INL/MIS-21-63258-Revision-0

20A44-121: Modeling and characterization of alpha-U to accelerate metallic fuels development

May 2024

Andrea M Jokisaari

Changing the World's Energy Future

Idaho National Laboratory

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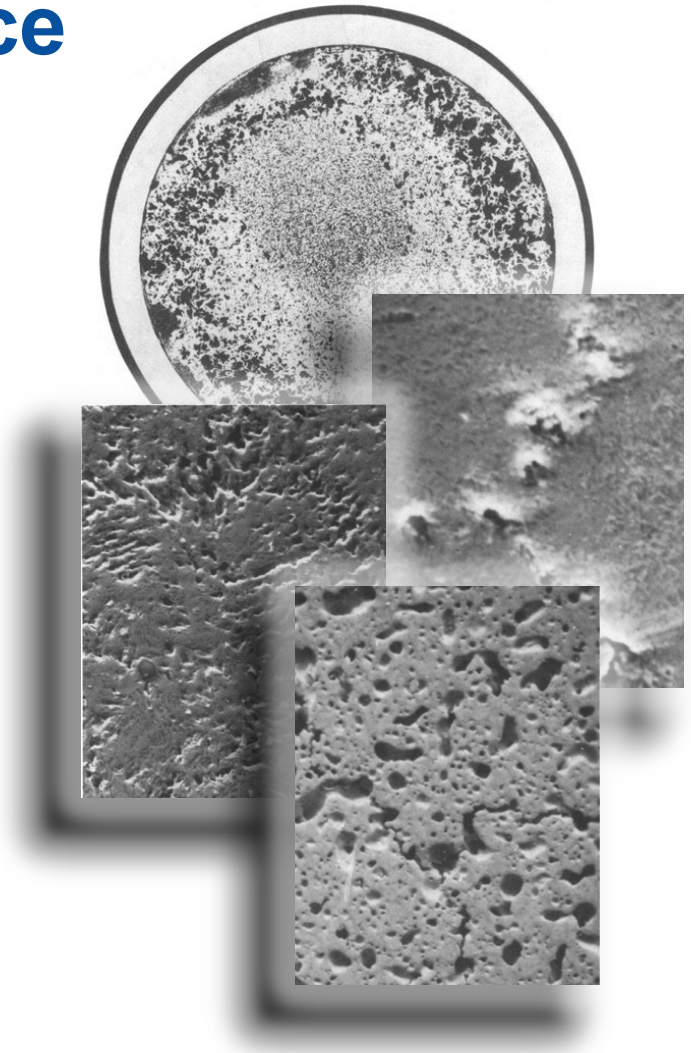
The Question:

What are the defects doing?

(Because they control everything...)

A modern study of α-uranium will benefit metallic fuel development and fundamental science

- Metallic fuel swelling is potentially lifetime-limiting, and fuel swells differently depending on the fuel temperature (phases present)
- Current predictive capability is limited
  - Existing fuel design
  - New possible designs and reactors
  - Heyday of α-uranium research was in the 1960s
- Basic understanding of α-uranium irradiation behavior is needed

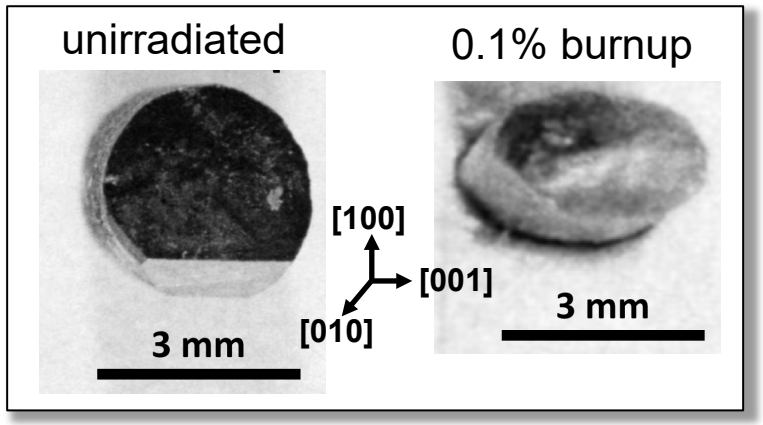


Met. Trans. A 21A (1990) 517

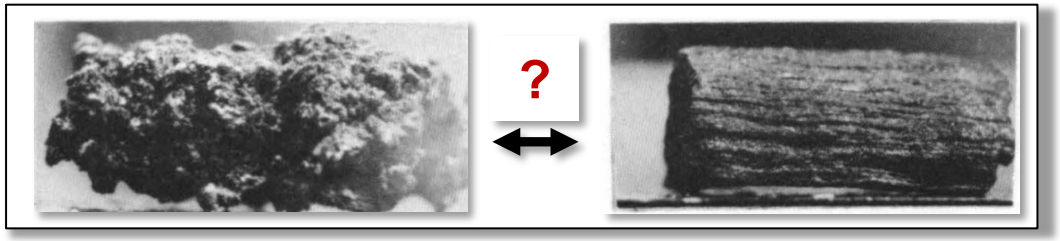
What are the defects doing?

