NEAMS fuels modeling for HTGRs: FY24 accomplishments and outlook for FY25

Presenter: Jacob Hirschhorn

Contributors (alphabetically): Larry Aagesen, Chaitanya Bhave, Somayajulu Dhulipala, Jacob Hirschhorn, Wen Jiang, Stephen Novascone, Antonio Recuero, Pierre-Clément Simon, Ryan Sweet, and Mathew Swisher

Outline

- NEAMS TRISO modeling background and overview
- Overview of FY24 activities
- FY24 activities detail
- FY24 engagement and broader impacts
- FY25 outlook

NEAMS
Nuclear Energy Advanced Modeling and Simulation

NEAMS TRISO modeling background and overview

2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024
Stage 1						Stage 2				Stage 3		
• Developed and implemented baseline TRISO modeling capabilities in BISON						• Improved internal mesh generation and Monte Carlo capabilities for TRISO simulations • Implemented PARFUME models in BISON • Began incorporating LLS-informed models for select TRISO properties/behaviors • Performed baseline BISON verification and validation (AGR-1, AGR-2, and IAEA CRP-6)				• Implemented fast integration and variance reduction methods for TRISO failure probability • Increased focus on LLS-informed model development, including for layer diffusivities and Pd penetration • Implemented various improvements to matrix property, particle debonding, and gap mass transport models • Expanded BISON validation cases to AGR-3/4 • Developed and implemented advanced uncertainty quantification methods to help identify high-priority improvements		

Looking ahead

- Expand BISON TRISO validation database to AGR-5/6/7, transient experiments, etc.
- Incorporate advanced behavioral models to enable failure probability calculations under realistic conditions
- Enhance and expand models for compact matrix performance

Based on works by W. Jiang.

Overview of FY24 activities

Engineering scale

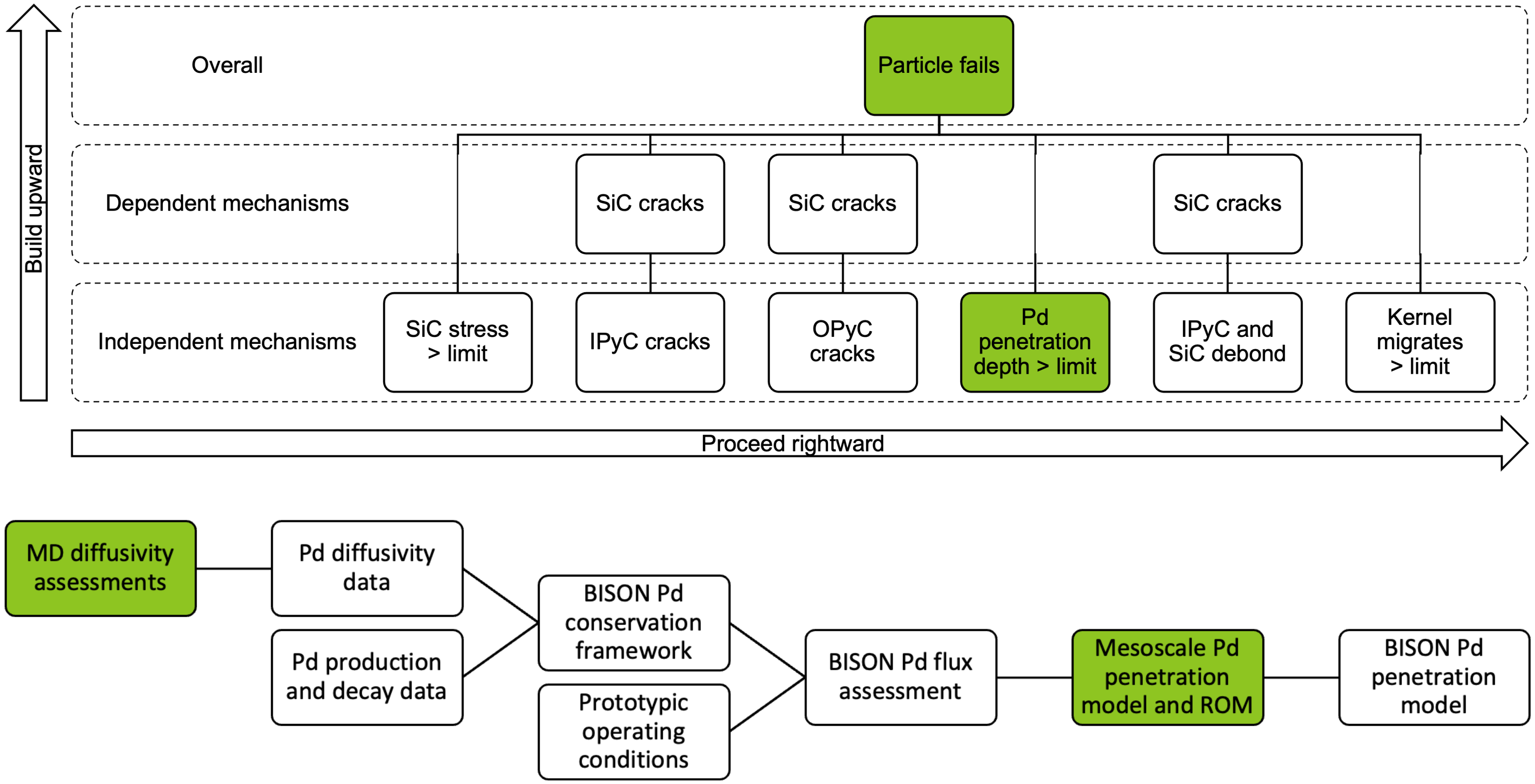
- INL/RPT-24-80567: Complete development of critical capabilities for TRISO fission product source term calculations and quantify mechanisms for Pd penetration of SiC
- INL/RPT-24-78711: Mortar-based cohesive zone model with application to TRISO particle debonding
- INL/RPT-24-79964: Bayesian analysis of TRISO fuel: quantifying model inadequacy, incorporating lower-length-scale effects, and developing parallel active learning capabilities

