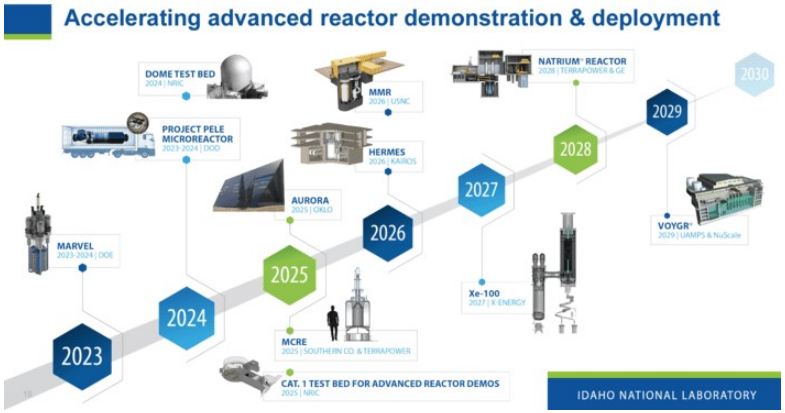
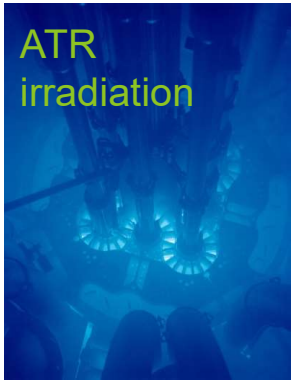
Materials & Fuels
Complex Advanced Data
Analytics (MFC ADA)

A Post Irradiation Examination Data Ecosystem for US Nuclear Energy

Idaho National Laboratory

Challenges and Opportunity for INL to support US Nuclear Industry











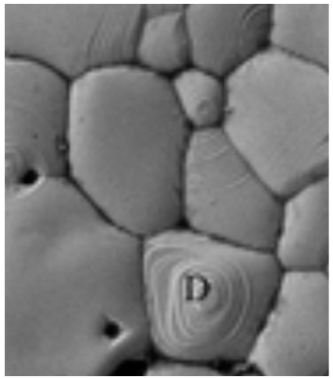
INL approach to PIE



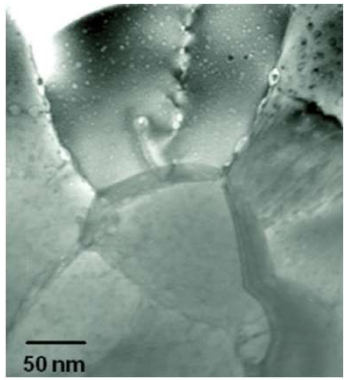
Fuel assembly 3 m



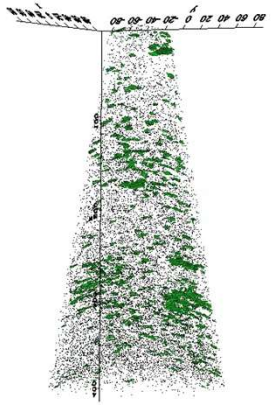
Fuel pellet
1 cm (10^{-2})



UO_2 grain 10 µm (10^{-5})ç



UO_2 grain boundary
2 nm (10^{-9})



Individual atoms 3 Å (10^{-10})

PIE capabilities span 10 orders of magnitude

INL multiscale approach PIE to support US NE mission

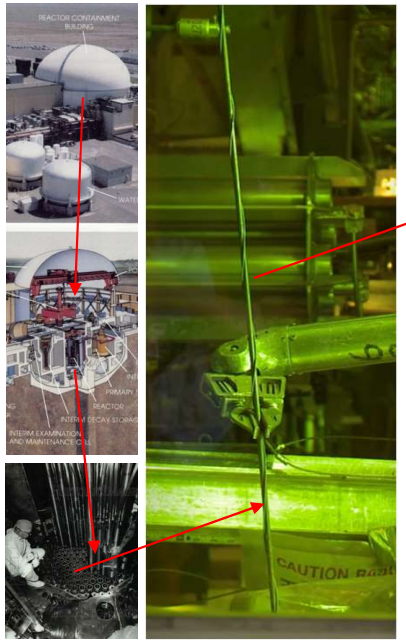
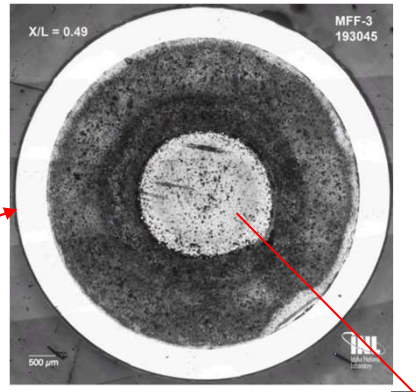
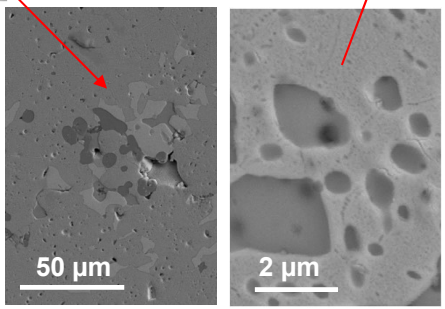


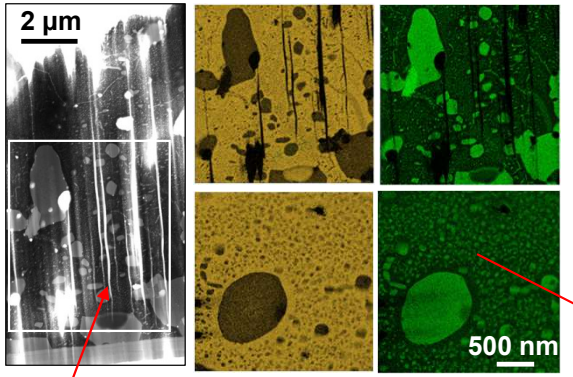
Photo observation of U-10Zr fuel pins irradiated in Fast Flux Test Facility (~1 m)



