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From atoms to advanced reactors: materials science and engineering at Idaho National Laboratory

September 2020

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Changing the World's Energy Future

Idaho National Laboratory

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Idaho Falls, Idaho 83415

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Andrea Jokisaari
Nuclear Science &
Technology Division

From Atoms to Advanced Reactors:

Materials Science and Engineering at Idaho National Laboratory

Idaho National Laboratory

My Education and Career

- BS, Ceramic and Materials Engineering, Clemson University
  - One year at l'Institut National Polytechnique de Grenoble
- MS, Materials Science and Engineering, University of Michigan
- PhD, Materials Science and Engineering, University of Michigan
- Postdoctoral fellow, Northwestern University and Argonne National Laboratory
- Computational Scientist, Idaho National Laboratory.

How I Got Here

- I started as an experimentalist…
  - Clemson Metals Laboratory undergraduate assistant
  - Undergraduate intern at Los Alamos National Laboratory (3x)
  - Clemson COMSET post-baccalaureate work
  - University of Michigan III-V semiconductor fabrication and characterization
- Who knew one semester of C++ in high school would be so useful?
  - University of Michigan phase-field modeling of fuel cladding (CASL)
  - Oak Ridge National Laboratory graduate internship (CASL)
  - Argonne National Laboratory/Northwestern University postdoc at CHiMaD for novel superalloys
  - INL computational scientist, MARMOT team
  - Deputy technical director, Nuclear Materials Development and Qualification Initiative.

Los Alamos NATIONAL LABORATORY EST. 1943

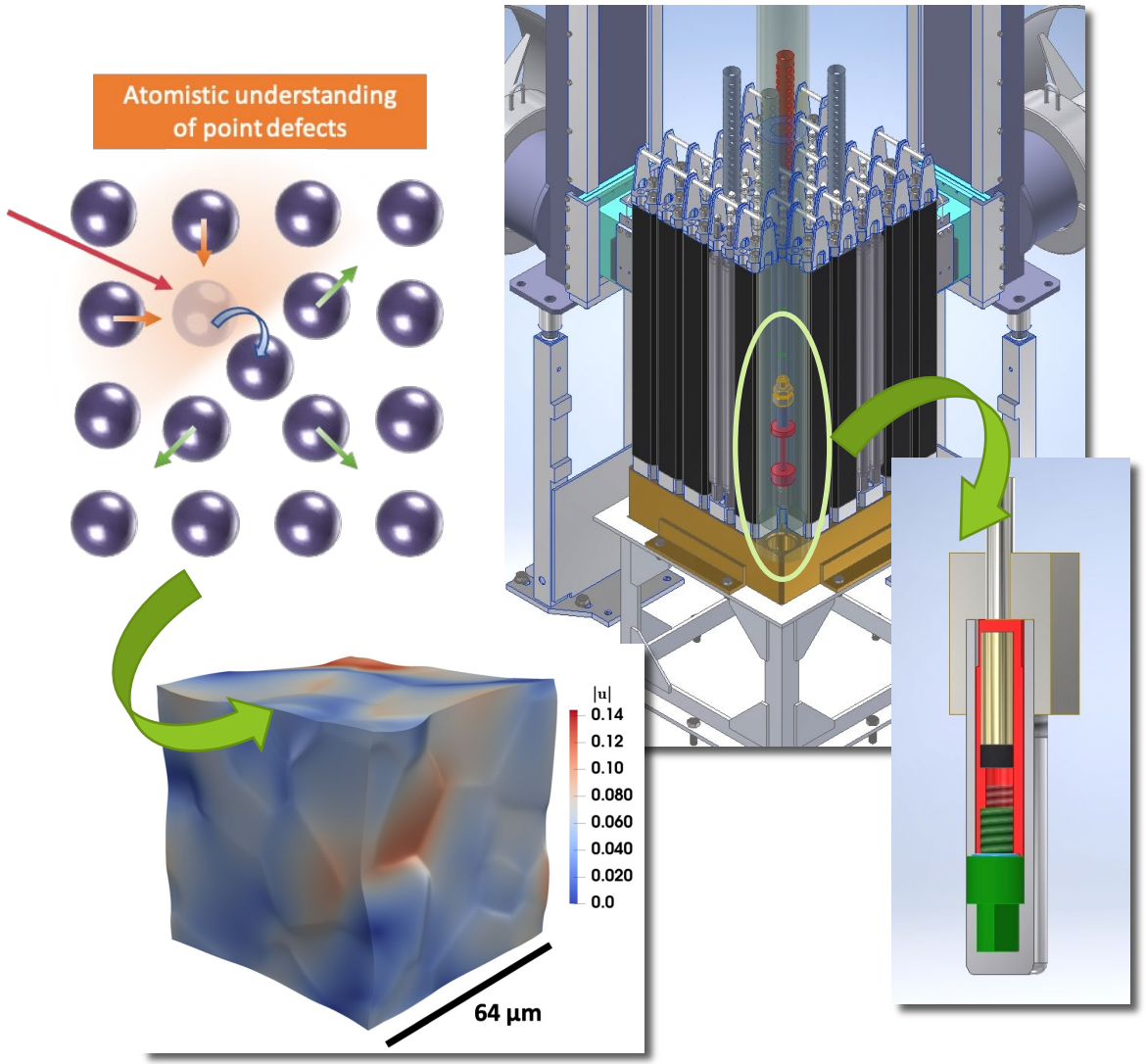
OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