Lower-length scale

- INL/RPT-24-80441: Lower length scale model for palladium attack of silicon carbide in TRISO fuel

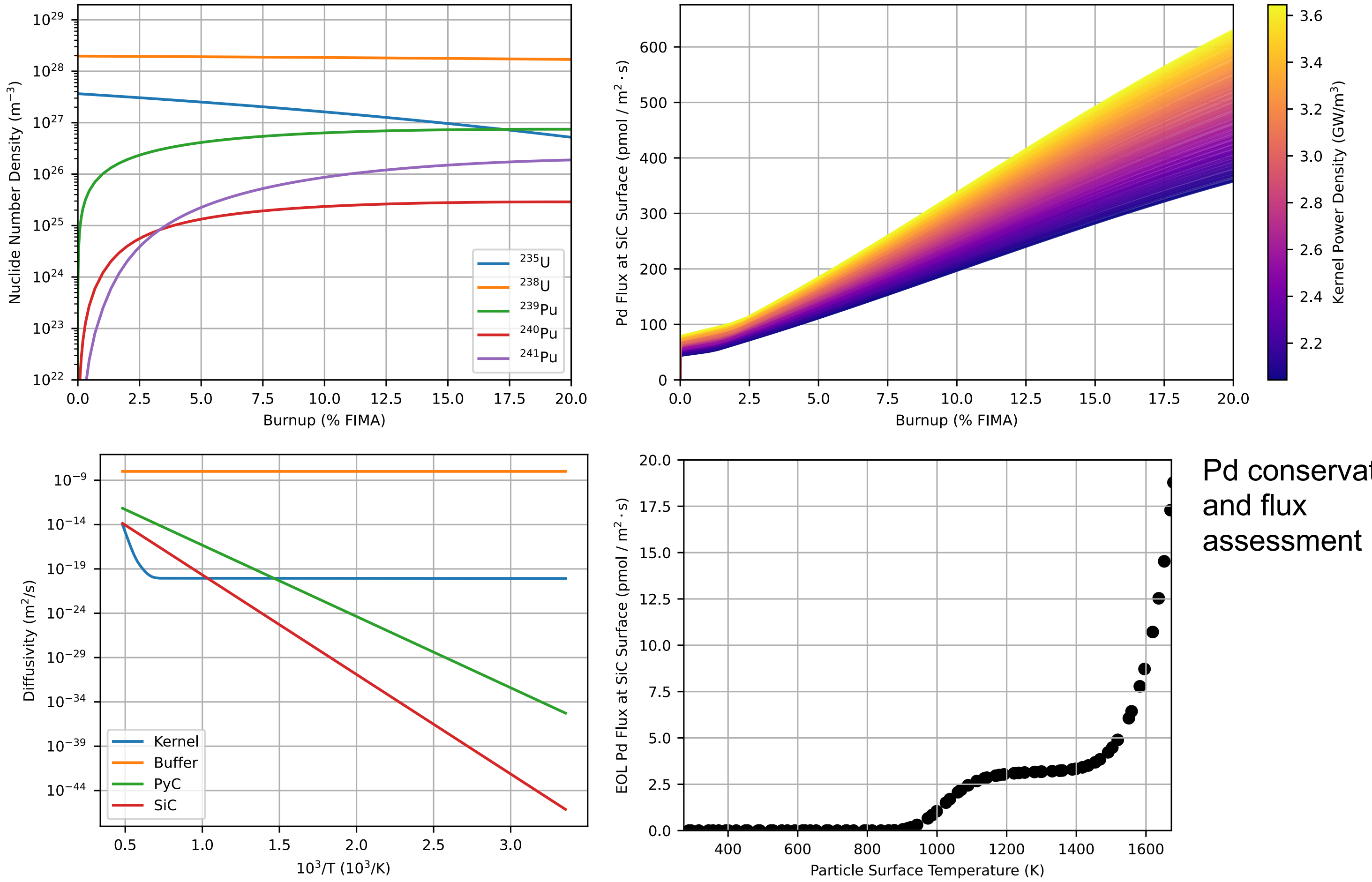
Pd and transport assessment (INL/RPT-24-80567)

