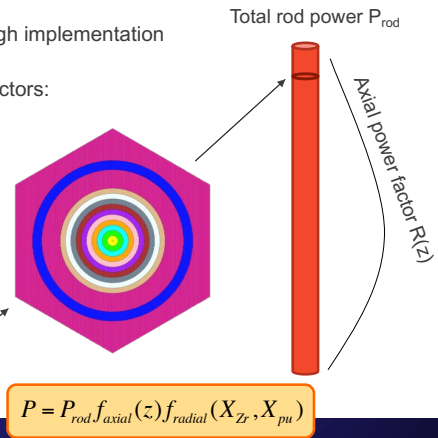
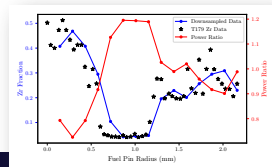


Advanced Simulation Aided Fuel Design



Radial Power Factor

- As zirconium and uranium move, the power profile of the pin will change
- Full coupling may be avoided through implementation of a “radial power factor”
- New power profile due to several factors:
 - Current Zr/Pu concentrations
 - Initial Zr/Pu concentrations
 - Initial U/Pu enrichments
 - Burnup dependence



$$P = P_{rod} f_{axial}(z) f_{radial}(X_{Zr}, X_{Pu})$$

11.4 Overview of Advanced Characterization Techniques

Assel Aitkaliyeva, University of Florida

UF Herbert Wertheim College of Engineering UNIVERSITY of FLORIDA

Manatee RESEARCH GROUP

Overview of the state-of-the-art (advanced characterization) techniques

*Metallic Fuels Meeting
November 15th, 2019
Assel Aitkaliyeva*

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Understanding material behavior

Chem bond Structure Properties Performance

Characterization Processing

ture

This image is in public domain.
Source: Wikimedia Commons, Materials Science Tetrahedron

Courtesy of M. Tonks

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PIE strategy & techniques

Courtesy of L. Capriotti

Scale of Exam Macro <1 μm

TOOLS

Visual Exams Neutron Radiography Dimensional Exams Gamma Spectrometry Fission Gas Release Optical Microscopy Chemistry Analysis Electron Microscopy SEM, TEM, EPMA Focused Ion Beam Atom Probe

Fuel Performance

Did it Fail Catastrophically How much did the geometry change Fission Product Migration Microstructure, Restructuring, FCCI Burnup, Actinide Balance Elemental distribution 3D microstructure Beyond Baseline

Number of Samples

A few pins The historic approach Section pins Select samples to EM FIB Sample Preparation

Baseline

100 μm

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Optical

2000 μm

FCCI

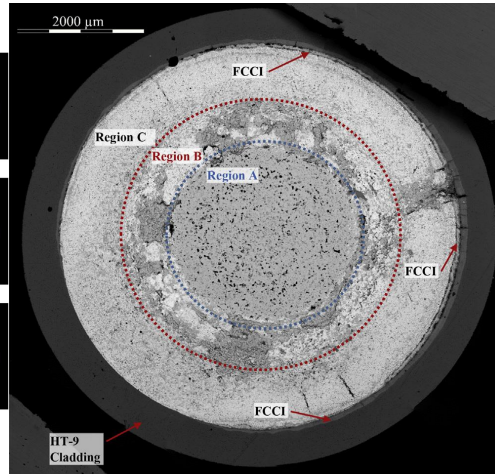
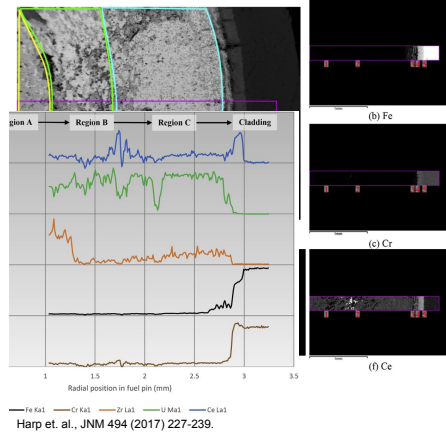
Region C Region B Region A

HT-9 Cladding

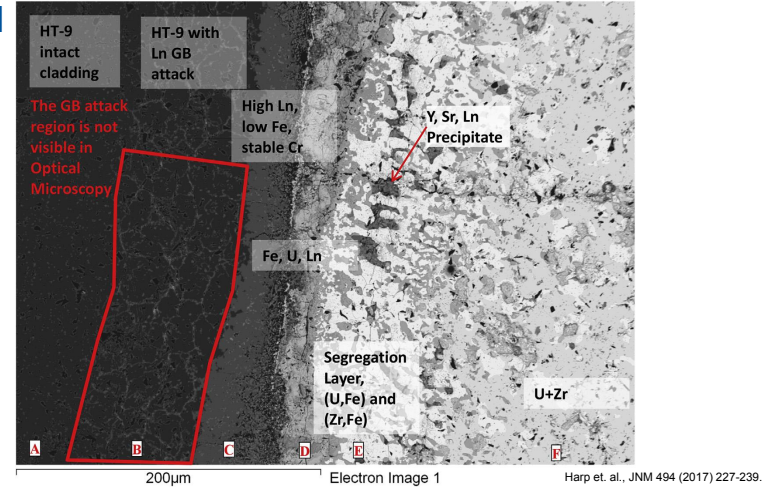
100 μm

Carmack et al., JNM 473 (2016) 167-177.
Harp et al., JNM 494 (2017) 227-239.

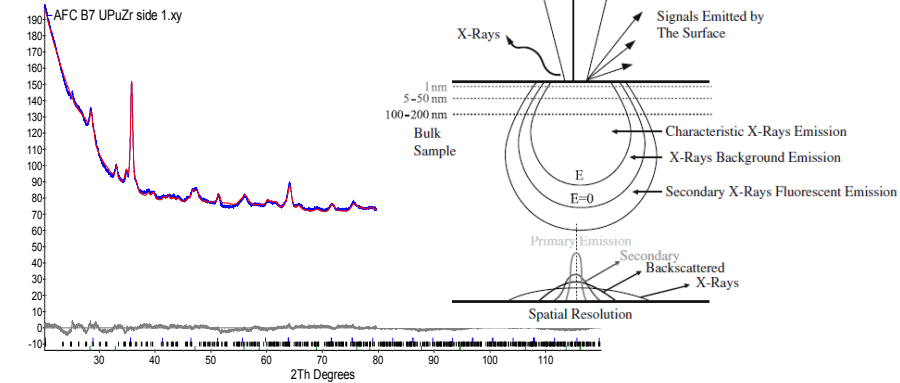
SEM



SEM

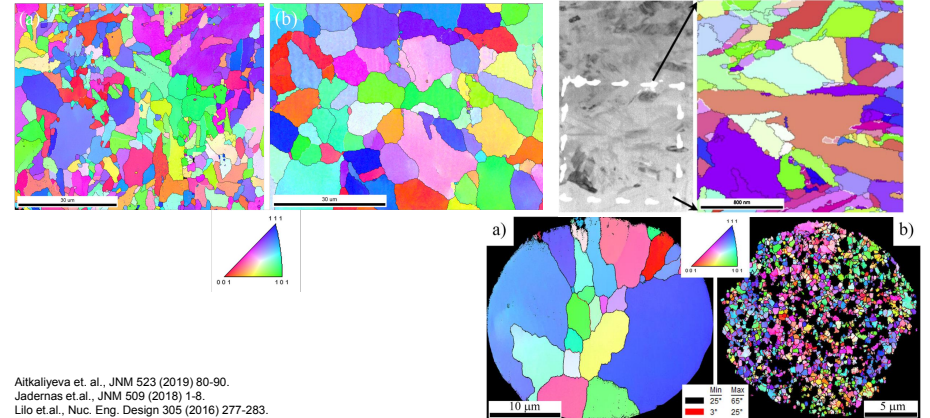


XRD



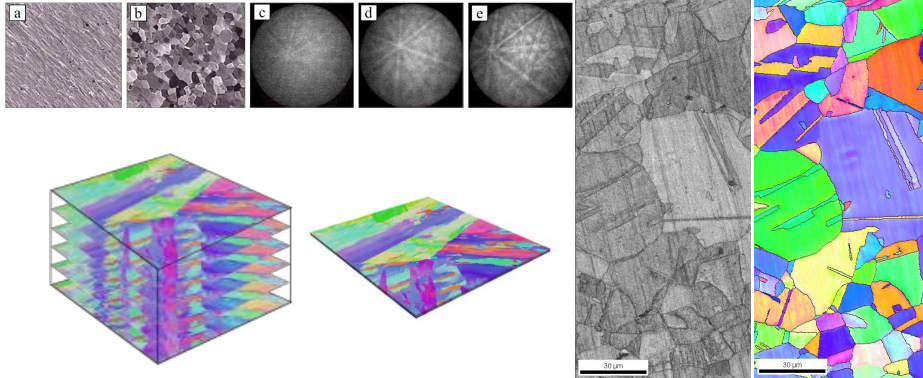
AFC report
Wright et al., JNM 526 (2019) 151745.