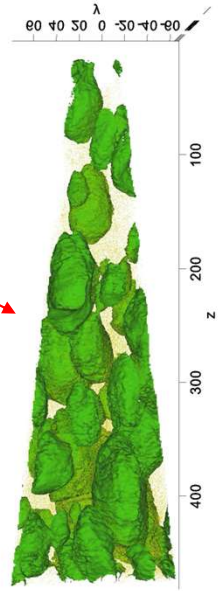
Optical microscopic examination (U-10Zr fuel) (1mm, 10^{-3} m)



Scanning electron microscopy characterization of U-10Zr grain and precipitate (1 µm, 10^{-6} m)



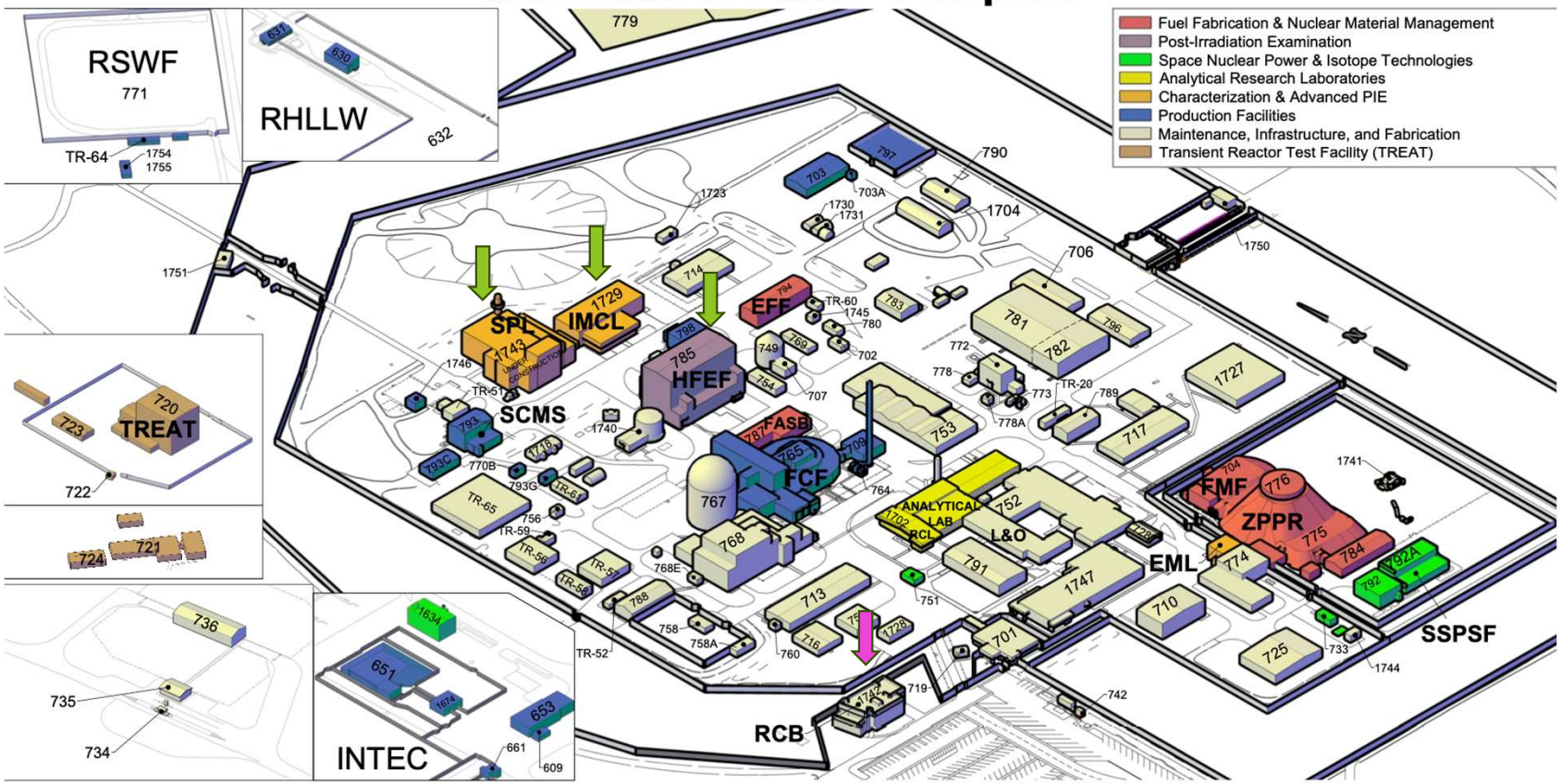
Transmission electron microscopy identification of Zr nano precipitate (2-5 nm, 10^{-9} m)



Atom probe tomography study of Zr atom distribution in 3D (3 Å, 10^{-10} m)