Northwestern

And What I Do Now

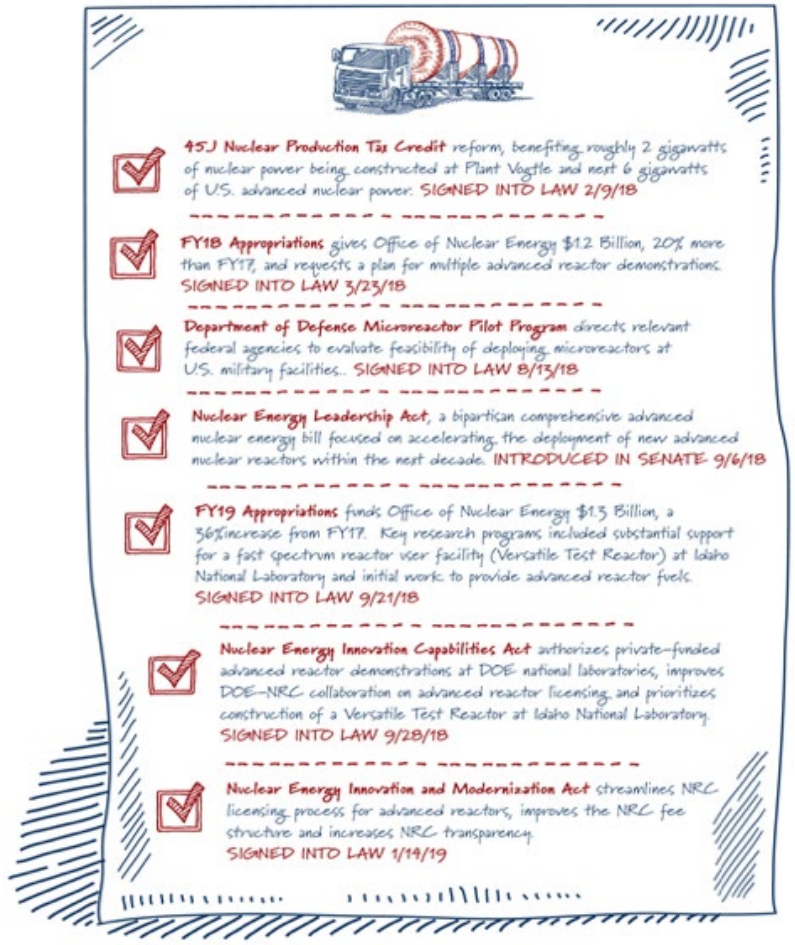
- I incorporate both experimentation and computation at INL
- Computational Scientist in the Computational Mechanics and Materials group, MARMOT team (January 2018)
  - MOOSE-based computational research
  - Mesoscale, physics-based modeling of nuclear fuels and structural materials
- LDRD on the irradiation damage in α-uranium (modeling and experiment)
- Deputy Technical Director, Nuclear Materials Development and Qualification Initiative (NMDQi).