EBSD



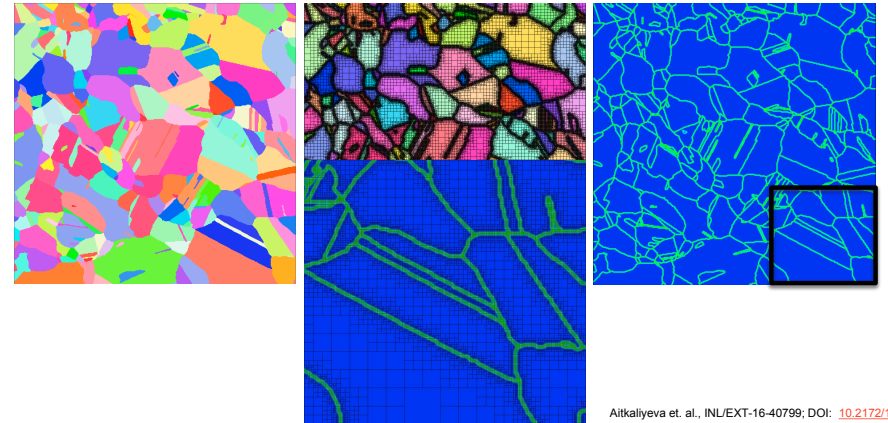
Aitkaliyeva et al., JNM 523 (2019) 80-90.
Jadernas et al., JNM 509 (2018) 1-8.
Lilo et al., Nuc. Eng. Design 305 (2016) 277-283.

EBSD tomography



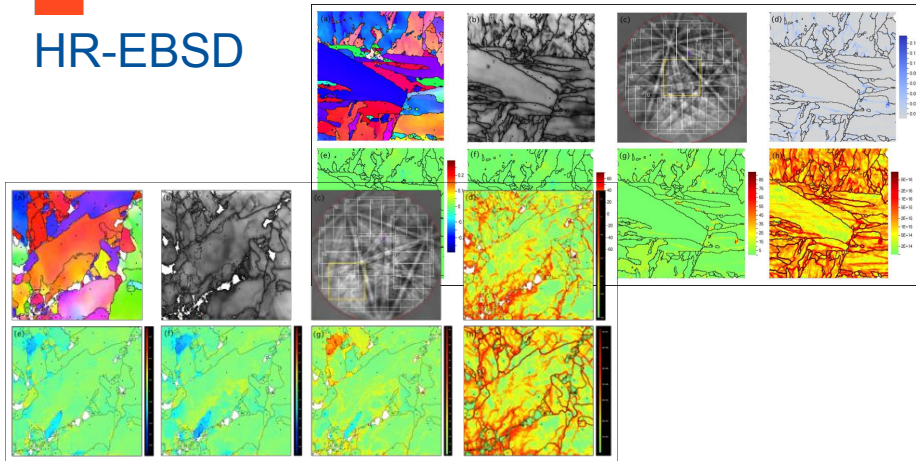
Aitkaliyeva et. al., INL/EXT-16-40799; DOI: [10.2172/1369528](https://doi.org/10.2172/1369528)

Integrating experimental data into MARMOT



Aitkaliyeva et. al., INL/EXT-16-40799; DOI: [10.2172/1369528](https://doi.org/10.2172/1369528)

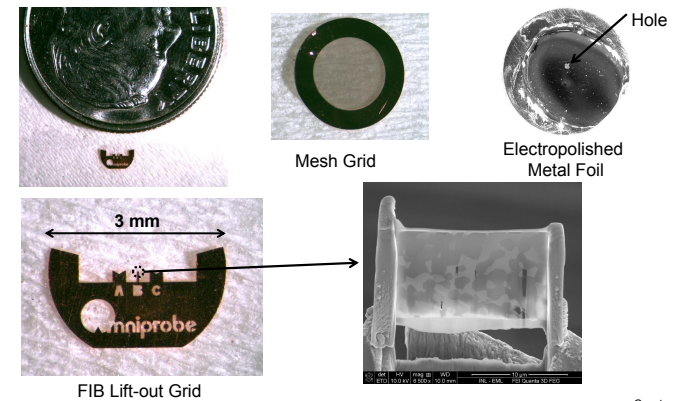
HR-EBSD



Aitkaliyeva et. al., INL/EXT-16-40799; DOI: [10.2172/1369528](https://doi.org/10.2172/1369528)

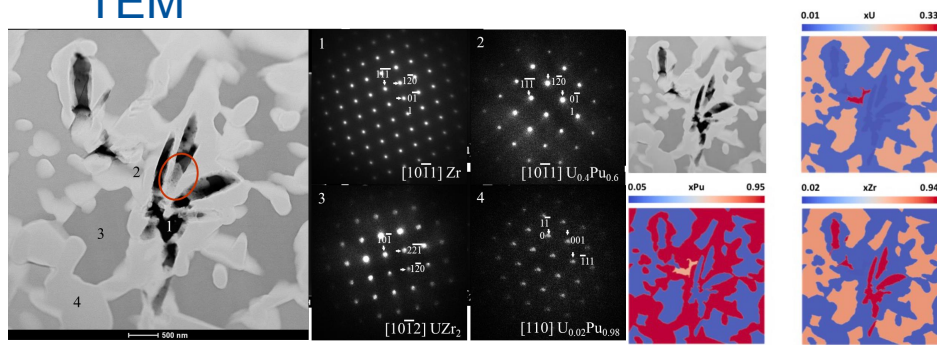
11

TEM Sample Types

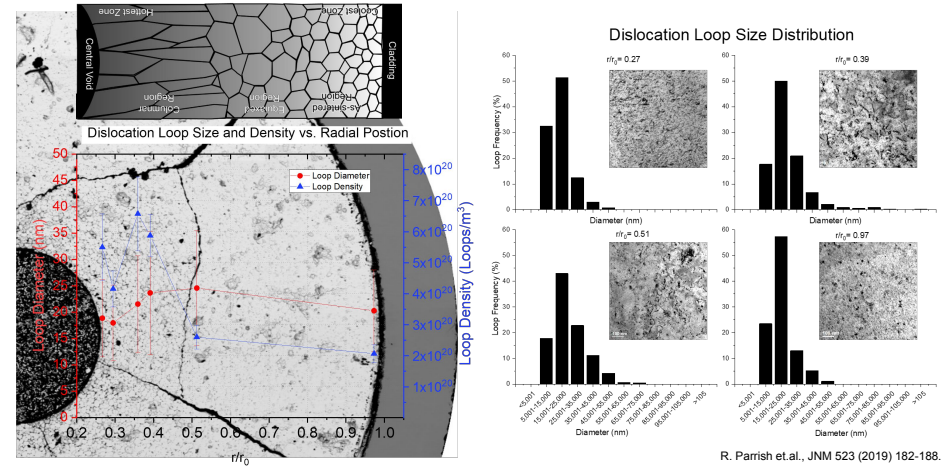


Courtesy of J. Cole and J. Gan

TEM

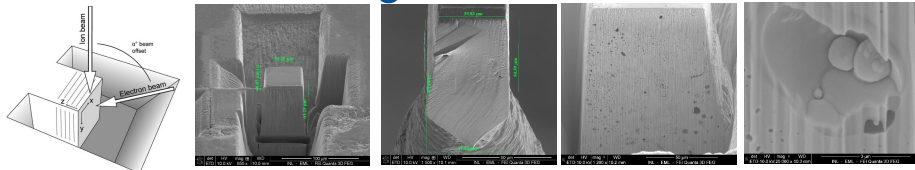


Aitkaliyeva et al., JNM 473 (2016) 75-82.
J. Hirschhorn et al., Annals of Nucl. Energy 518 (2019) 80-94.