- Pd fission products can migrate to and react with the SiC, degrading
  - Structural integrity
  - Fission product retention
- Empirical models
  - Correlate to temperature
  - Were fit to data with considerable scatter
- A mechanistic multiscale modeling framework is being developed



Pd and transport assessment (INL/RPT-24-80567)

- Developed a fuel burnout- and breeding-dependent Pd source term
- Developed a Pd conservation framework using diffusivities from LANL and the literature to model Pd transport, production, and loss
- Assessed Pd fluxes at the SiC surface for a range of particle designs and operating conditions
- The results were used to inform lower-length scale model development



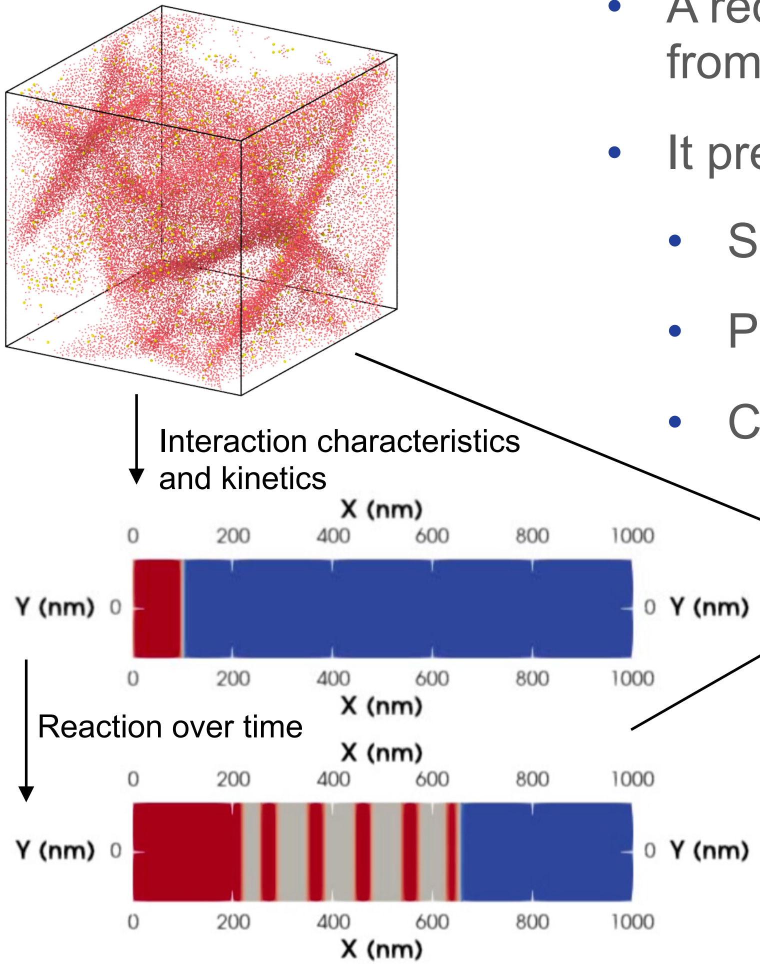
Pd conservation and flux assessment

J. Hirschhorn, et al. INL/RPT-24-80567.

U.S. DEPARTMENT of ENERGY | Office of Nuclear Energy

Mechanistic LLS-informed Pd modeling (INL/RPT-24-80441)

- Molecular dynamics analyses of polycrystalline SiC were conducted to assess
  - Potential energies associated with Pd in various microstructural positions
  - Corresponding diffusivities
- A phase-field model was developed to predict formation of Pd silicides using the
  - Pd flux assessed at the engineering scale
  - Properties assessed at the atomistic scale



Simulation results demonstrate that interaction microstructure (lamellar versus precipitates) depends on the spatial heterogeneity of the applied mass flux

- A reduced order model (ROM) was developed from the phase-field model for use in BISON
- It predicts Pd penetration as a function of
  - SiC grain structure
  - Pd and SiC reactant kinetics
  - Change in Pd flux with penetration depth

$$P_{Pd}(t) = \sqrt[3]{\frac{18V_m f r_{SiC}^2}{\pi}\int_{t=0}^{t} J_{Pd}(t)dt + r_{SiC}^3} - r_{SiC},$$