Coupled modeling and experiments to provide new understanding of α-U

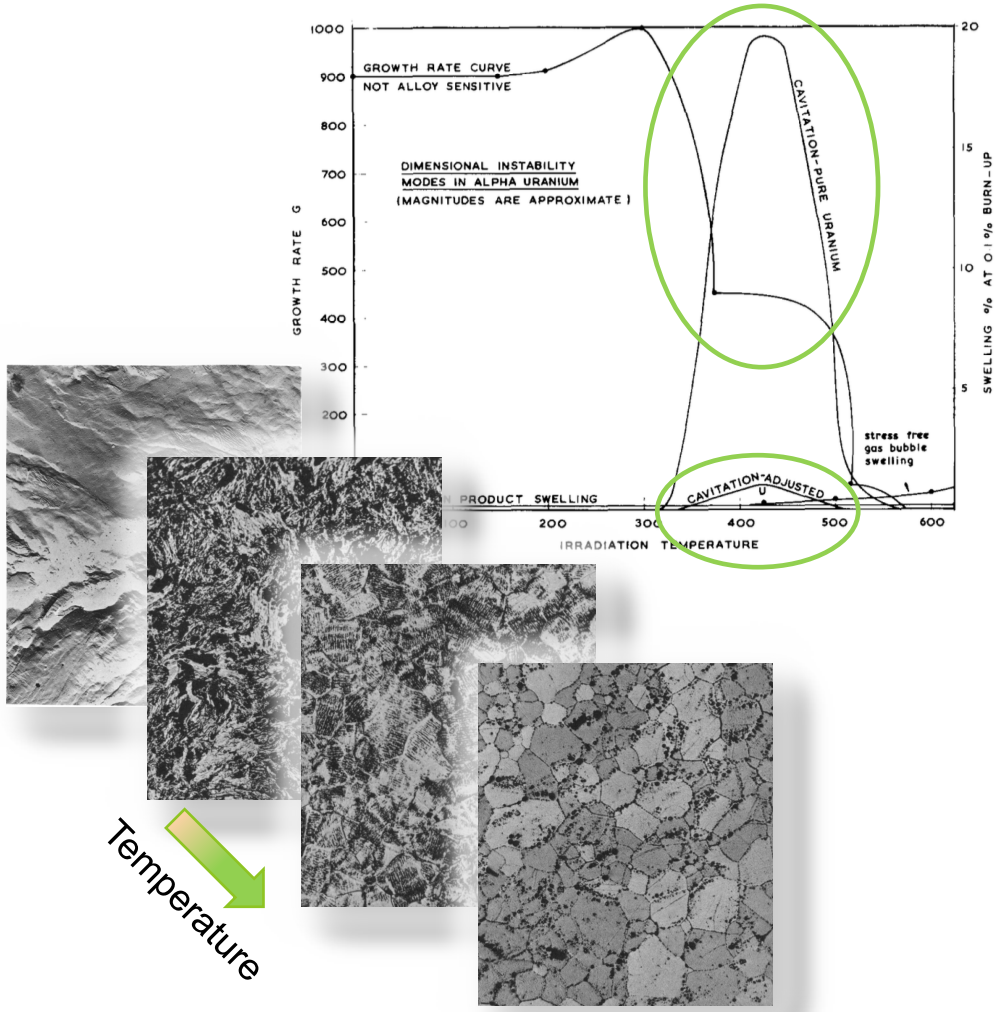
- Atomistic-to-mesoscale modeling links time and length scales
- In-situ furnace controls irradiation conditions