Demonstrating Advanced Reactors is an INL Mission

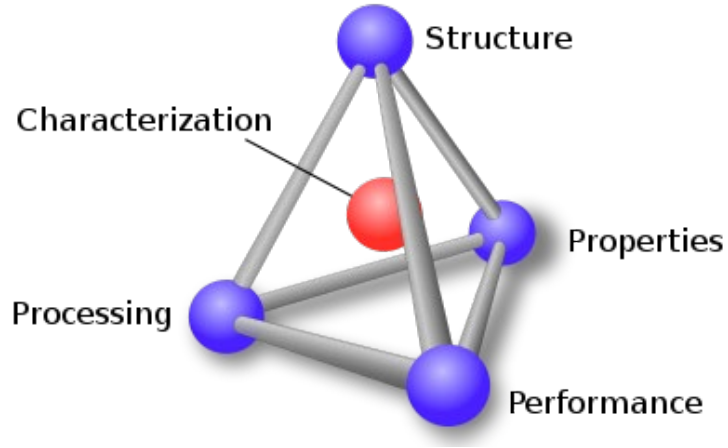
- Strong interest in clean energy is driving renewed interest in nuclear
- INL's unique combination of infrastructure, geography, and capabilities enables our mission
- Materials are crucial and success requires multidisciplinary effort.

"*I'm thrilled that senators from both sides of the aisle have come together to support advanced nuclear. This is exactly the kind of leadership our country needs to both solve the climate challenge and reassert our leadership in this important industry.*"
Bill Gates, March 2019