Incorporates the thermodynamics of Pd silicide formation to describe the depth of interaction region as a function of mass flux

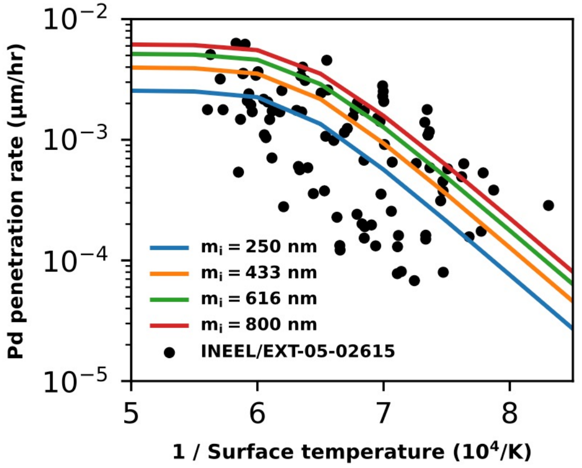
$$f = \frac{m_i D_{Pd}^{GB}}{2d_{GB}D_{Pd}^{GB} + (m_i - 2d_{GB})D_{Pd}^{bulk}}.$$

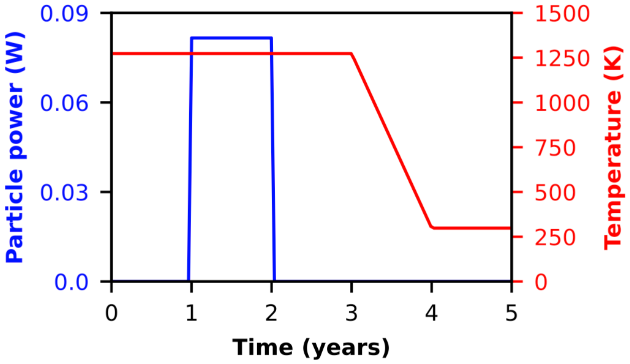
Accounts for microstructural and geometric effects

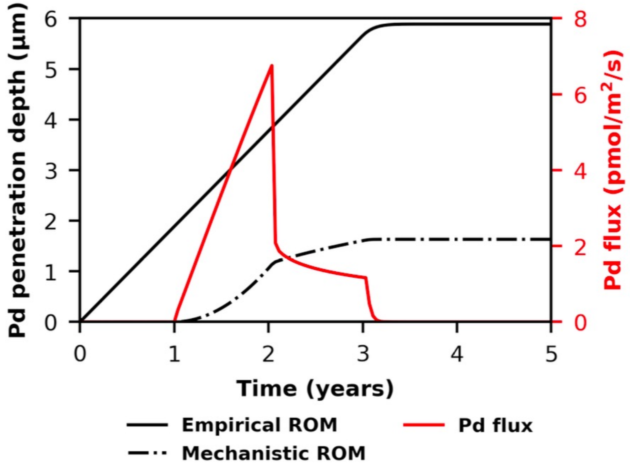
Mechanistic LLS-informed Pd modeling (INL/RPT-24-80441)

- Preliminary demonstration and validation exercises exhibit the expected behaviors
  - The ROM predicts reasonable Pd penetration rates and suggests possible explanations for the data scatter
  - The ROM offers improves performance over the empirical correlation for time-varying operating conditions due to its sensitivity to Pd inventory and mass flux
- FY25 work will focus on
  - Investigating the impacts of Ag on Pd–SiC thermodynamics and kinetics
  - Refining the phase-field model and the associated BISON ROM
  - Validating the models to legacy data and quantifying uncertainties