Paine, ANL-5676, 1958



Leggett, HW-79559, 1963

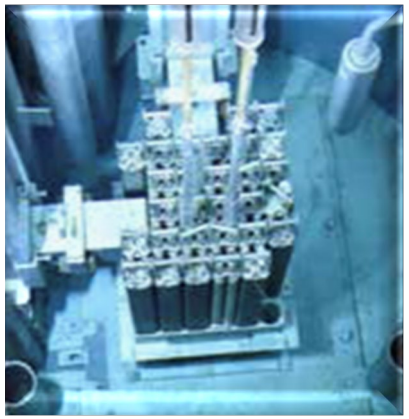


Acta Metall. 23 (1975) 101

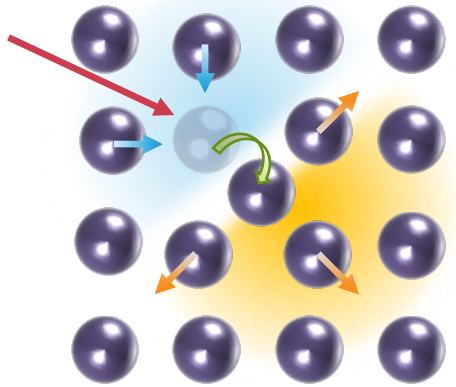
Advancing the state of the art for fuel and reactor materials

- Novel approach to link length and time scales necessary to model long-term microstructure evolution under irradiation
- Furthering basic science of irradiation effects on materials and supporting the development and deployment of next-generation reactors worldwide
  - BES-GBS project
  - NMDQi
  - NEAMS (Marmot, Bison)
  - Industry (Oklo)
- Strengthen internal connections at INL between modeling and experiment

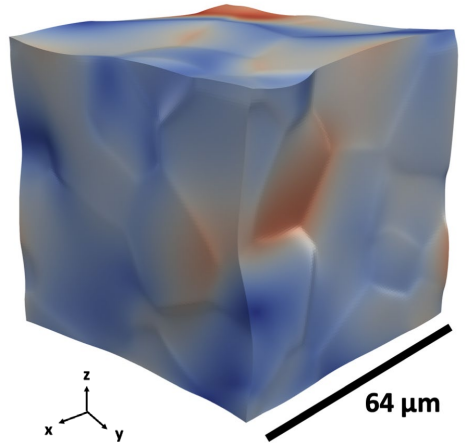
NRAD hot-stage irradiation



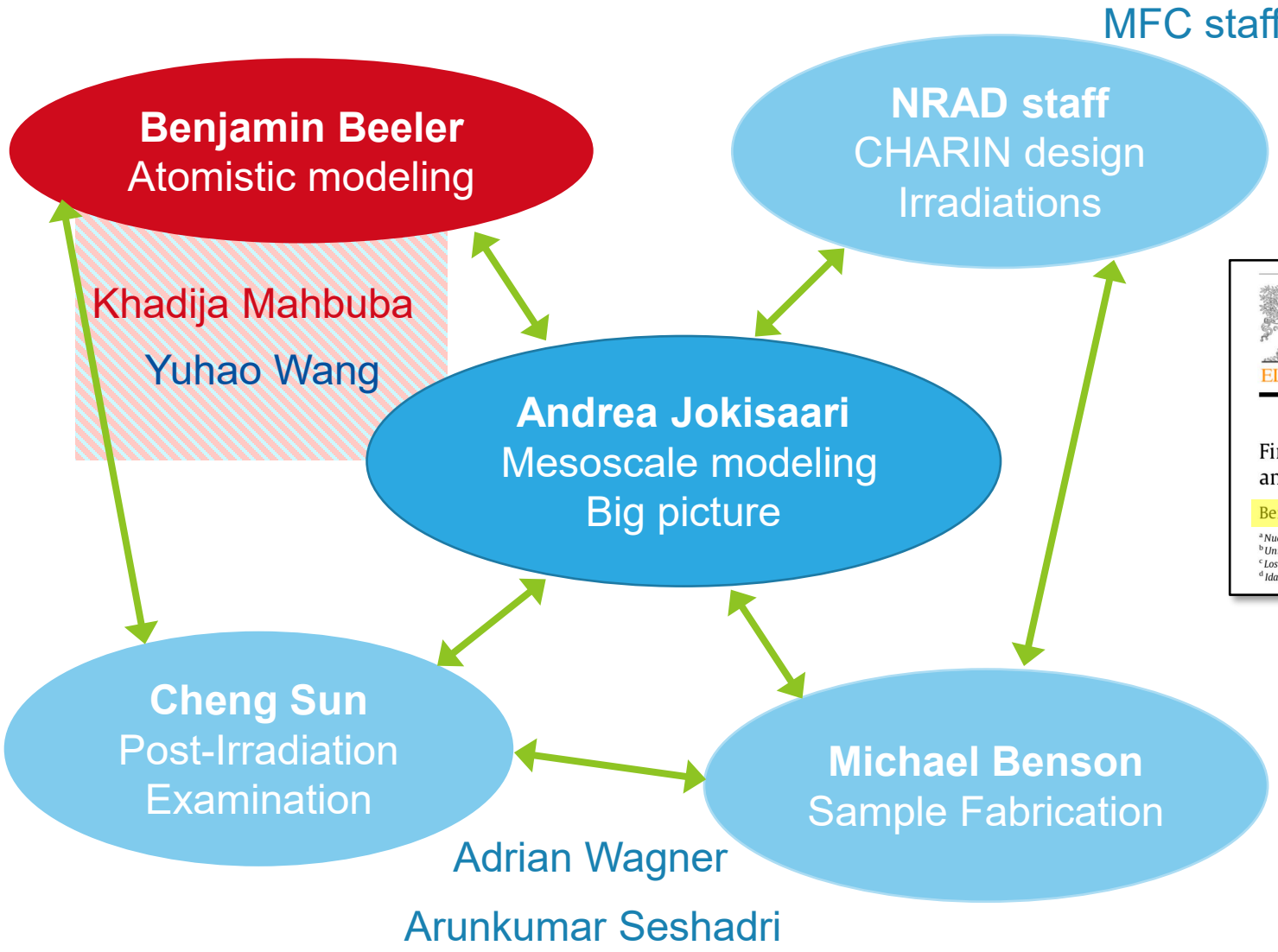
Atomistic understanding of point defects