R. Parrish et al., JNM 523 (2019) 182-188.

Other advantages of FIB



SE micrographs

Precipitates

IQ maps

Pores

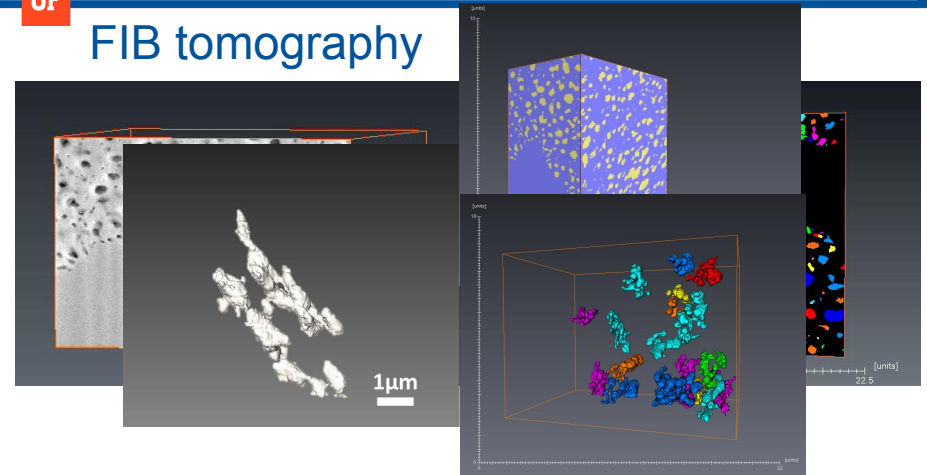
IPF maps

Grains

3D
microstructure

Aitkaliyeva, unpublished

FIB tomography



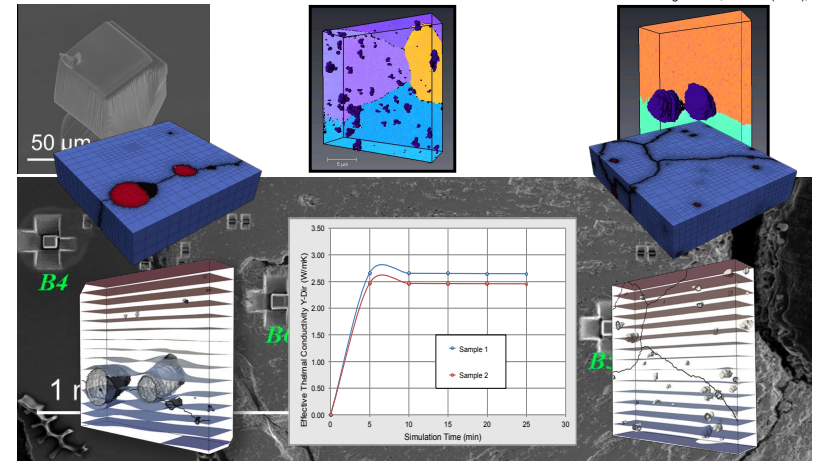
B.D. Miller, et al., J. Nucl. Mater. 510, 431 (2018)

FIB tomography - EBSD

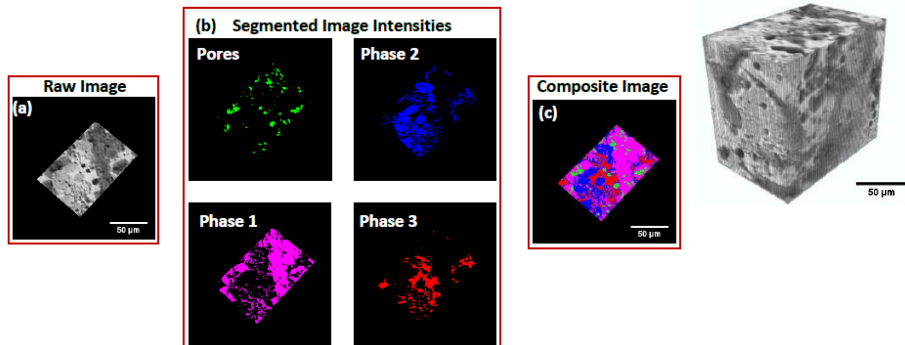


McKinney, under preparation

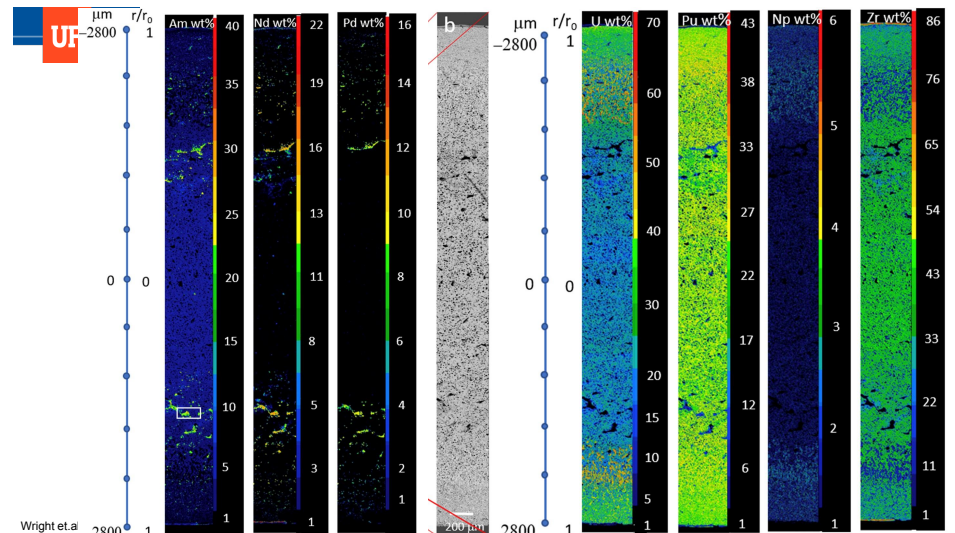
Aitkaliyeva, unpublished
Teague et al., JOM 66 (2014), 2569-2577



Tomography

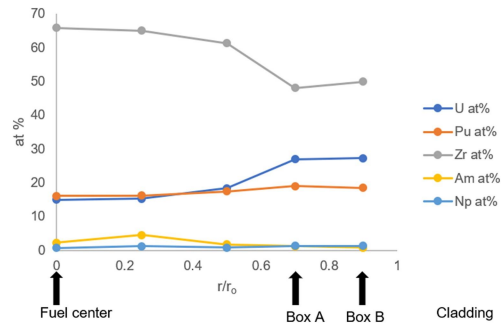


Okuniewski et al.

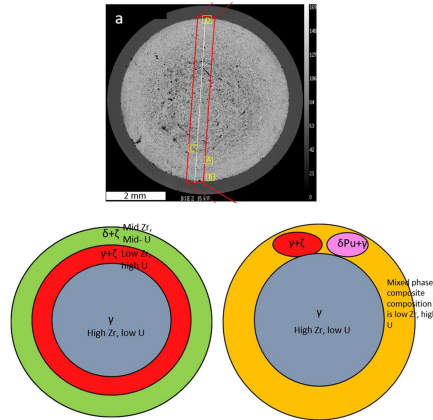


Wright et al.