PIE capabilities span 10 orders of magnitude

Materials & Fuels Complex

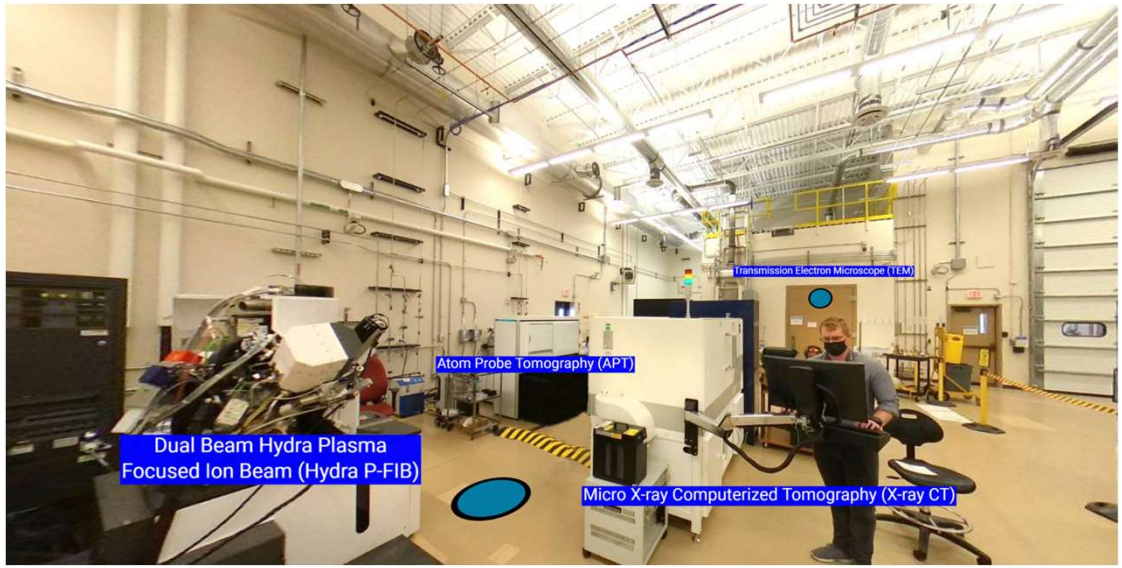


IMCL PIE capability

KEY CAPABILITIES/INSTRUMENTS:

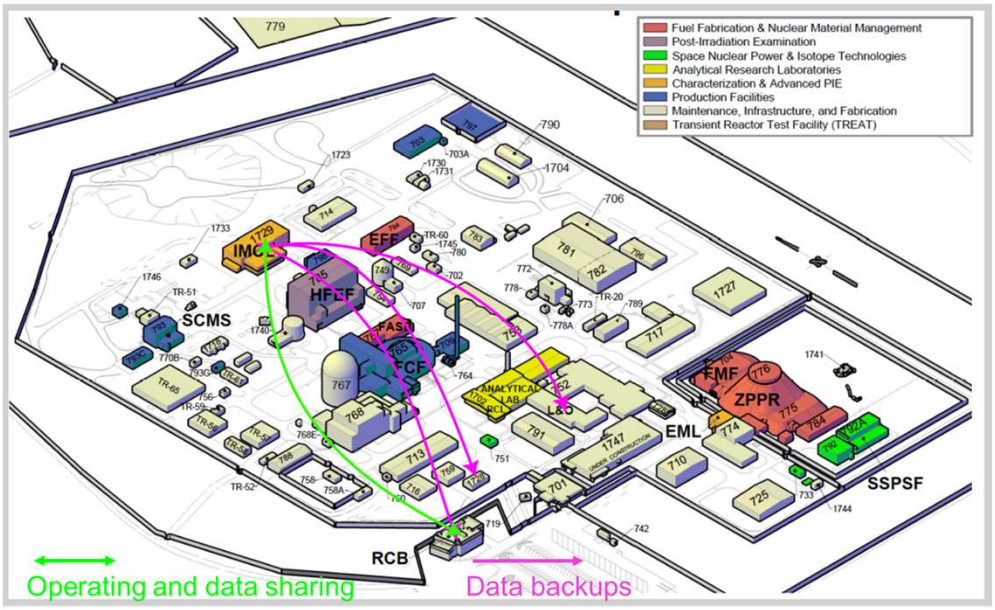
Application	Instrument	Capabilities	Configuration
Sample Preparation	SSPA - Shielded sample preparation area	Optical microscope, polishing and grinding, sample cutting in hot cell, glovebox, and hood	Shielded
Advanced Microscopy, Microchemistry, Micromechanical Testing	SEM - JEOL 7600	High-resolution scanning electron microscope (SEM) equipped with electron back-scatter diffraction, energy dispersive X-ray spectroscopy (EDS) and wavelength dispersive spectroscopy (WDS) detectors	Benchtop
	EPMA - Shielded Cameca SX100R	Quantitative compositional analysis of solid specimens on a micrometer spatial scale. Detectors and electronics are shielded to 3 Ci of 137 Cs to allow for trace element detection. Measures elements from B to Cm.	Shielded
	STEM - FEI Titan Scanning Transmission Electron Microscope	Equipped with probe corrector, super-X EDS, electron energy loss spectroscopy (EELS), DENSolutions D6 heating holder (1573 K), tomography holders, vacuum transfer holder, Hysitron PI-95 PicoIndenter	Benchtop
	APT - LEAP 5000 Atom Probe	3D imaging and chemical analysis at sub-nanometer scale	Benchtop
	FIB - FEI Quanta 3D FEG Focus Ion Beam	Preparation of minute samples for TEM, APT, and micromechanical testing	Shielded
	FIB - Thermo G3 Plasma Focus Ion Beam	Preparation of block samples for rapid 3D reconstruction, micromechanical testing, and microscale thermal property testing	Shielded
	FIB - Thermo G4 Helios Hydra Plasma Focus Ion Beam with TOF-SIMS	Equipped with secondary ion mass spectrometer (SIMS), EDS, and electron backscatter diffraction (EBSD) for sample preparation, imaging, microstructural, and chemical analysis	Benchtop





Recent development: IMCL Remote Console and Data Centralization

(2 years 1.6 M)

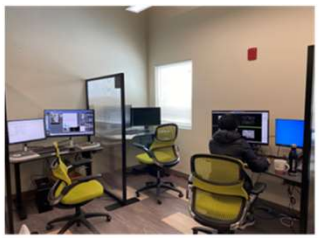


Researchers from RCB remote operating the instruments of IMCL; access and share the data from instruments.