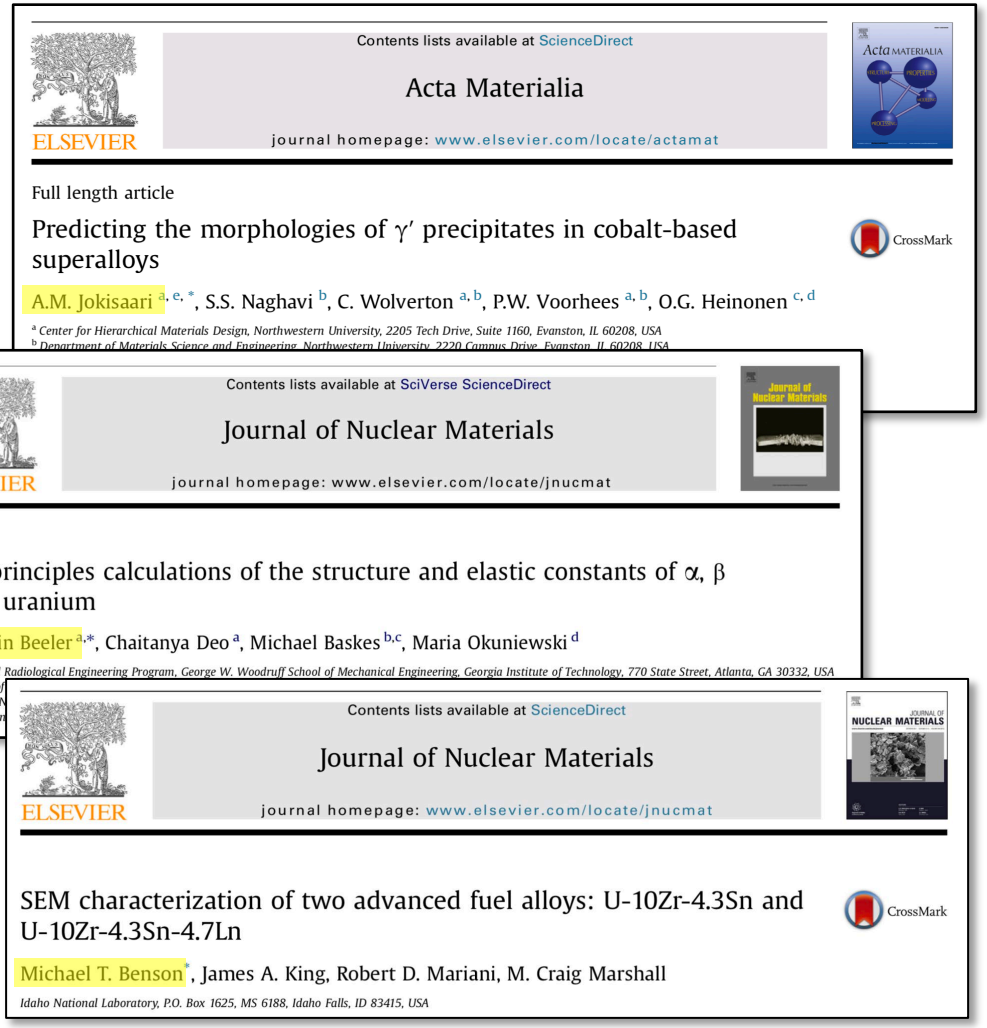


Microstructure behavior under irradiation



Team members have synergistic expertise





Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

Full length article

Predicting the morphologies of γ′ precipitates in cobalt-based superalloys

A.M. Jokisaari [a, e, *], S.S. Naghavi [b], C. Wolverton [a, b], P.W. Voorhees [a, b], O.G. Heinonen [c, d]