EPMA

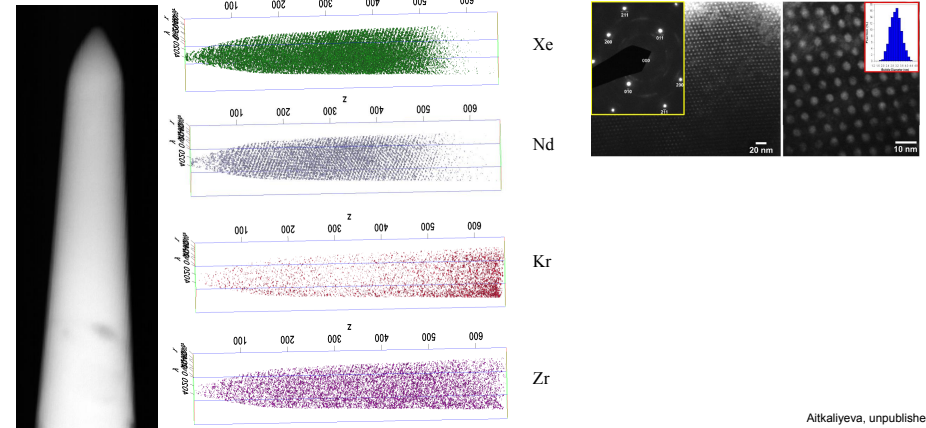


Cladding



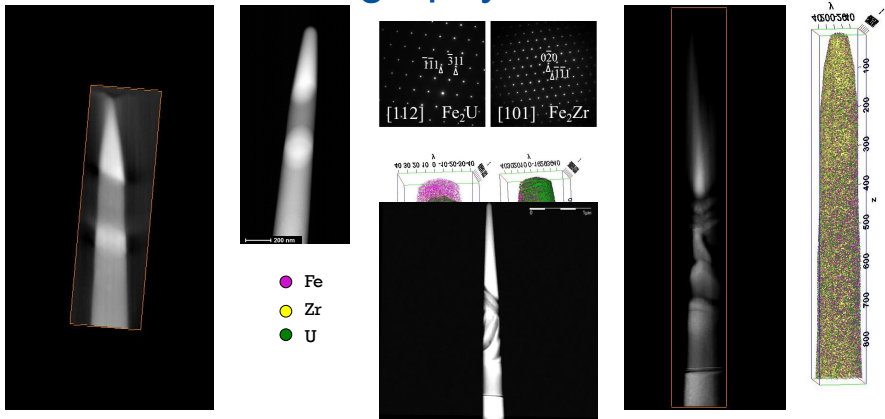
Wright et al., JNM 526 (2019) 151745.

Atom probe tomography



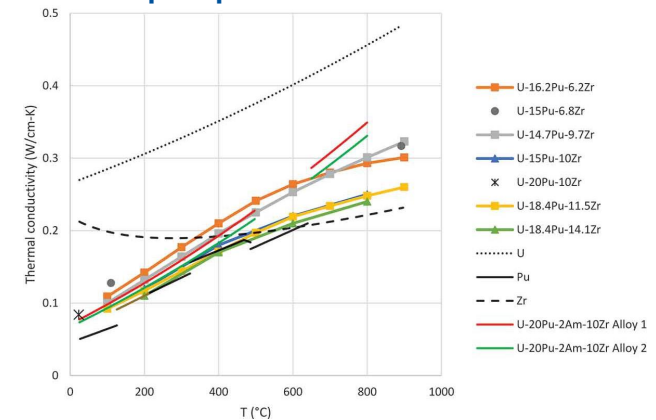
Aitkaliyeva, unpublished

Electron tomography

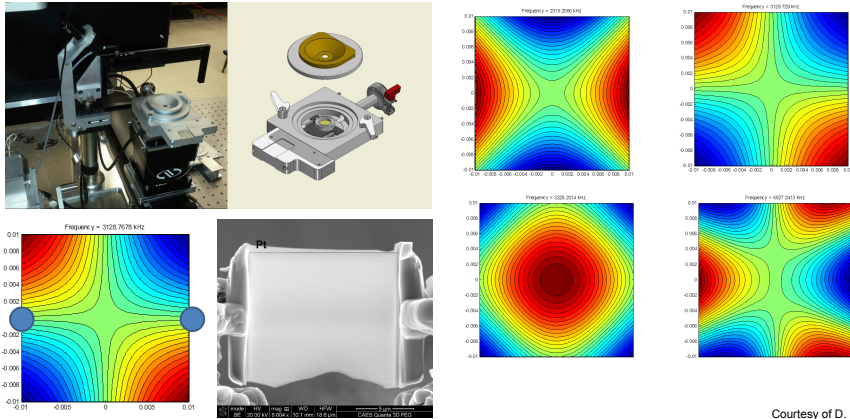


Aitkaliyeva, unpublished

Thermal properties

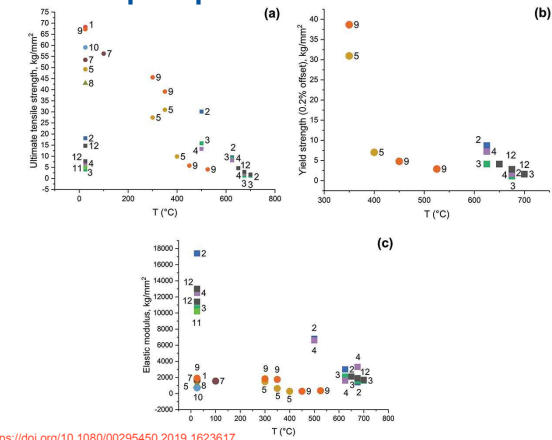
Janney et al., Nuclear Technol. 2019 <https://doi.org/10.1080/00295450.2019.1623617>

TCM

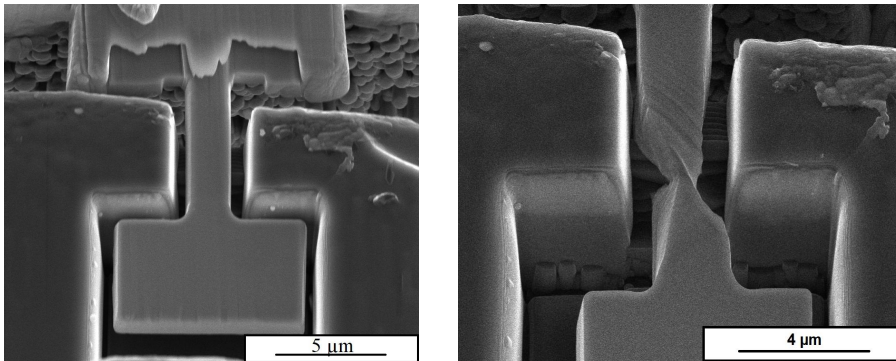
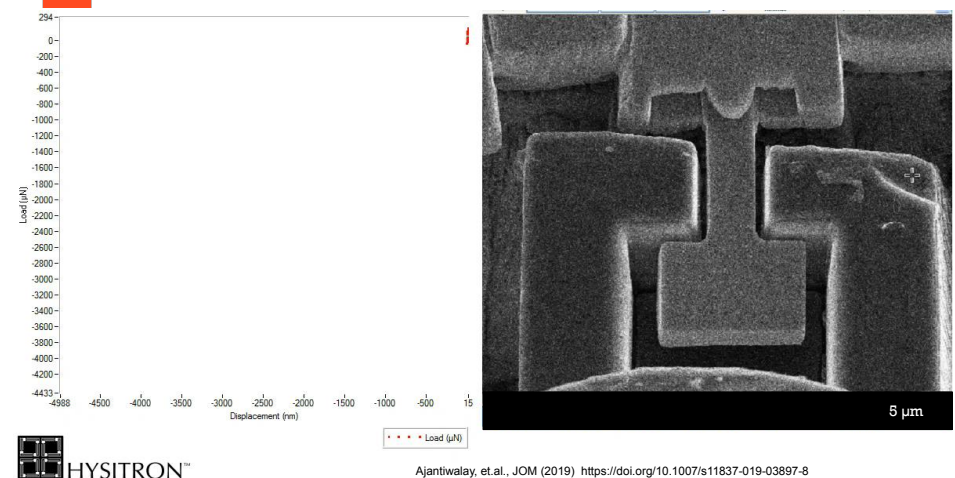