1. Secure nuclear research data and instruments
2. Better protect researchers from contamination risk
3. Effective use of MFC nuclear facilities
4. Rapid recycle of users, visitors, interns, and postdocs
5. More flexibility to support program needs



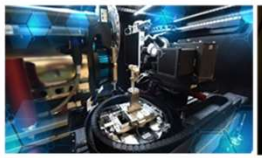
RCB Remote Access Area



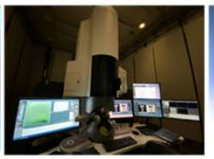
Researchers are remote working on G4 and TEM-EELS



G3 and G4 PFIB



X-ray



TEM



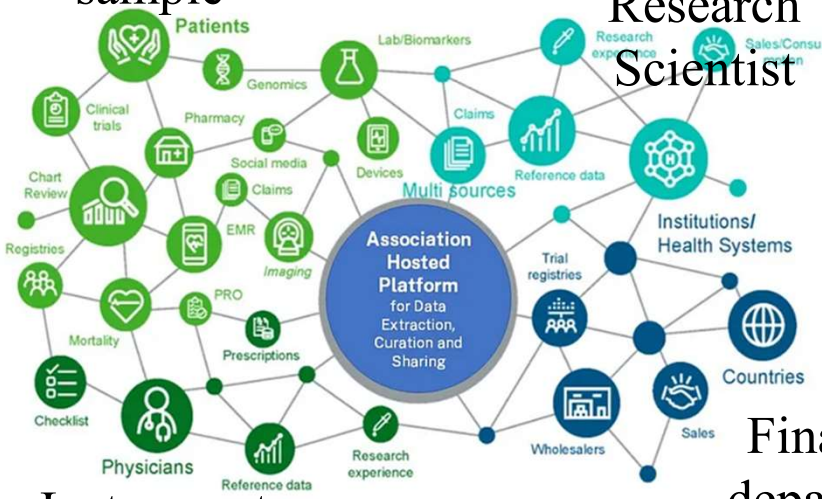
LEAP/APT

Challenges for microscopist

- Understand the microscopy
- Be able to implement, or at least be aware of, analysis algorithms to extract the most and often hard to get information from the large data.
  - Data analysis
  - reconstruction
  - Automation
- Gap between microscopy and biological wings are being bridged.
- Gap between microscopy and nuclear materials research is being recognized but being bridged from data perspective.

sample

Research Scientist

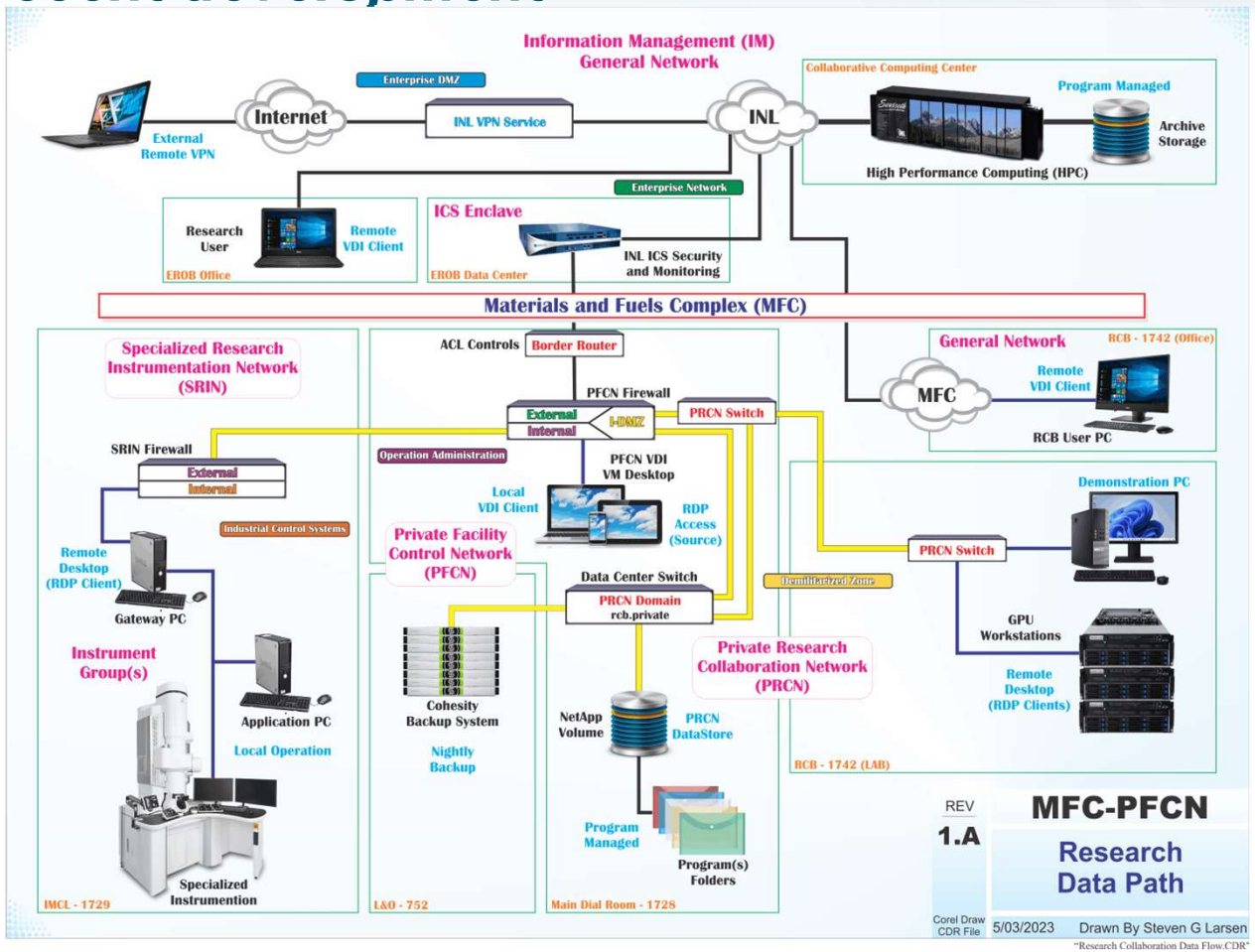


Data Ecosystem Map for Health Care — Source IQVIA and Association Ventures

Financial department

Instrument scientist

Our most recent development



Our recent data Science/ ML / AI journal publications



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The Advanced Characterization, Post Irradiation Examination, and Materials Informatics for the Development of Ultra High-burnup Annular U-10Zr Metallic Fuel