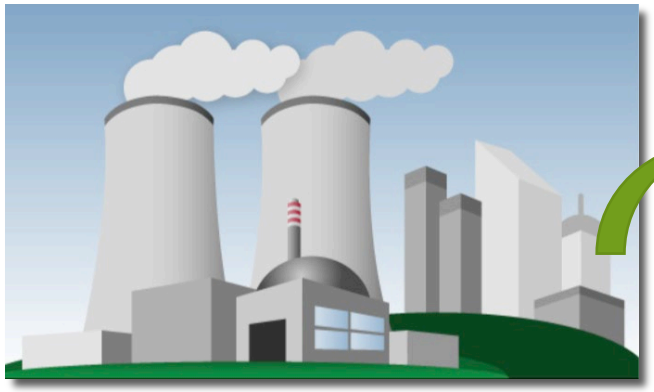


Source: Clear Path Action

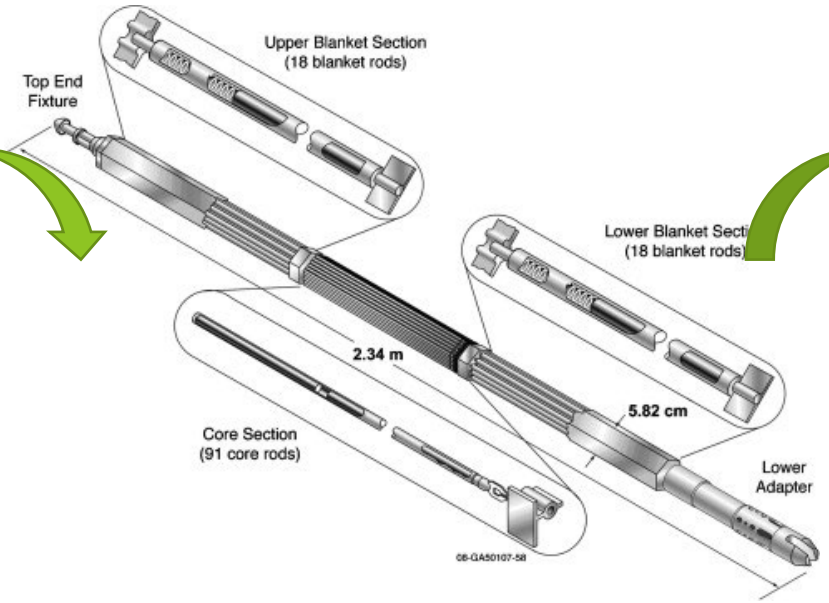
From Atoms to Advanced Reactors



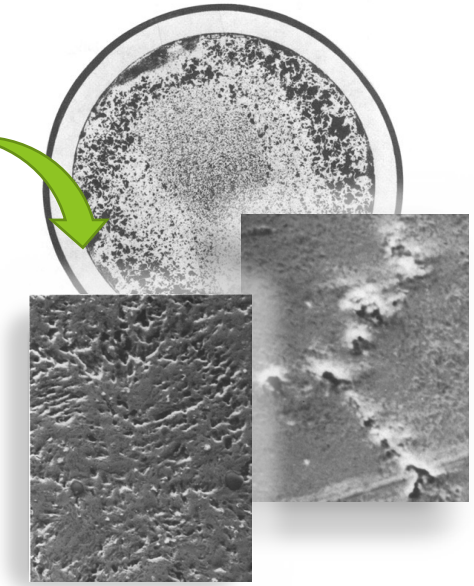
Reactor installation



Fuel assembly



Fuel rod

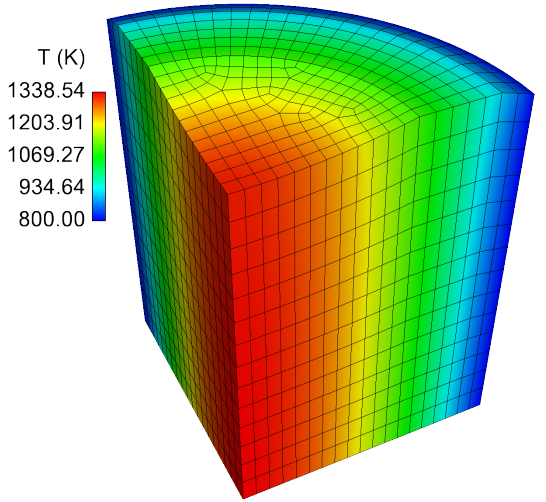


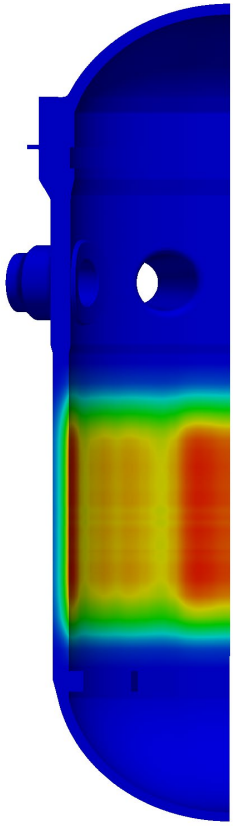
Operating requirements

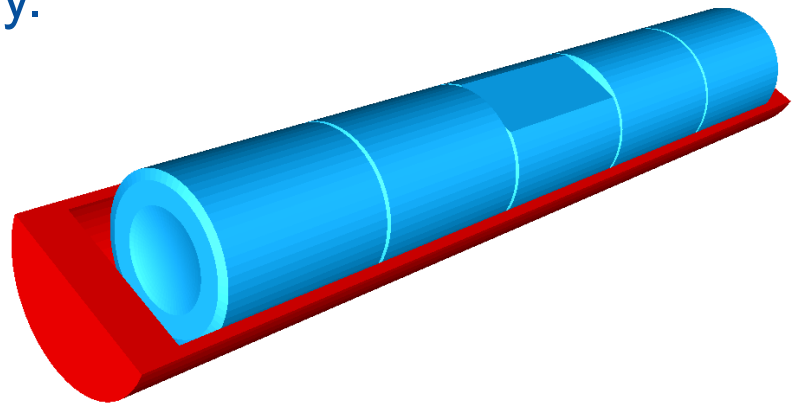
ASTM requirements

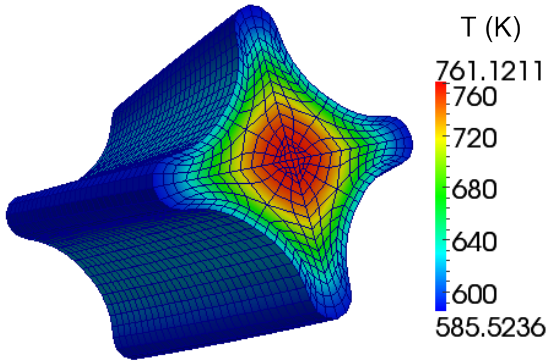
Reactor Fuel Performance Modeling

- BISON and GRIZZLY are INL codes for fuel and structural modeling
- LWR and advanced reactor capabilities (TRISO, metallic, accident-tolerant fuels)
- BISON is used by NASA, the Nuclear Regulatory Commission, Karios Power, Oklo, Westinghouse, and the Canadian Nuclear Laboratory.