Courtesy of D. Hurley

Mechanical properties

Janney et al., Nuclear Technol. 2019 <https://doi.org/10.1080/00295450.2019.1623617>

In-situ tensile tests

Ajantiwalay, et al., JOM (2019) <https://doi.org/10.1007/s11837-019-03897-8>


HYSITRON™

Ajantiwalay, et al., JOM (2019) <https://doi.org/10.1007/s11837-019-03897-8>

11.5 Lower Length-Scale Simulation of U-Zr and U-Pu-Zr Fuels

Michael Tonks, University of Florida


Jacob Hirschhorn, University of Florida


Herbert Wertheim College of Engineering
 UNIVERSITY of FLORIDA

Lower Length-Scale Modeling and Simulation of U-Zr and U-Pu-Zr Fuels

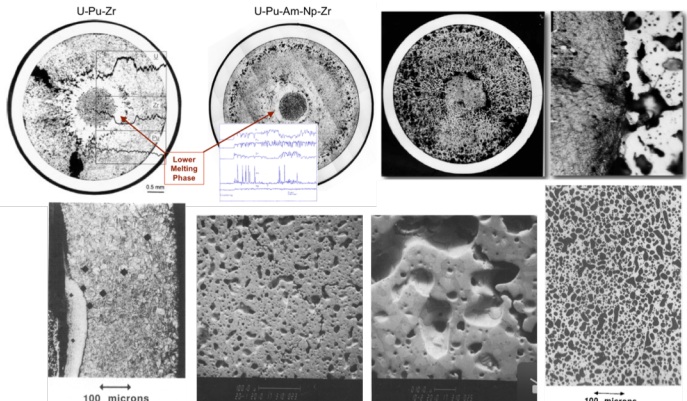
Michael Tonks, Jacob Hirschhorn
Department of Materials Science and Engineering

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Herbert Wertheim College of Engineering
 DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

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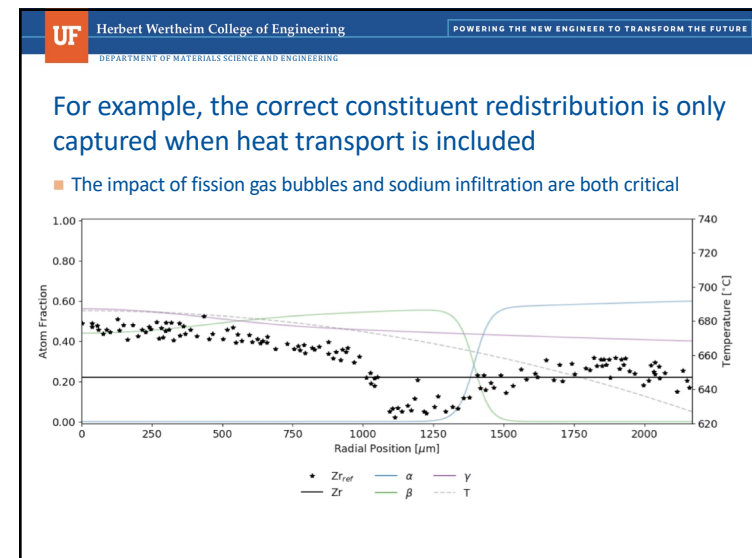
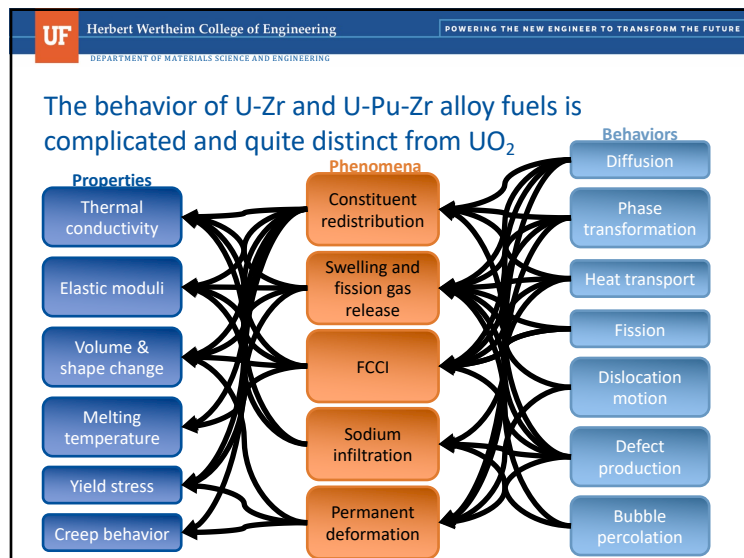
The development and optimization of U-Zr and U-Pu-Zr fuels will require a mechanistic understanding of the fuel

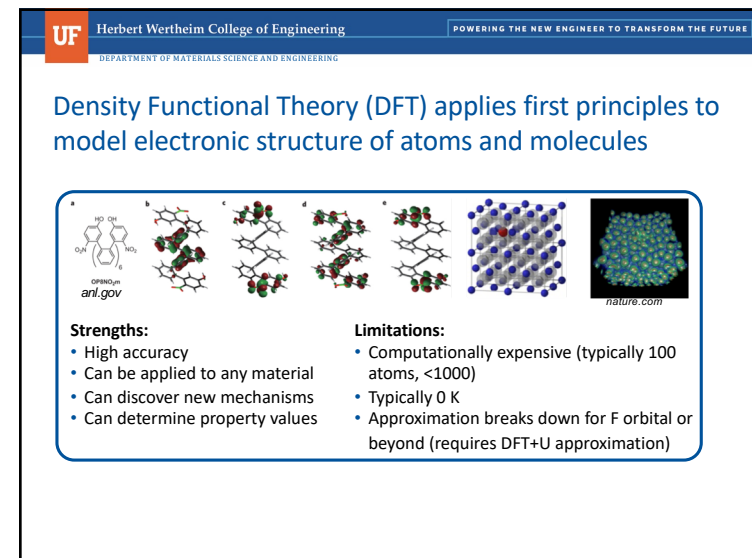
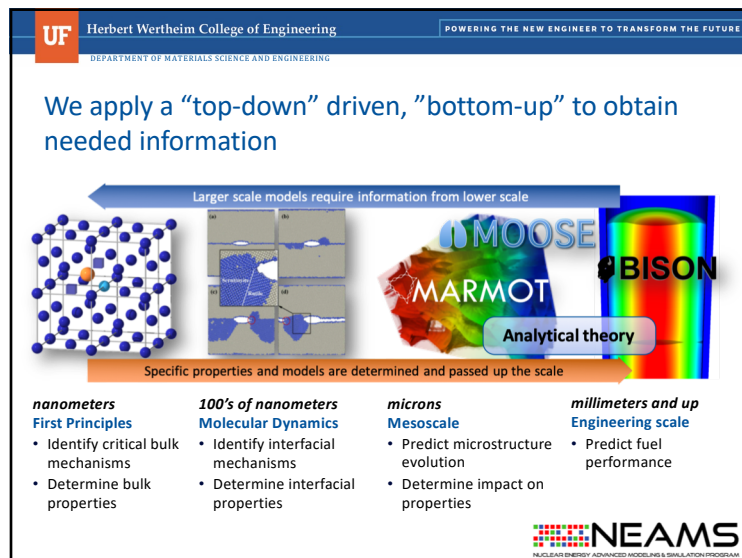
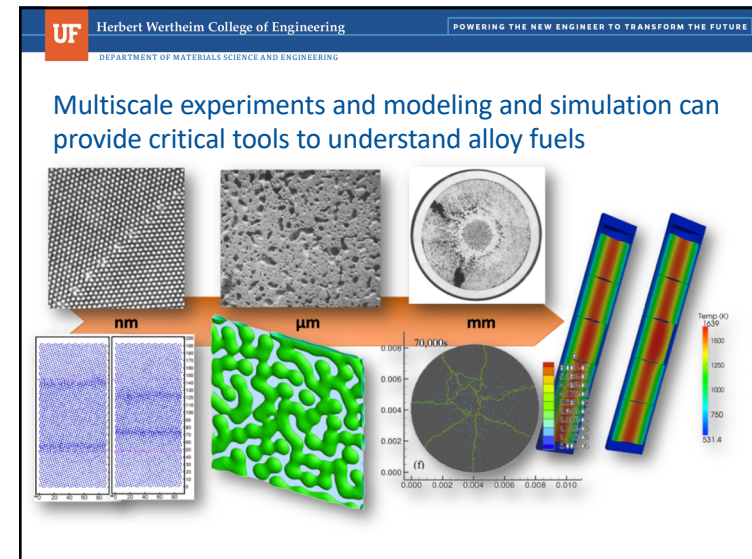
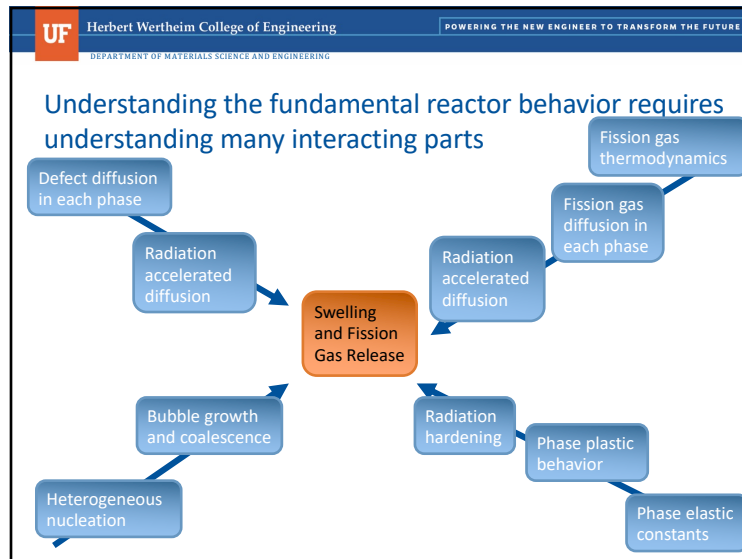