Tiankai Yao[1]*, Fei Xu[1], Fidelma G. Di Lemma[1], Mukesh Bachhav[1], Fei Teng[1], Daniel J. Murry[1], Michael T. Benson[1] and Luca Capriotti[1]

[1] Idaho National Laboratory (DOE), United States

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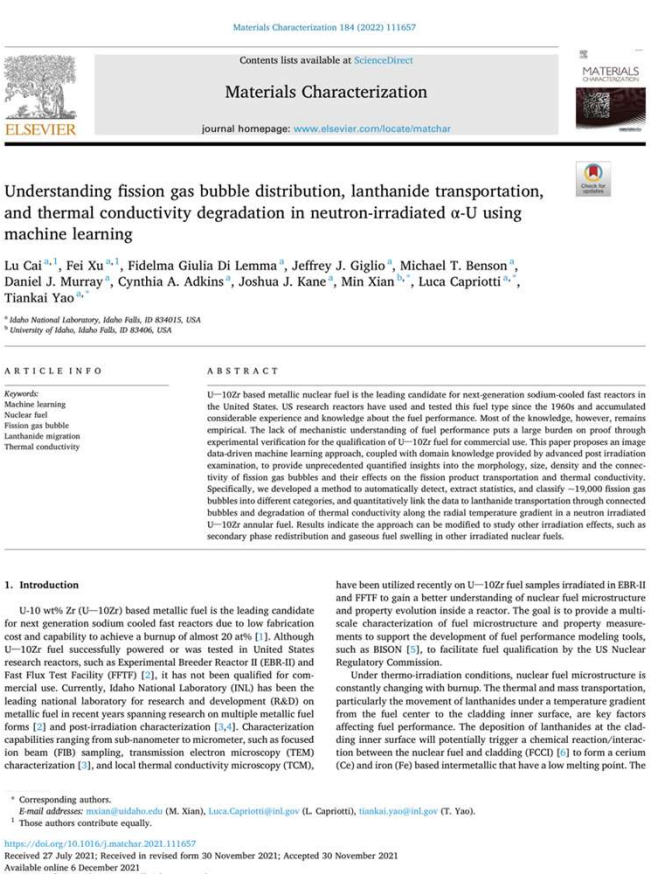
U-Zr-based metallic fuel is a promising fuel candidate for Gen IV fast spectrum reactors. Through a historical irradiation campaign, the sodium thermal boned U-10Zr design can achieve a burnup of 10% fissions per initial heavy metal atom (FIMA), newer fuel designs are pushing the burn-up limit to 20% or even 30% FIMA. To achieve the higher burnup and eliminate the pyrophoric sodium simultaneously, a prototypical annular fuel has been designed, fabricated, cladded with HT-9 in the Materials & Fuels Complex, and irradiated in the Advanced Test Reactors of Idaho National Laboratory (INL) to a peak burnup of 3.3% FIMA. During irradiation, the mechanical contact between fuel and cladding acts as heat dissipation paths. The irradiation lasted for 132 days in the reactor. Recently, both the achieved fresh and irradiated fuel samples were characterized using advanced characterization methods developed in the Irradiated Materials Characterization Laboratory of INL. This paper showcases the application of advanced characterization and materials informatics to study the irradiation effects on metallic fuel. Future work will focus on further implementation of advanced characterization and statistical data mining to help better fuel performance modeling and support U-Zr-based metallic fuel qualification for advanced reactors.

People also looked at

Assessing the interfacial corrosion mechanism of Inconel 617 in chloride molten salt corrosion using multi-modal advanced characterization techniques
Trishelle M. Copeland-Johnson, Daniel J. Murray, Guoping Cao and Lingfeng He

Neptunium mononitride as a target material for Pu-238 production
Kathryn M. Peruski

A review of void and gas bubble superlattices self-organization under irradiation
Yongfeng Zhang



Materials Characterization 184 (2022) 111657

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Understanding fission gas bubble distribution, lanthanide transportation, and thermal conductivity degradation in neutron-irradiated α-U using machine learning

Lu Cai[a,1], Fei Xu[a,1], Fidelma Giulia Di Lemma[a], Jeffrey J. Giglio[a], Michael T. Benson[a], Daniel J. Murray[a], Cynthia A. Adkins[a], Joshua J. Kane[a], Min Xian[b,*], Luca Capriotti[a,*], Tiankai Yao[a,*]

[a] Idaho National Laboratory, Idaho Falls, ID 834015, USA
[b] University of Idaho, Idaho Falls, ID 83406, USA

ARTICLE INFO

Keywords:
Machine learning
Nuclear fuel
Fission gas bubble
Lanthanide migration
Thermal conductivity

ABSTRACT

U—10Zr based metallic nuclear fuel is the leading candidate for next-generation sodium-cooled fast reactors in the United States. US research reactors have used and tested this fuel type since the 1960s and accumulated considerable experience and knowledge about the fuel performance. Most of the knowledge, however, remains empirical. The lack of mechanistic understanding of fuel performance puts a large burden on proof through experimental verification for the qualification of U—10Zr fuel for commercial use. This paper proposes an image data-driven machine learning approach, coupled with domain knowledge provided by advanced post irradiation examination, to provide unprecedented quantified insights into the morphology, size, density and the connectivity of fission gas bubbles and their effects on the fission product transportation and thermal conductivity. Specifically, we developed a method to automatically detect, extract statistics, and classify ~19,000 fission gas bubbles into different categories, and quantitatively link the data to lanthanide transportation through connected bubbles and degradation of thermal conductivity along the radial temperature gradient in a neutron irradiated U—10Zr annular fuel. Results indicate the approach can be modified to study other irradiation effects, such as secondary phase redistribution and gaseous fuel swelling in other irradiated nuclear fuels.