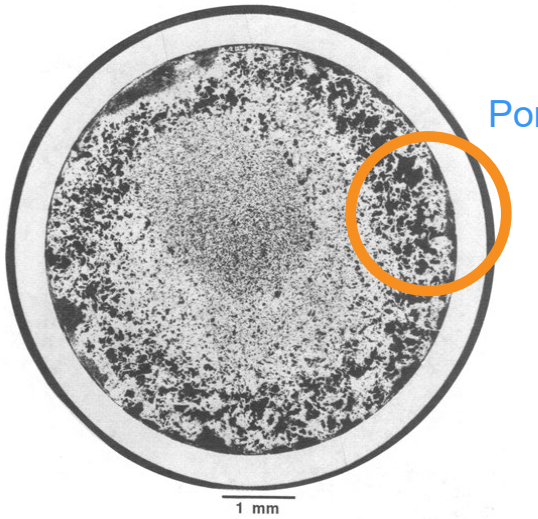






Physics-based U-Pu-Zr Fuel Performance

- U-Pu-Zr fuel is proposed for several advanced reactors, such as Oklo and the Versatile Test Reactor
- Legacy of EBR-II data, new analysis from MFC
- Engineering-scale materials science: creating insights from lower length scales
- Model and code development for BISON.



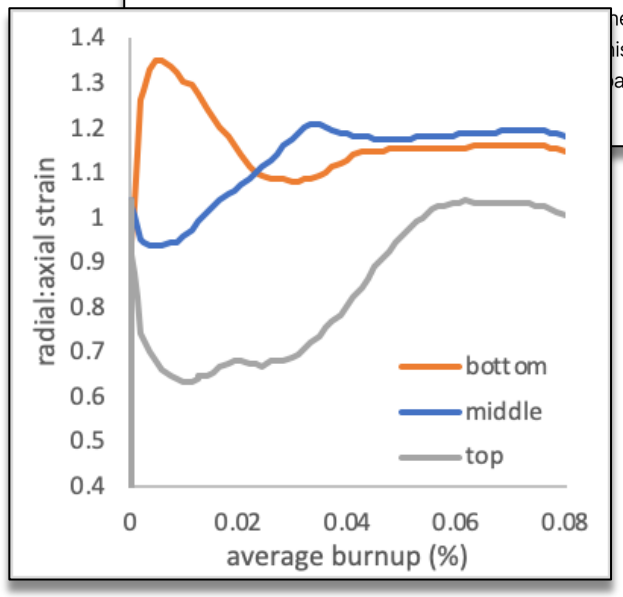
Porous outer structure

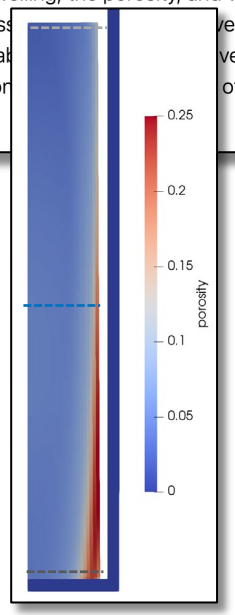
UPuZr Low-Temperature Swelling

Calculates swelling increment due to low-temperature swelling in UPuZr.

Description

`UPuZrLowTemperatureSwelling` computes a swelling increment to account for swelling arising from the presence of α-uranium in U-Pu-Zr systems. It is designed to be used in conjunction with a gaseous swelling model such as in `UPuZrGaseousSwelling` as well as with a joiner class, `UPuZrPorosityEigenstrain`, that computes the swelling, the porosity, and volumetric