Comparison to legacy experimental data



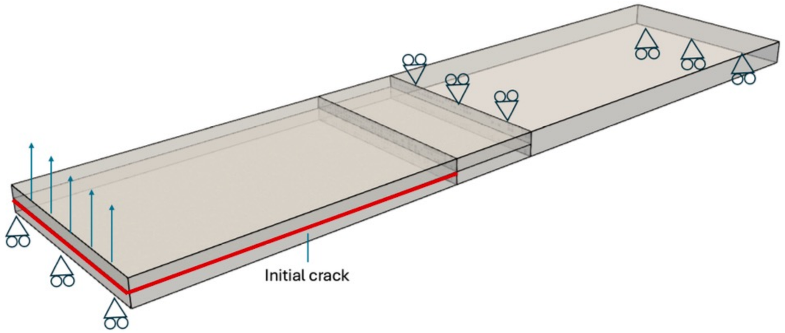


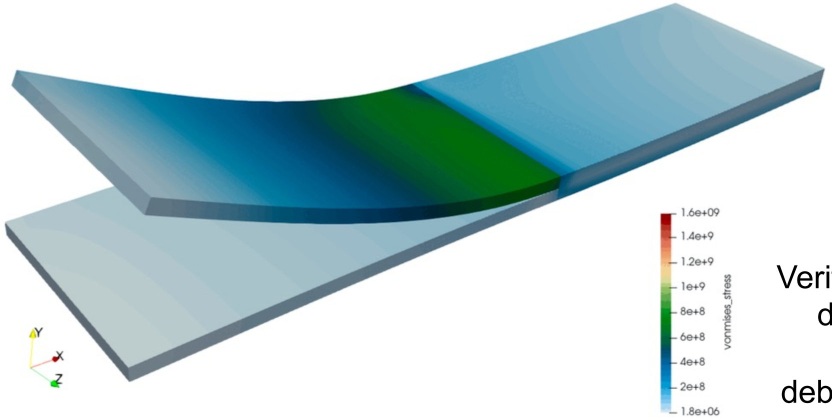


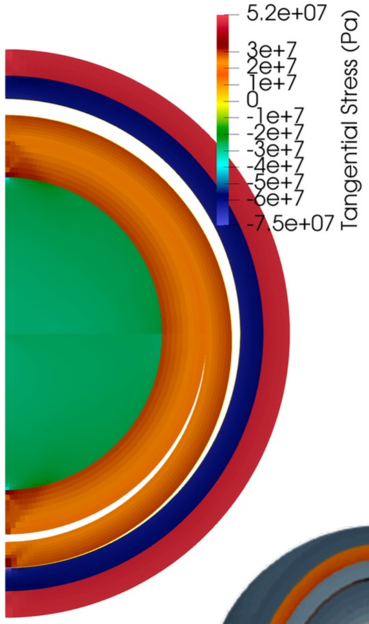
Realistic dependencies on particle Pd inventory and temperature

Mortar cohesive zone debonding modeling (INL/RPT-24-78711)

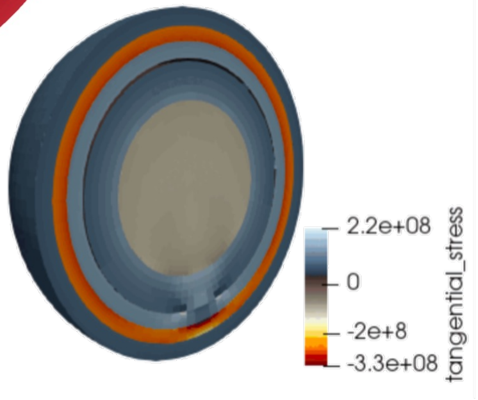
- A preliminary mortar formulation for cohesive zone modeling was developed, implemented, and demonstrated
- The model improves the robustness and accuracy of TRISO debonding calculations, enabling more realistic simulations of
  - Asymmetric particle temperature distributions due to partial debonding
  - Fission product transport
  - Cascading multiphysics failure behaviors







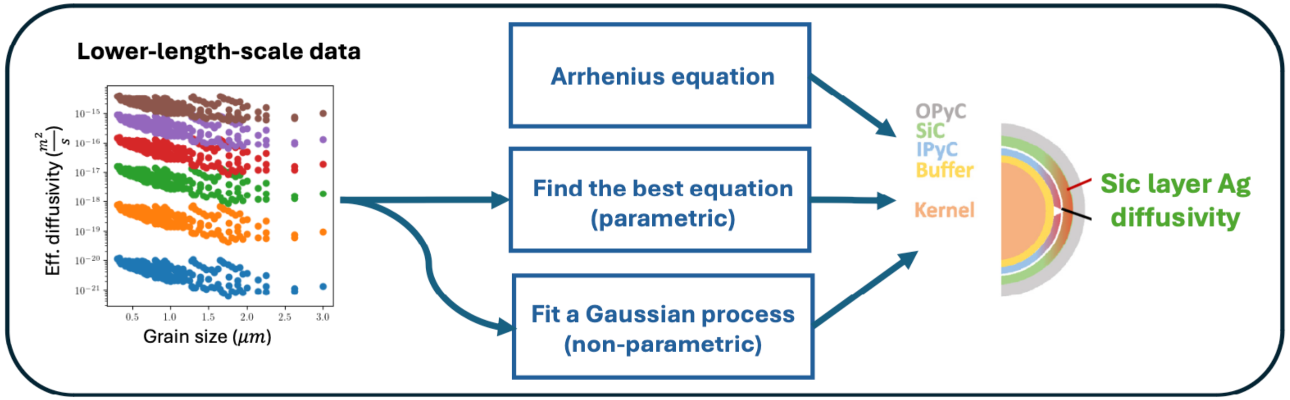
Verification exercises demonstrate more realistic partial debonding behaviors