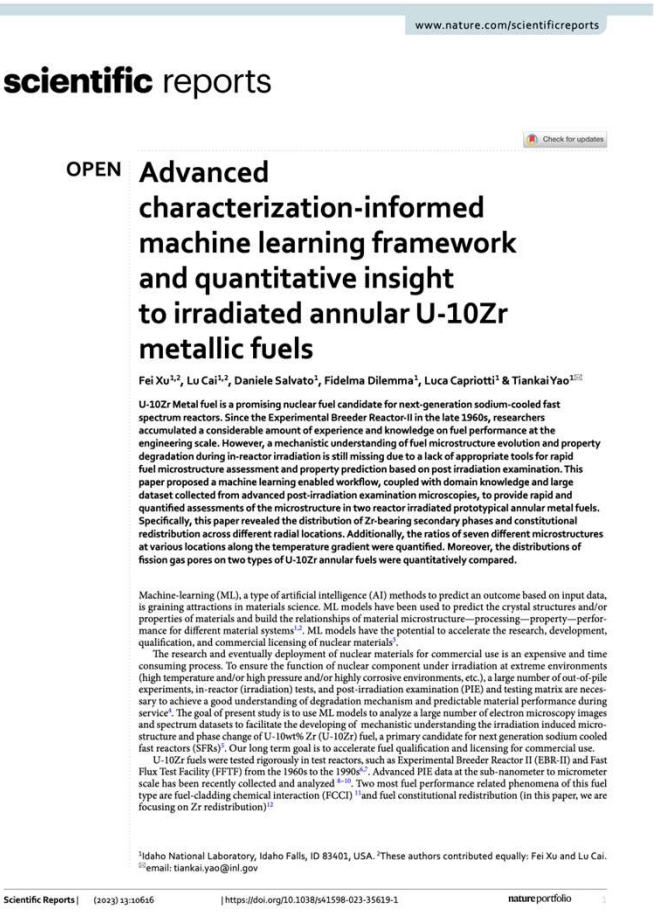
1. Introduction

U-10 wt% Zr (U—10Zr) based metallic fuel is the leading candidate for next generation sodium cooled fast reactors due to low fabrication cost and capability to achieve a burnup of almost 20 at% [1]. Although U—10Zr fuel successfully powered or was tested in United States research reactors, such as Experimental Breeder Reactor II (EBR-II) and Fast Flux Test Facility (FFTF) [2], it has not been qualified for commercial use. Currently, Idaho National Laboratory (INL) has been the leading national laboratory for research and development (R&D) on metallic fuel in recent years spanning research on multiple metallic fuel forms [2] and post-irradiation characterization [3,4]. Characterization capabilities ranging from sub-nanometer to micrometer, such as focused ion beam (FIB) sampling, transmission electron microscopy (TEM) characterization [3], and local thermal conductivity microscopy (TCM), have been utilized recently on U—10Zr fuel samples irradiated in EBR-II and FFTF to gain a better understanding of nuclear fuel microstructure and property evolution inside a reactor. The goal is to provide a multi-scale characterization of fuel microstructure and property measurements to support the development of fuel performance modeling tools, such as BISON [5], to facilitate fuel qualification by the US Nuclear Regulatory Commission.

Under thermo-irradiation conditions, nuclear fuel microstructure is constantly changing with burnup. The thermal and mass transportation, particularly the movement of lanthanides under a temperature gradient from the fuel center to the cladding inner surface, are key factors affecting fuel performance. The deposition of lanthanides at the cladding inner surface will potentially trigger a chemical reaction/interaction between the nuclear fuel and cladding (FCCI) [6] to form a cerium (Ce) and iron (Fe) based intermetallic that have a low melting point. The

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E-mail addresses: mxian@uidaho.edu (M. Xian), Luca.Capriotti@inl.gov (L. Capriotti), tiankai.yao@inl.gov (T. Yao).
[1] Those authors contribute equally.

https://doi.org/10.1016/j.matchar.2021.111657
Received 27 July 2021; Received in revised form 30 November 2021; Accepted 30 November 2021
Available online 6 December 2021
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Advanced characterization-informed machine learning framework and quantitative insight to irradiated annular U-10Zr metallic fuels

Fei Xu[1,2], Lu Cai[1,2], Daniele Salvato[1], Fidelma Dilemma[1], Luca Capriotti[1] & Tiankai Yao[1]✉

U-10Zr Metal fuel is a promising nuclear fuel candidate for next-generation sodium-cooled fast spectrum reactors. Since the Experimental Breeder Reactor-II in the late 1960s, researchers accumulated a considerable amount of experience and knowledge on fuel performance at the engineering scale. However, a mechanistic understanding of fuel microstructure evolution and property degradation during in-reactor irradiation is still missing due to a lack of appropriate tools for rapid fuel microstructure assessment and property prediction based on post irradiation examination. This paper proposed a machine learning enabled workflow, coupled with domain knowledge and large dataset collected from advanced post-irradiation examination microscopies, to provide rapid and quantified assessments of the microstructure in two reactor irradiated prototypical annular metal fuels. Specifically, this paper revealed the distribution of Zr-bearing secondary phases and constitutional redistribution across different radial locations. Additionally, the ratios of seven different microstructures at various locations along the temperature gradient were quantified. Moreover, the distributions of fission gas pores on two types of U-10Zr annular fuels were quantitatively compared.

Machine-learning (ML), a type of artificial intelligence (AI) methods to predict an outcome based on input data, is graining attractions in materials science. ML models have been used to predict the crystal structures and/or properties of materials and build the relationships of material microstructure—processing—property—performance for different material systems[1,2]. ML models have the potential to accelerate the research, development, qualification, and commercial licensing of nuclear materials[3].