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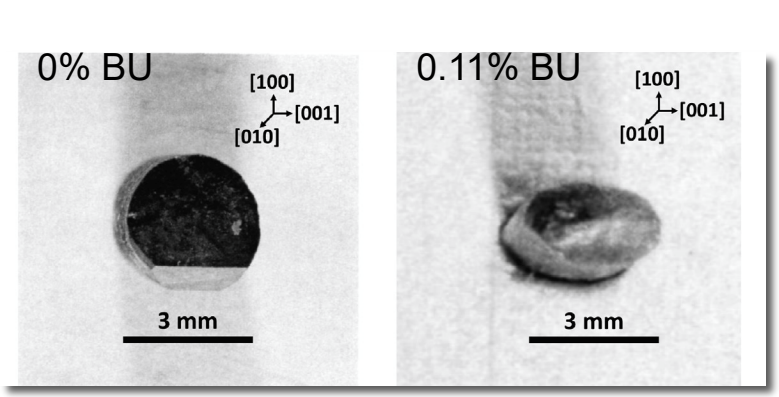
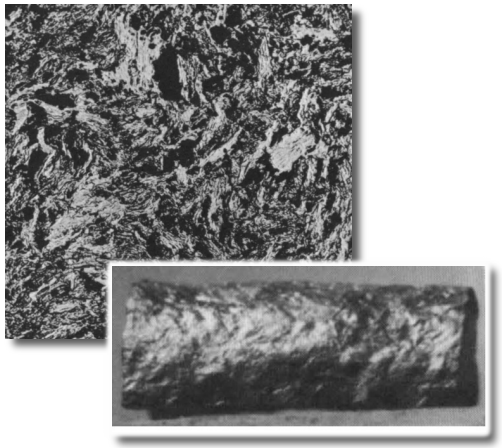
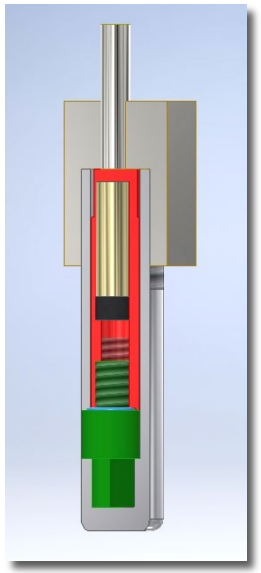
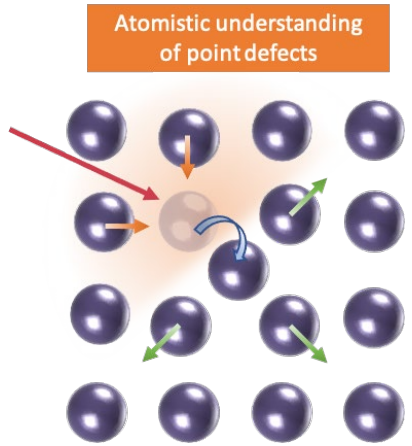
Irradiation & Thermal-induced Microstructure Changes