[a] Center for Hierarchical Materials Design, Northwestern University, 2205 Tech Drive, Suite 1160, Evanston, IL 60208, USA

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Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

First principles calculations of the structure and elastic constants of α, β and γ uranium

Benjamin Beeler [a,*], Chaitanya Deo [a], Michael Baskes [b,c], Maria Okuniewski [d]

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[b] University of

[c] Los Alamos N

[d] Idaho Nation

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

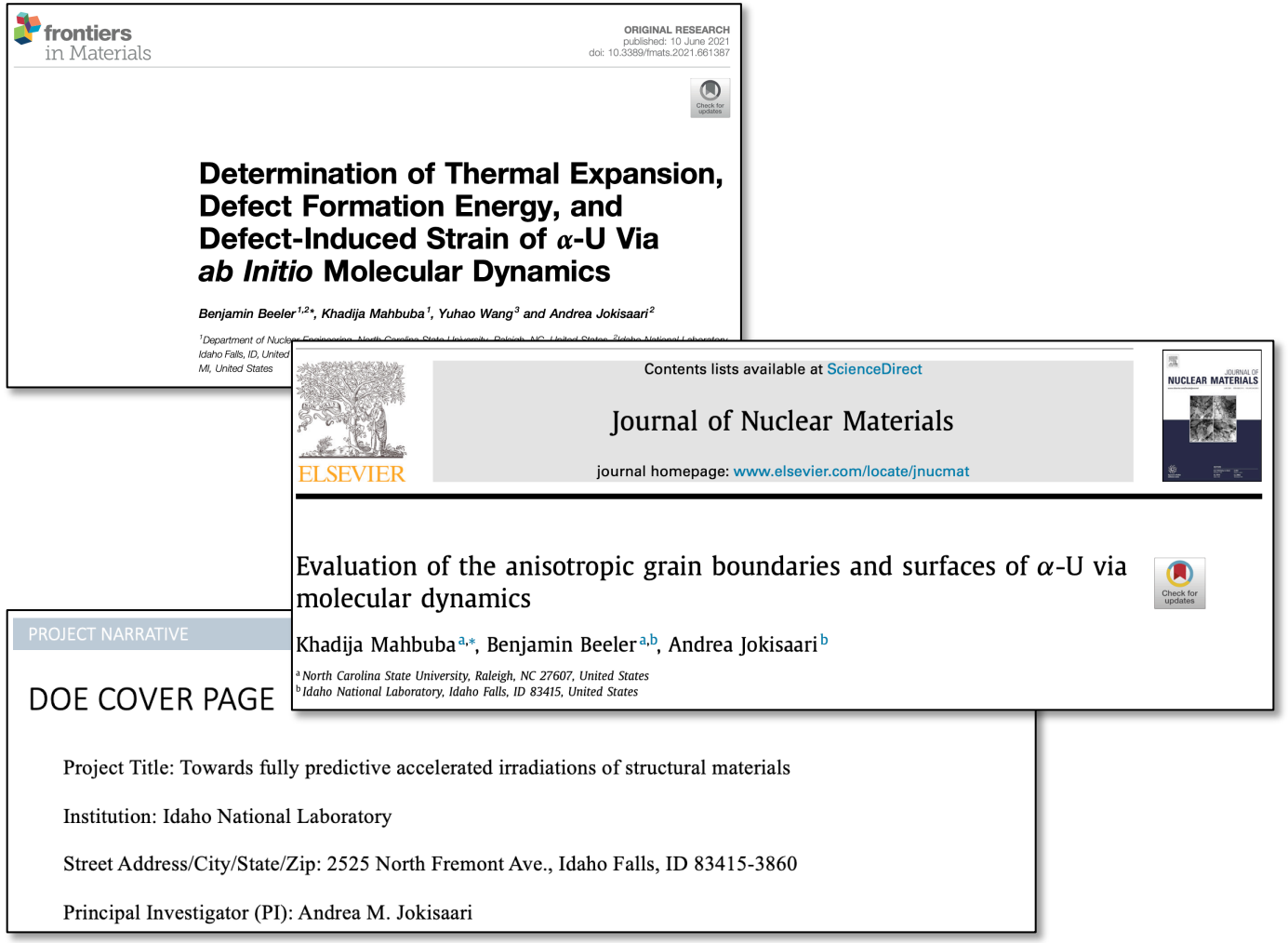
SEM characterization of two advanced fuel alloys: U-10Zr-4.3Sn and U-10Zr-4.3Sn-4.7Ln