U-Pu-Zr U-Pu-Am-Np-Zr

Lower Melting Phase

100 microns





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DFT and *ab initio* molecular dynamics (AIMD) has been used to investigate various behaviors of uranium

- DFT has a low temperature mechanical instability in γ -U that can be overcome with AIMD
- Compared the cohesive energies and volumes of α - and γ -U
 - DFT: S. K. Xiang, et al., *J. Nucl. Mater.* 375 (2008) 113
- Point defects (self defects, Zr, fission gas) were investigated
 - DFT: B. Beeler, et al., *J. Phys.: Condens. Matter* 22 (2010) 505703
 - DFT: B. Beeler, et al., *J. Nucl. Mater.* 425 (2012) 2.
 - DFT: G.-Y. Huang, B. Wirth, *J. Phys.: Cond. Mat.* 23 (2011) 205402.
 - DFT: G.-Y. Huang, B. Wirth, *J. Phys.: Cond. Mat.* 24 (2012) 415404.
 - AIMD: B. Beeler, D. Andersson, C. Jiang, Y. Zhang (2019) SUBMITTED to *J. Nucl. Mater.*
- Properties of β -U were investigated
 - DFT: B. Beeler, et al., *J. Nucl. Mater.* 433 (2013) 143.
 - DFT: J.H. Li, et al., *J. Alloys Compd.* 516 (2012) 139.
- Equation of state
 - AIMD: R. Hood, L. Yang, J. Moriarty, *Phys. Rev. B* 78 (2008) 024116.

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DFT has also been applied to investigate behaviors of plutonium

- Modeling Pu with DFT is complicated by the delocalized nature of its f electrons
- Phonon dispersion
 - Wong, J. et al. *Science* 301, 1078 (2003)
 - Dai, X., et al., *Science* 300, 953 (2003).
- Elastic constants
 - Söderlind et al., *Phys. Rev. B* 70, 144103 (2004).
- Electronic structure
 - Liu et al., *Physica B* 405, 3717 (2010). 23. Li, T.-S., He, B., Li, G.,
 - Xu et al., *Acta Phys. -Chim. Sin.* 5, 75 (2015).

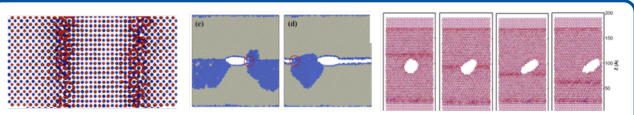
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DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING

DFT has not been applied to the alloys very much, primarily due to the γ -U instability

- This could be overcome with AIMD or lattice dynamics methods, but it hasn't happened yet
- Ground state properties of U-Pu and Pu-Zr solid solution systems
 - A. Landa, et al., *J. of Nucl. Mater.* 393 (2009) 141
- Structural, electronic, and elastic properties of equiatomic U-Zr alloys
 - Zhang, C-B, et al. *J. of Nucl. Mater.* 496 (2017): 333-342.

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Molecular dynamics (MD) simulates atoms by solving Newton's equations based on a potential function



Strengths:

- Much more computationally efficient than DFT
- Regularly used to model millions of atoms at finite temperatures and across time

Limitations:

- Small time scales (nanoseconds)
- Small length scales (<400 nm)
- A unique potential function must be developed for each material
- Potentials are never perfect
- Hard to model complex systems

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There are several potentials for available for relevant to U-Zr and U-Pu-Zr fuels

- Pure uranium potentials
 - EAM - D. Smirnova, et al., *Phys. Metals and Metall.* 113 (2012) 107
 - EAM - M. Pascuet, et al., *J. Nucl. Mater.* 424 (2012) 158
 - MEAM - B. Beeler, et al., *J. Phys.: Condes. Matter* 24 (2012) 075401
 - ADP - D. Smirnova, et al., *Phys. of Metals and Metall.* 116 (2015) 445
 - COMB - Y. Li, et al. *Journal of Physics: Condensed Matter* 24.23 (2012): 235403.
- Uranium-zirconium potential
 - A. Moore, et al., *J. of Nucl. Mater.* 467 (2015) 802
- Uranium-xenon potential
 - B. Beeler, et al., *ASTM STP 1547: Effects of Radiation on Nuclear Materials*, 25th Volume (2012) 231

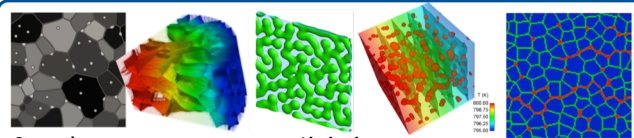
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These potentials have been used to look at many different phenomena

- Vibrational density of states
 - Fidanyan, K. S., and V. V. Stegailov. *J. Physics: Conference Series*. Vol. 774. No. 1. IOP Publishing, 2016.
- Lattice expansion
 - Y. Li, et al., *J. of Nuclear Materials* 475 (2016) 6
- Point defect formation and migration
 - D. Smirnova, A. Kuksin, S. Starikov, *J. of Nuclear Materials* 458 (2015) 304
 - Antropov, A. S., et al. *J. Physics: Conference Series*. Vol. 1133. No. 1. 2018.
- Displacement energies
 - B. Beeler, et al., *J. of Nuclear Materials* 508 (2018) 181
 - Chen, E.Y., et al., *Computational Materials Science* 157 (2019): 75-86.
- Cascade behavior
 - Y. Miao, et al., *J. of Nuclear Materials* 456 (2015) 1
 - Zhou, Ning, et al., *J. of Nuclear Materials* 526 (2019): 151769.
- Phase microstructure
 - Moore, A. P., et al. *Acta Materialia* 115 (2016): 178-188.
- Misfit Dislocations
 - Chen, E.Y., et al. *Computational Materials Science* 154 (2018): 194-203.