A. Recuero, et al. INL/RPT-24-78711.

Bayesian analysis of model inadequacy (INL/RPT-24-79964)

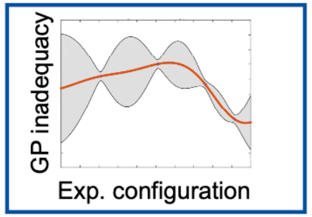
- Parametric and non-parametric methods for incorporating LLS-informed TRISO models into BISON were assessed against empirical Ag diffusivities
- A new Bayesian framework was developed, implemented, and applied to AGR-1. AGR-2. and AGR-3/4 data and assessments, allowing quantification of uncertainties associated with
  - Model inadequacy (including physics and operating conditions)
  - Model parameters
  - Experimental noise



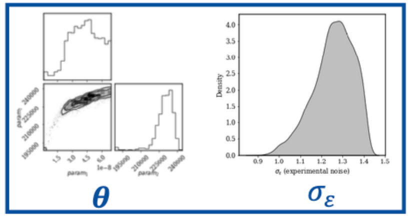
Module 1
Best estimate of the model parameters $\boldsymbol{\theta}$

Standard Bayesian calibration
or
Deterministic optimization

Module 2
GP inadequacy term hyper-parameters $\boldsymbol{\gamma}_\delta$

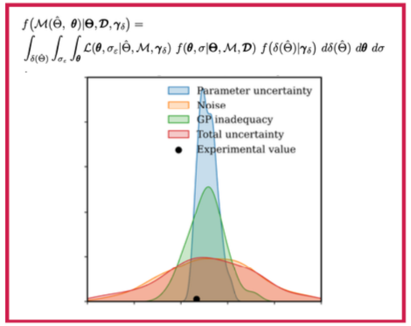


Module 3
Inverse UQ of $\{\boldsymbol{\theta}, \sigma_\varepsilon\}$



Bootstrapping the experimental data into two batches for fitting the GP inadequacy term and performing inverse UQ. Associated sensitivity analyses.

Module 4
Posterior predictive distribution



Uncertainty contributions can be applied to identify high-priority improvements

FY24 engagement and broader impacts

DOE programs

- Advanced Reactor Technologies
  - Supported development of multi-scale simulations for TRISO transient fuel performance and experiment design/interpretation
- Advanced Gas Reactor
  - Supported development of preliminary nuclide-specific fission product source terms with Griffin
  - Supported development of multi-scale simulations for AGR-3/4 re-irradiation experiments

Industry and academia

- Delivered BISON trainings
  - For general audiences in a university setting
  - Directly to industry partners
- Participated in various direct industry collaborations
  - Provided continuing routine and on-demand support
  - Literature review and BISON upkeep
  - VTB upkeep
- FY24 journal articles to date: 1 published, 2 in preparation/review

Overview of FY25 activities

Engineering scale

- Implement user-friendly mortar debonding models for TRISO coating layers using Advanced Gas Reactor Program material property data and apply uncertainty quantification to begin to assess model adequacy and data needs
- Update and refine TRISO assessment input files to better represent recent developments and to be consistent for TRISO simulations
- Develop assessments for particle fuel transient experiments and separate effects tests
- Begin to assess thermal, mass, and particle-particle stress interactions at the compact scale to provide guidance for follow-on work focused on matrix performance

Lower-length scale

- Investigate high-temperature Pd-Ag-SiC interaction mechanisms using molecular dynamics and incorporate them into the Pd penetration phase-field model
- Complete expansion of the existing multiscale low-temperature Pd penetration model to account for high temperatures and Ag interactions, validate models against experimental data, and quantify uncertainties associated with its predictions

FY26 and beyond

- Near-term NEAMS Fuels TRISO priorities
  - **Demonstrate the ability to model observed failure behaviors** by validating Pd penetration models to AGR and separate effects data and incorporating them into failure probability calculations
  - **Bolster the existing BISON validation database** by developing and extending assessments for steady-state, transient, and separate effects experiments
  - **Support qualification, licensing, and further development** through broad and systematic application of uncertainty quantification
  - **Increase prediction accuracy** by investing in material property and behavioral model development for pyrolytic carbon, SiC, and UCO
- We are here for you, and we need your feedback
- Questions and comments: Jacob.Hirschhorn@inl.gov