Michael T. Benson*, James A. King, Robert D. Mariani, M. Craig Marshall

Idaho National Laboratory, P.O. Box 1625, MS 6188, Idaho Falls, ID 83415, USA

Generating scientific and engineering output that will impact the future

- Modeling and simulation focusing on understanding point defect behavior and interplay of multiple phenomena on microstructure evolution
- Obtain experimental data about the change in defect behavior with temperature and the influence of grain boundaries/internal sinks
- New in-situ irradiation furnace (CHARIN) being developed
- Journal publications and conference presentations
- Catalyzed BES-EC proposal by PI



frontiers in Materials

ORIGINAL RESEARCH
published: 10 June 2021
doi: 10.3389/fmats.2021.661387

Determination of Thermal Expansion, Defect Formation Energy, and Defect-Induced Strain of α-U Via *ab Initio* Molecular Dynamics

Benjamin Beeler[1,2], Khadija Mahbuba[1], Yuhao Wang[3] and Andrea Jokisaari[2]*

[1]Department of Nuclear Engineering, North Carolina State University, Raleigh, NC, United States, [2]Idaho National Laboratory, Idaho Falls, ID, United States, [3]University of Michigan, Ann Arbor, MI, United States

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

ELSEVIER

Evaluation of the anisotropic grain boundaries and surfaces of α-U via molecular dynamics

Khadija Mahbuba[a,*], Benjamin Beeler[a,b], Andrea Jokisaari[b]

[a] North Carolina State University, Raleigh, NC 27607, United States
[b] Idaho National Laboratory, Idaho Falls, ID 83415, United States

PROJECT NARRATIVE

DOE COVER PAGE

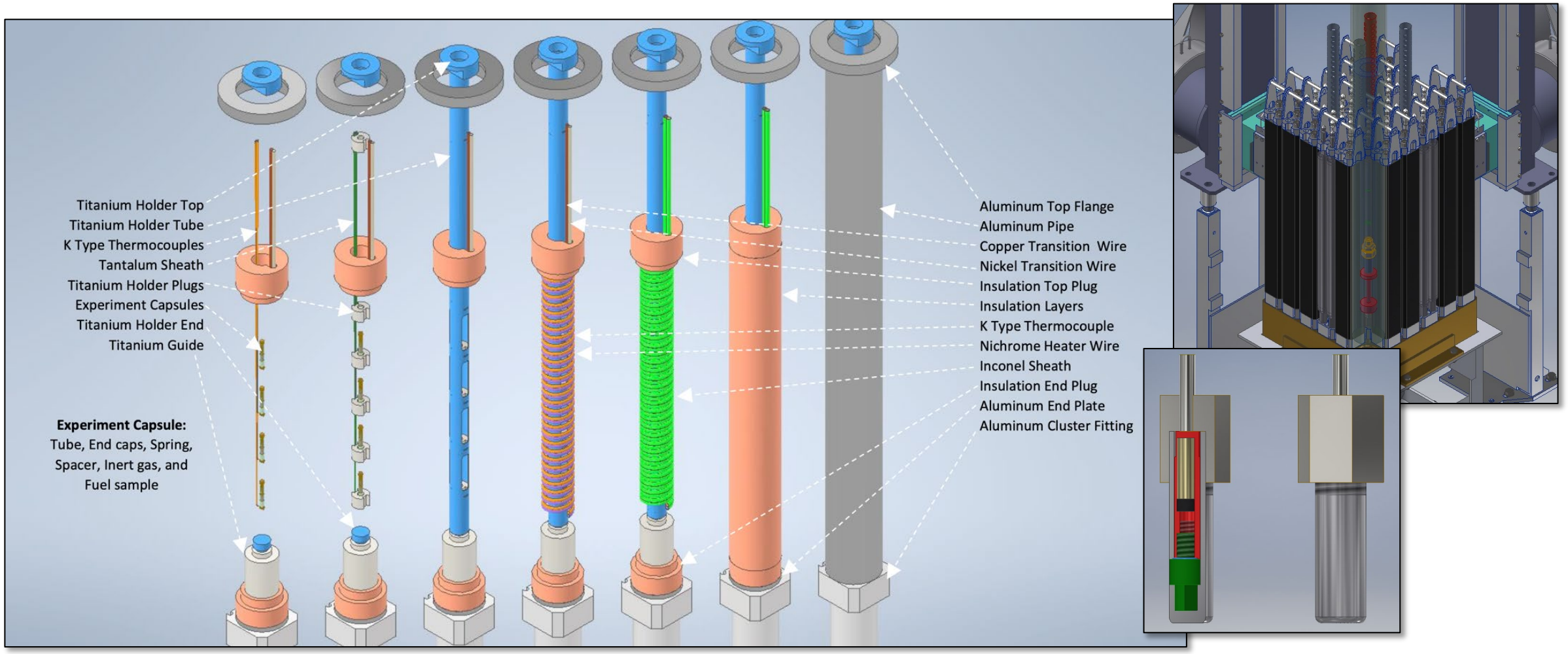
Project Title: Towards fully predictive accelerated irradiations of structural materials