The research and eventually deployment of nuclear materials for commercial use is an expensive and time consuming process. To ensure the function of nuclear component under irradiation at extreme environments (high temperature and/or high pressure and/or highly corrosive environments, etc.), a large number of out-of-pile experiments, in-reactor (irradiation) tests, and post-irradiation examination (PIE) and testing matrix are necessary to achieve a good understanding of degradation mechanism and predictable material performance during service[4]. The goal of present study is to use ML models to analyze a large number of electron microscopy images and spectrum datasets to facilitate the developing of mechanistic understanding the irradiation induced microstructure and phase change of U-10wt% Zr (U-10Zr) fuel, a primary candidate for next generation sodium cooled fast reactors (SFRs)[5]. Our long term goal is to accelerate fuel qualification and licensing for commercial use.

U-10Zr fuels were tested rigorously in test reactors, such as Experimental Breeder Reactor II (EBR-II) and Fast Flux Test Facility (FFTF) from the 1960s to the 1990s[6,7]. Advanced PIE data at the sub-nanometer to micrometer scale has been recently collected and analyzed [8–10]. Two most fuel performance related phenomena of this fuel type are fuel-cladding chemical interaction (FCCI) [11]and fuel constitutional redistribution (in this paper, we are focusing on Zr redistribution)[12]

[1]Idaho National Laboratory, Idaho Falls, ID 83401, USA. [2]These authors contributed equally: Fei Xu and Lu Cai. ✉email: tiankai.yao@inl.gov

Proposed Architecture for Advanced Data Analytics

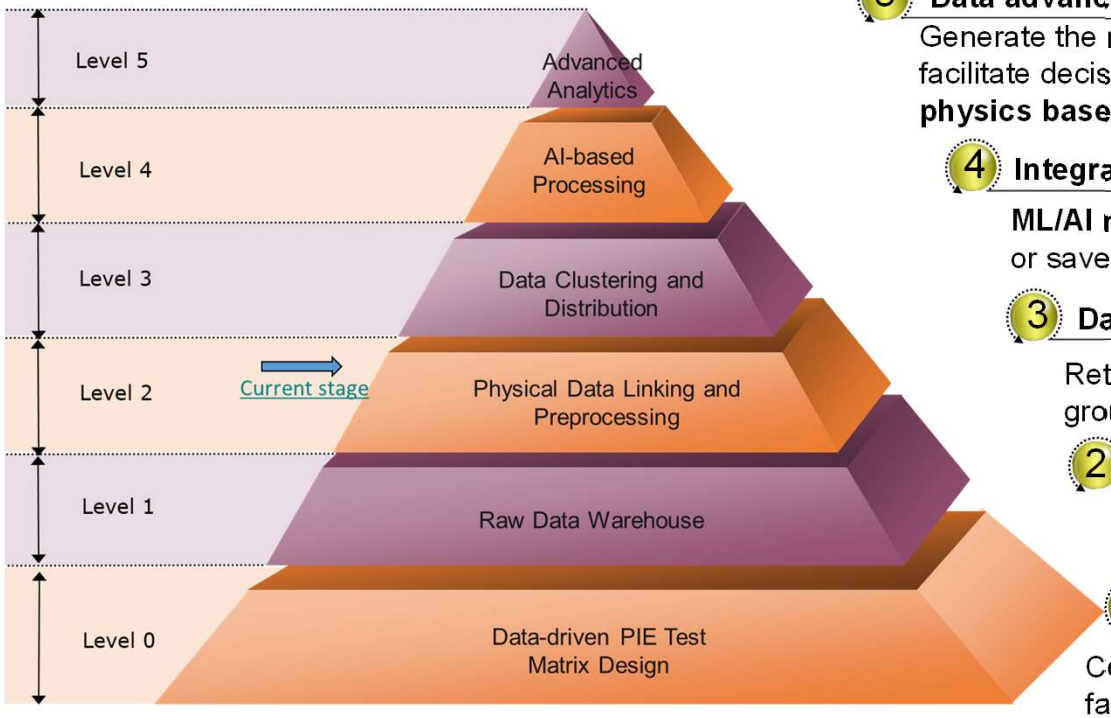


Figure 1: Six levels of data integration and processing to achieve advanced analytics at MFCADA, and the level where MFC currently resides

5 Data advanced analytics

Generate the results from ML/AI models for the reports and publications to facilitate decision-making. **Our analytics results can be directly used by physics based models, such as BISON and MOOSE.**

4 Integrating models

ML/AI models to process either real-time data from instruments or saved historical data.

3 Data management

Retrieved data on different needs and clustered into different groups/research topics

2 Label data with existing physical information

Data tagging through sample ID, instrument, facility, projects, et al.