Improve understanding and predictive capabilities

Facilitate qualification, licensing, and deployment

Support operating margin reduction

U.S. DEPARTMENT of ENERGY

Office of Nuclear Energy

Uranium nitride fuels

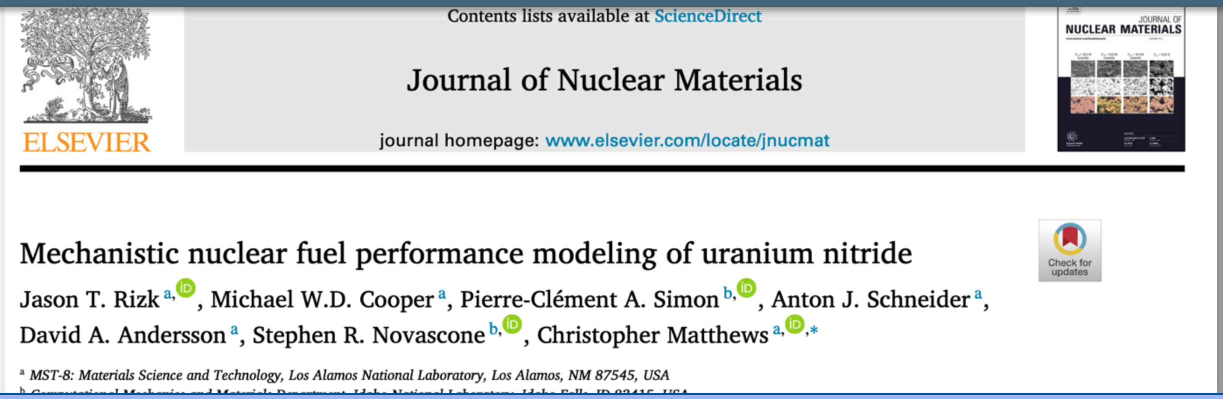
Presenter: Christopher (Topher) Matthews

Contributors: Michael Cooper, Anton Schneider, P.C. Simon

Uranium Nitride: Recent Accomplishments

- Developed first-of-a-kind mechanistic model for UN fission gas release and swelling
  - Revived dislocation model in BISON
  - Adapted lower-length scale UN parameters
- Quantitatively capturing swelling behavior in UN
- Expanded assessment data base and high burnup extension forthcoming in FY25

Uranium nitride capable BISON ready for external users


ELSEVIER

Contents lists available at ScienceDirect

Journal of Nuclear Materials

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

Mechanistic nuclear fuel performance modeling of uranium nitride

Jason T. Rizk [a], Michael W.D. Cooper [a], Pierre-Clément A. Simon [b], Anton J. Schneider [a], David A. Andersson [a], Stephen R. Novascone [b], Christopher Matthews [a,*]

[a] MST-8: Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Continuing work focused on 1) chemistry dependence, 2) porosity dependence, and 3) application to TRISO

Lower Length Scale (DFT & EP)
- Defect stability and kinetics
  - U_i, V_U
  - N_i, V_N
  - {$2U_i$}
  - {$Xe:2V_U$}
  - etc.

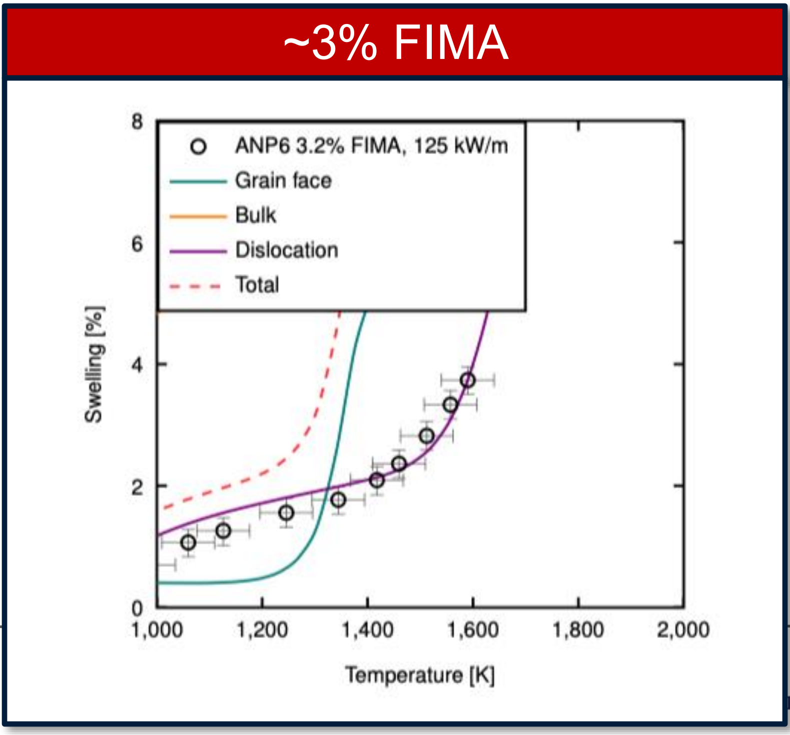
- Defect stability & mobility

Meso-Scale (Centipede)
- Free Energy Cluster Dynamics (FECD)
  - Defect concentrations (irradiation-enhanced)
  - Self-diffusivity
  - Gas atom diffusivity
  - Defect clusters
  - Perfect interstitial dislocation loops
- Sensitivity to temperature, chemistry, and irradiation