Institution: Idaho National Laboratory

Street Address/City/State/Zip: 2525 North Fremont Ave., Idaho Falls, ID 83415-3860

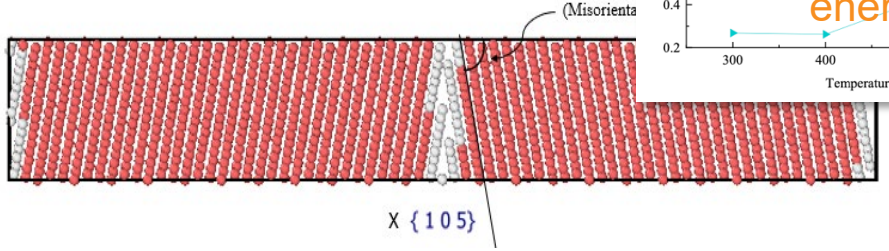
Principal Investigator (PI): Andrea M. Jokisaari

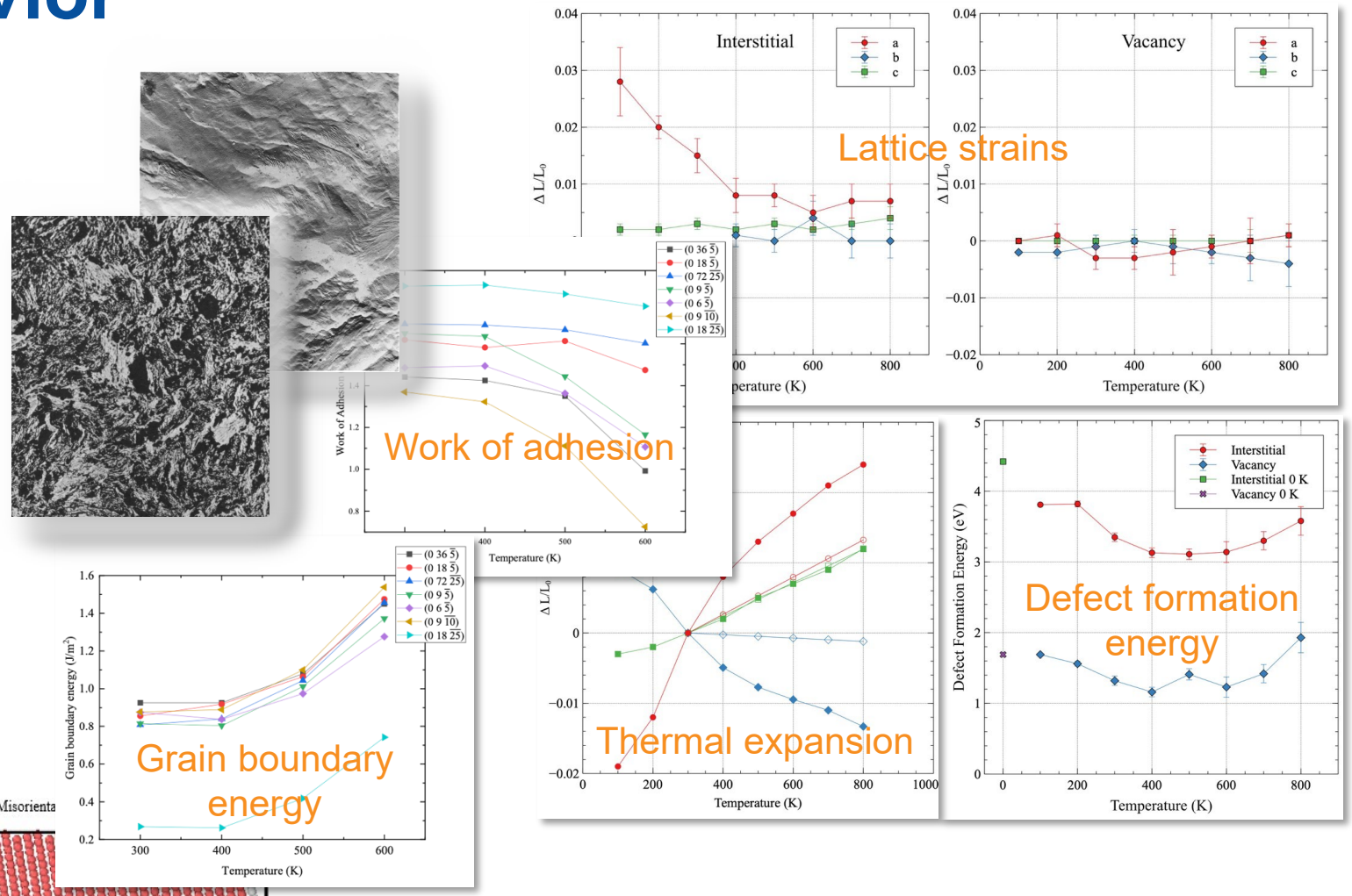
CHARIN furnace efficiently uses neutrons for high-fidelity materials testing