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The phase field method predicts microstructure evolution by evolving continuous variables to minimize free energy



Strengths:

- Predicts microstructure evolution without numerical issues
- Easily couples to other physics
- Quantitative and material specific

Limitations:

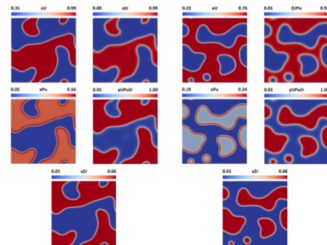
- All interfaces are diffuse (finite width)
- A free energy must be developed for each new system
- Mechanisms must be built into the model

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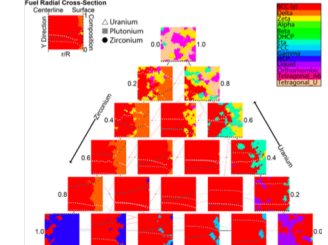
The phase field method has been applied to model constituent redistribution and phase transformation

- Cox, Jordan J., et al. *Metallurgical and Materials Transactions A* 49.12 (2018): 6457-6468.
- Hirschhorn, Jacob, et al. *Annals of Nuclear Energy* 124 (2019): 490-502.
- Hirschhorn, Jacob, et al. *Journal of Nuclear Materials* (2019).

Hirschhorn, Jacob, et al.

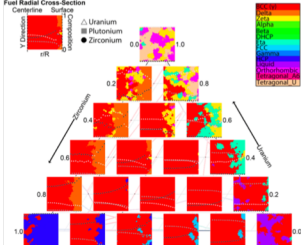


(a) Decomposition of 50:50Pu-50Zr at 900°C.



(b) Decomposition of 50:50Pu-50Zr at 800°C.

Cox, Jordan J., et al.

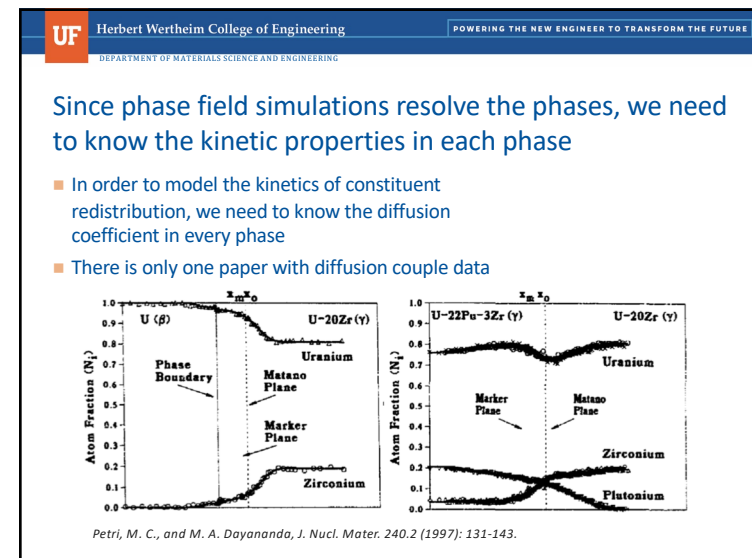
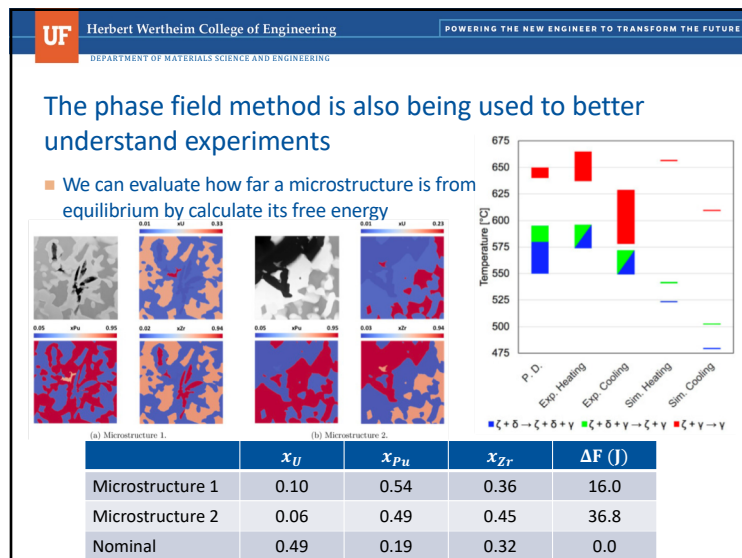
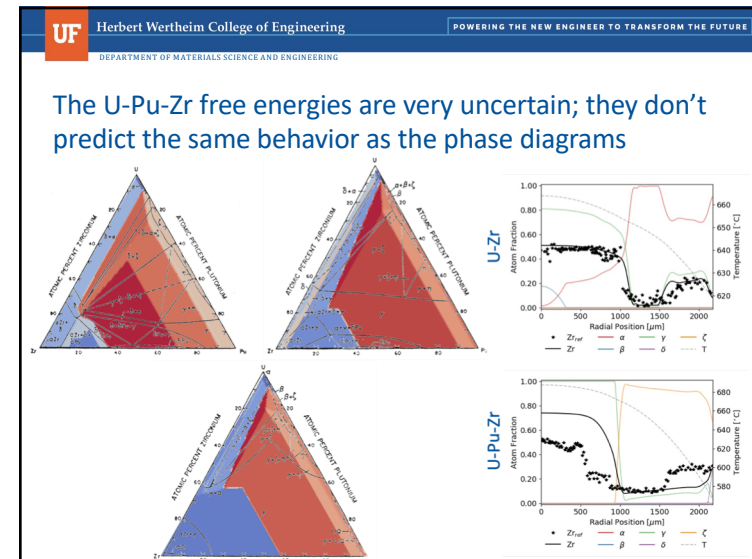


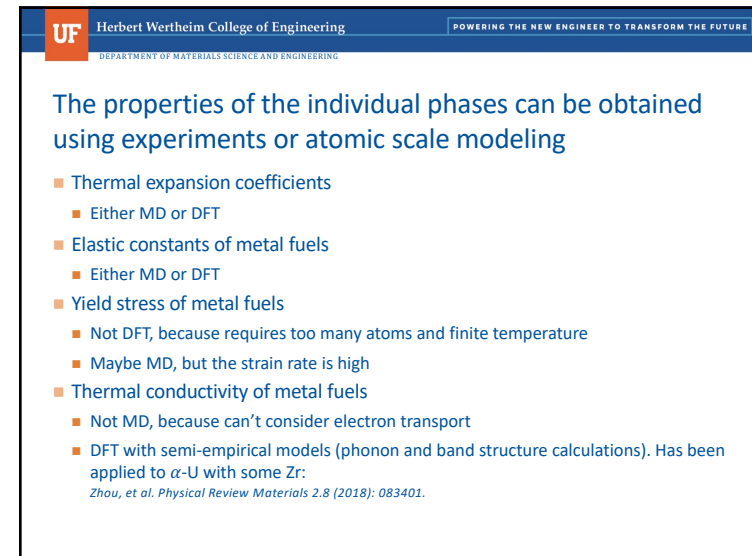
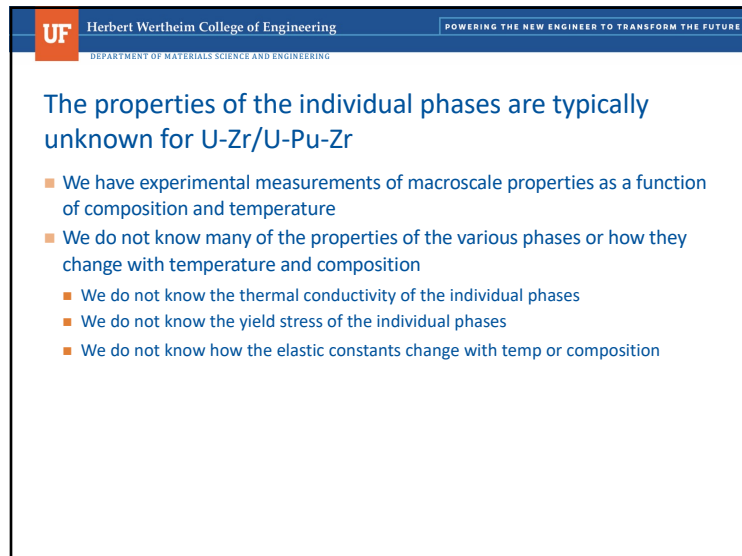
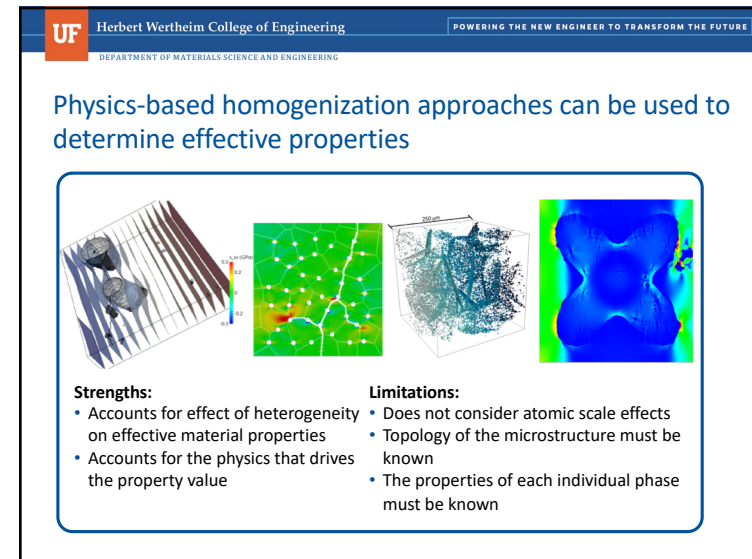
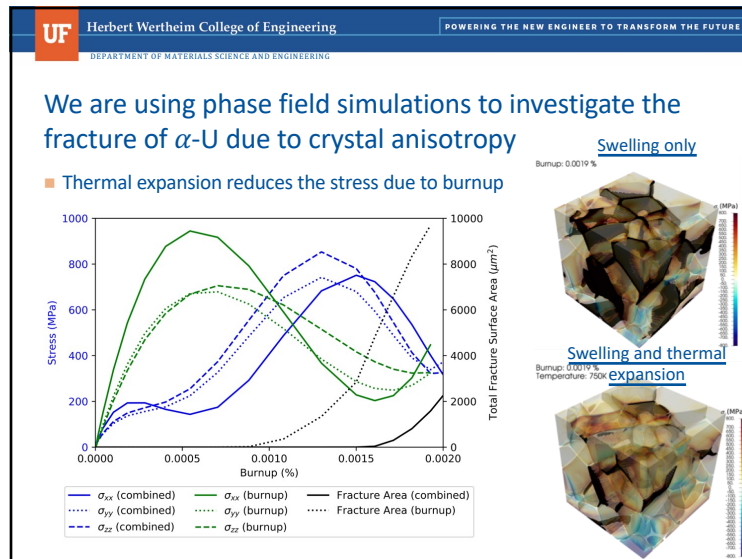
Phase diagram showing the decomposition of 50:50Pu-50Zr at 900°C.