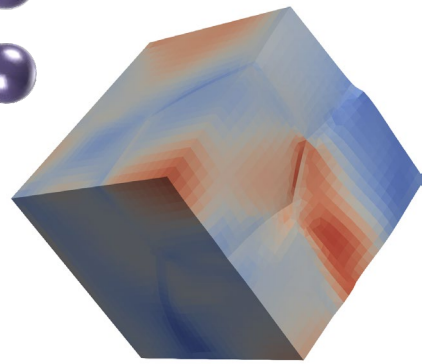




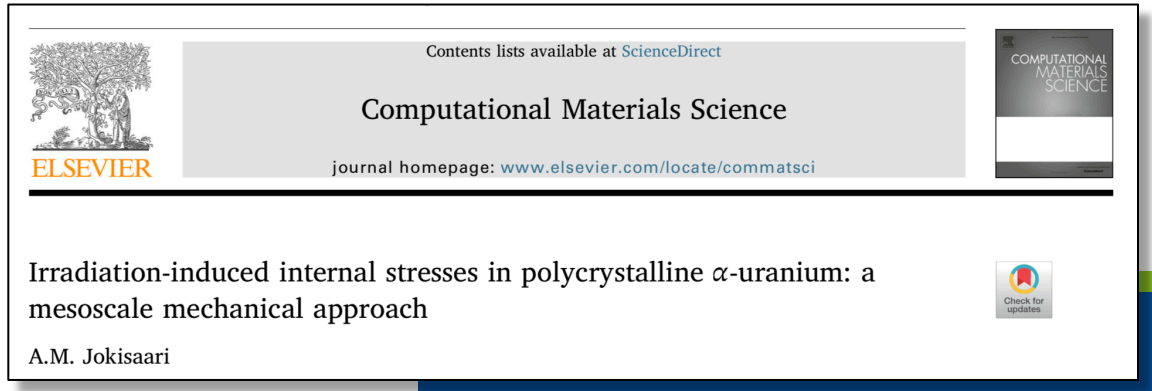
CHARIN sample holder



Plastic strain localization in α-U



- Atomistic and microstructural investigation of the physics of U-Pu-Zr fuel swelling and on other fuels
- Physics-based microstructure models mean new fuel designs can be modeled correctly
- Basic physical understanding advances in irradiation materials science
- Combines modeling and experiment.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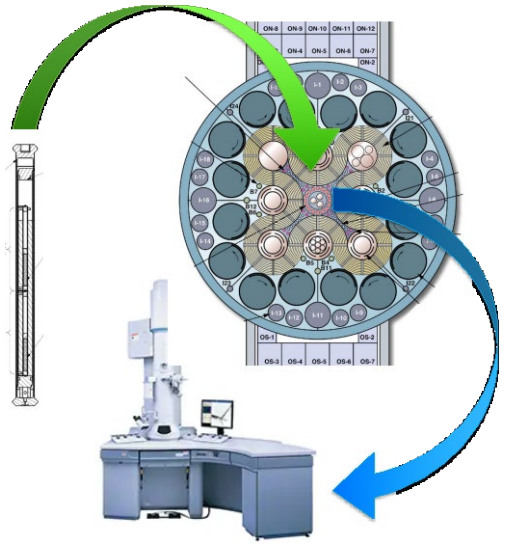
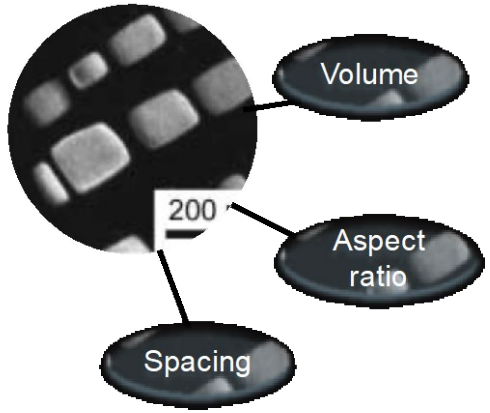
Irradiation-induced internal stresses in polycrystalline α-uranium: a mesoscale mechanical approach

A.M. Jokisaari

Nuclear Materials Discovery and Qualification Initiative Brings a New Paradigm

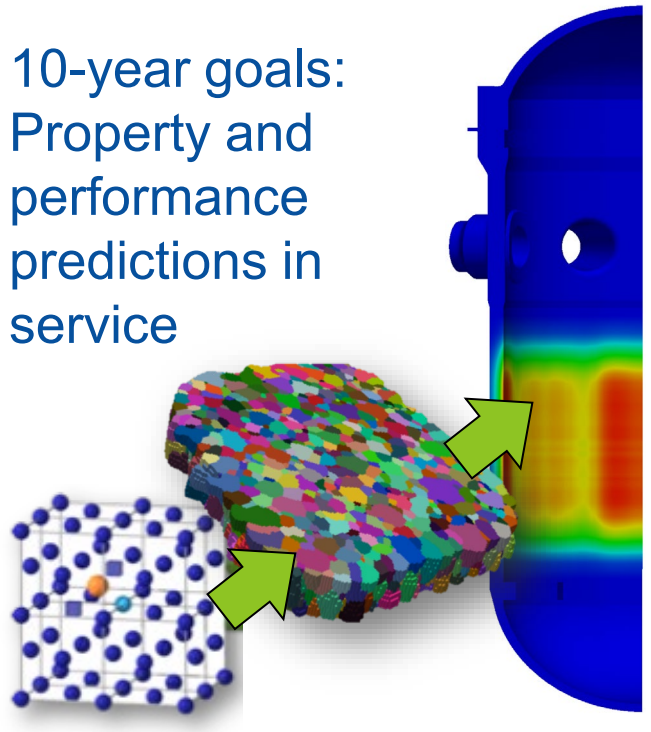
Physics-based modeling along with rapid testing and characterization links microstructures and service conditions to properties





Machine learning can harness data in new ways to improve predictions

10-year goals: Property and performance predictions in service



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