Atomistic investigations suggest several mechanisms for irradiation behavior

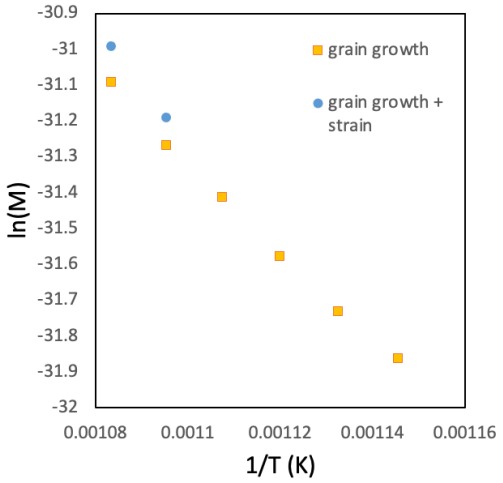
- Extensive characterization of atomistic properties of orthorhombic α-U to understand its anisotropic nature
- Fruitful collaboration between NCSU and INL
  - Two graduate students supported
- Future work involves characterizing grain boundary sink behavior, multi-defect lattice strains

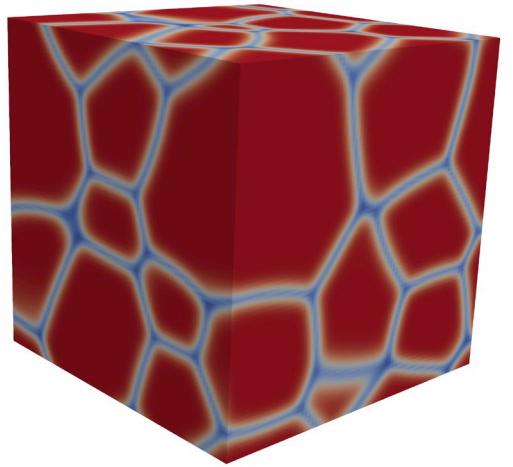


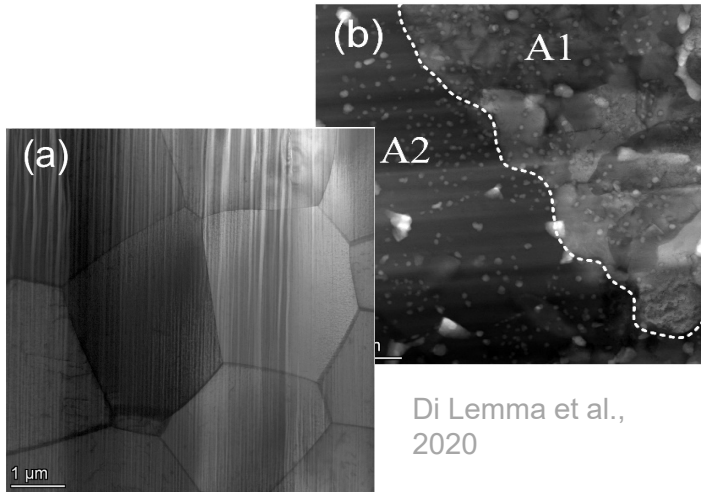


Microstructure evolution simulations are shedding light on thermomechanical behaviors

- Examining impact of thermal strain anisotropy on grain growth using average grain boundary energy and anisotropic thermal strains
  - Grain growth kinetics
  - Texture evolution
- Future work will focus on defect evolution







Di Lemma et al., 2020