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There have been various thermodynamic assessments using experimental and DFT data

- Uranium-Zirconium**
 - Leibowitz, et al. *J. Nuclear Materials* 167 (1989): 76-81.
 - Masaki, et al. *J. alloys and compounds* 271 (1998): 636-640.
 - Chevalier, et al. *Calphad* 28.1 (2004): 15-40.
 - W Xiong, et al. *J. Nucl. Mater.* 443.1-3 (2013): 331-341.
- Uranium-Plutonium-Zirconium**
 - Kurata, *Calphad* 23.3-4 (1999): 305-337.
 - Agarwal, R., and V. Venugopal. No. BARC--2004/E/009. Bhabha Atomic Research Centre, 2004.
 - Perron, A., et al. *J. Nuclear Materials* 454.1-3 (2014): 81-95.
 - Perron, A., et al. *J. Nuclear Materials* 458 (2015): 425-441.

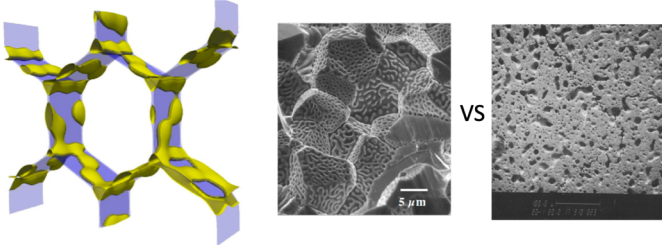




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The phase field method has been widely used for fission gas behavior, but we need more info for U-Zr/U-Pu-Zr



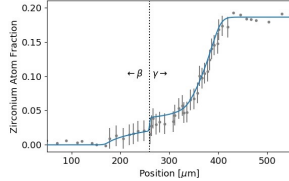
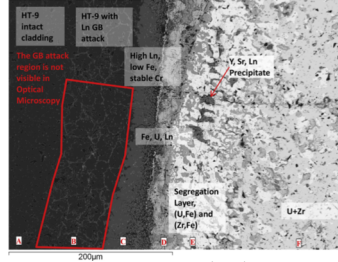
- The fission gas behavior is very different than in UO_2
 - We need to know the fission gas diffusion rates in each phase
 - We also need to know the impact of phase interfaces on the gas behavior
 - Plasticity or creep could also impact the behavior

Aagesen et al. *Computational Materials Science* 161 (2019): 35-45.

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Fuel cladding chemical interaction (FCCI) could be modeled with phase field, but more information is needed

- For both Lanthanide transport into cladding and Fe into fuel requires
 - Free energy of the system
 - Interfacial properties
 - Kinetic parameters

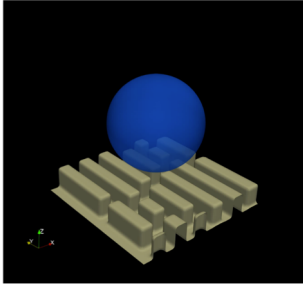
Xu et al. *Acta Phys. -Chim. Sin.* 5, 75 (2015).

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Sodium infiltration has a large impact on the thermal conductivity of the material

- Modeling sodium infiltration will depend on various other behaviors
 - Fission gas bubble interconnection
 - Fuel-liquid sodium interfacial energy

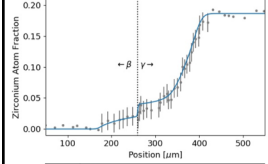
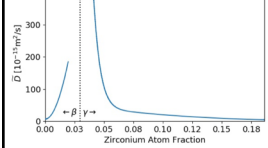


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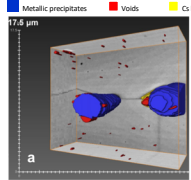
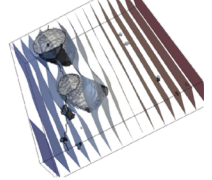
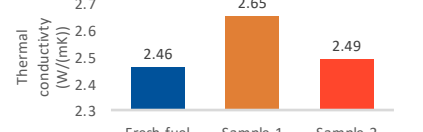
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Simulations can be used to interpret experiments, extracting parameters by calibrating the model to data

We fit diffusion coefficients to the data using the phase field method

Calculated thermal conductivities of reconstructed MOX microstructures showed the importance of defects below the resolution of the EBSD

Sample	Thermal conductivity (W/(mK))
Fresh fuel	2.46
Sample 1	2.65
Sample 2	2.49

— Current Work + Experiment

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Atomistic and mesoscale modeling and simulation can play a major role in gaining further understanding of this fuel type

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The behavior of U-Zr and U-Pu-Zr alloy fuels is complex and quite distinct from UO₂.

Atomistic

- Thermal expansion
- Thermal conductivity
- Thermal stability
- Thermal expansion
- Thermal conductivity
- Thermal stability
- Thermal expansion
- Thermal conductivity
- Thermal stability

Mesoscale

- Thermal expansion
- Thermal conductivity
- Thermal stability
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- Thermal stability

Macroscale

- Thermal expansion
- Thermal conductivity
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Atomistic and mesoscale simulations inform the development of analytical materials models

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Mesoscale

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Density Functional Theory (DFT) applies first principles to model electronic structure of atoms and molecules

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Mesoscale

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Molecular dynamics (MD) simulates atoms by solving Newton's equations based on a potential function

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The phase field method models microstructure evolution in domains from 100 nm to 100 microns

Atomistic

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Mesoscale

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Physics-based homogenization approaches can be used to determine effective properties

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