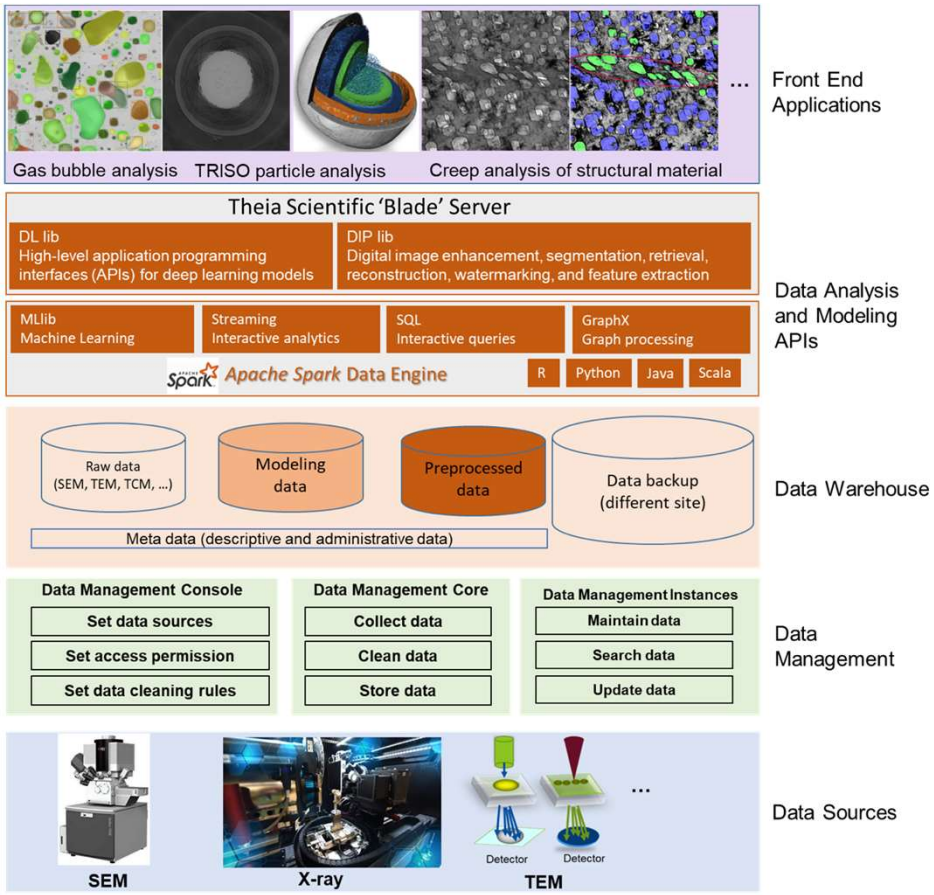
1 Data centralize

Collecting raw data from multiple instruments located at different facilities. All raw data is centralized, backed up, and controlled by internal/external access

0 Data-drive AI models guide PIE test matrix design

The results from advanced analytics will guide more efficient test matrix design.

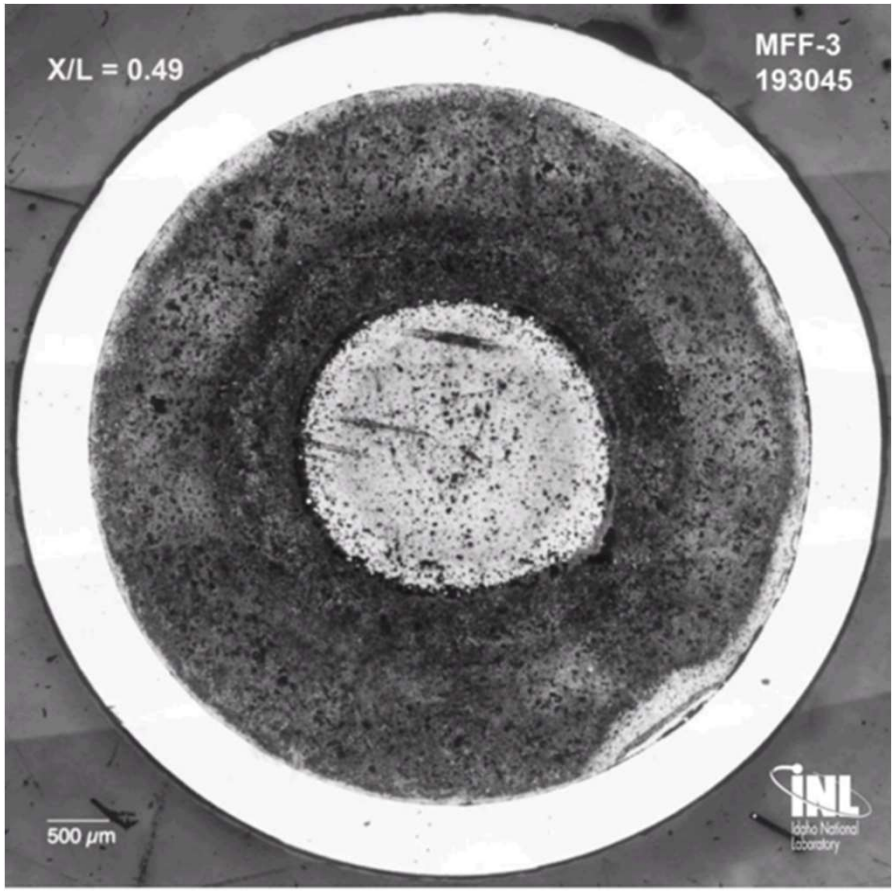
The vision of the PIE data ecosystem

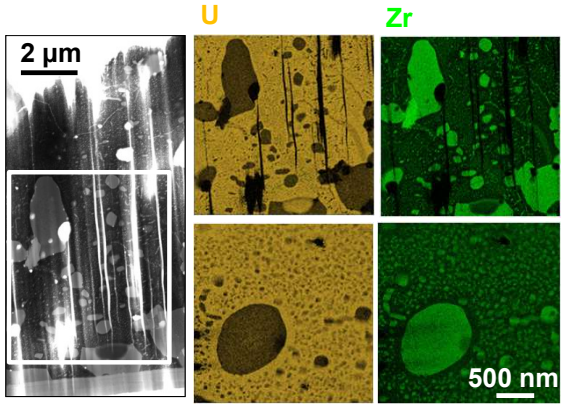




- **Model development and integration**
  Expand more new models to the data engine and finalize the user interface and test on real tasks
- **User interface**
  Develop a web application with the functions of data retrieval, user-friendly model applications, and visualization analysis
- **Data engine**
  Prepare the hardware for the data analysis server and install the Apache data engine on the blade and the existing libraries and models
- **Data Management**
  Build the data links, and provide basic and essential functions to support managing and securing data based on projects/tasks

Together, we can make things happen





Transmission electron microscopy identification of Zr nano precipitate (2-5 nm, 10^{-9} m)