CALPHAD calculations

- Sink strength

Engineering-Scale (BISON)
- SIFGRS: Fission Gas Model
  - Fission gas concentration
  - Bubble formation and growth
  - Collection along dislocations and grain boundaries
  - Fission gas release
  - Swelling

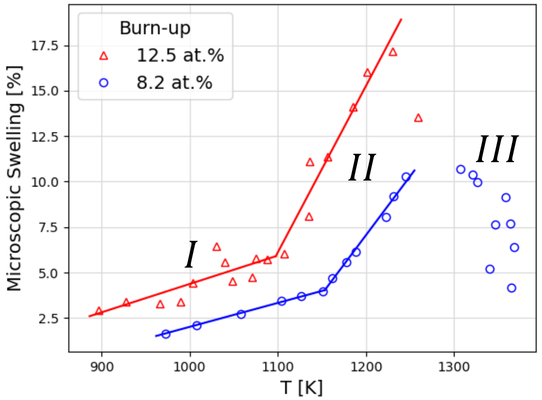


UN Modeling Approach: Capture breakaway swelling first

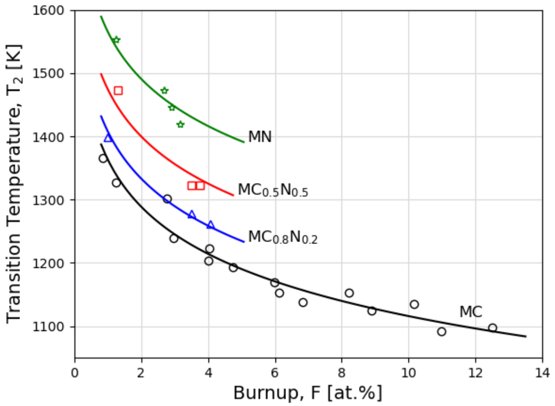
Mechanistic modeling allowed for mechanism not to be picked a priori

Experimental observation: “Breakaway Swelling”

- Sudden change in the rate that microscopic swelling increases with temperature once a threshold temperature is reached (Region $I \rightarrow II$)
- Greater burn-up causes lower transition temperatures



Microscopic swelling in MC



The transition temperature ($I \rightarrow II$) for breakaway swelling in MCN fuel

- Region II associated with both larger intra- and inter-granular bubbles
- Third region (III) of decreased swelling after a greater threshold temperature
  - Large interconnected grain boundary bubbles
  - Release of gas from grain interior into porosity

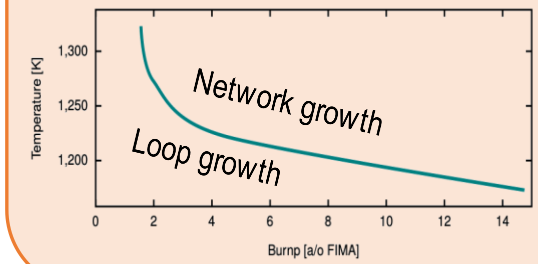
Need to understand this phenomenon for mechanistic fuel performance model

M. Colin, M. Coquerelle, I. L. F. Ray, C. Ronchi, C. T. Walker, H. Blank, *Nuclear Technology* 63, 442, 1983

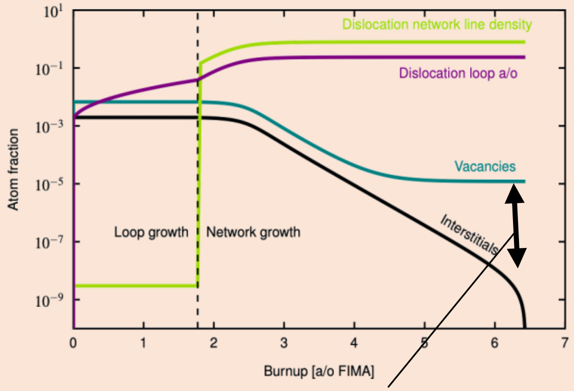
Mechanism(s) responsible for the transition?

Extended defects consume point defects?

- The dislocation network more efficiently traps interstitials
- Vacancies trap at bubbles instead of annihilating through recombination



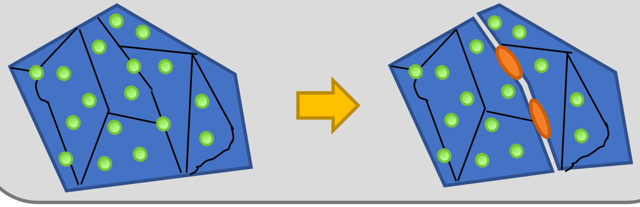
Calculated defect concentrations



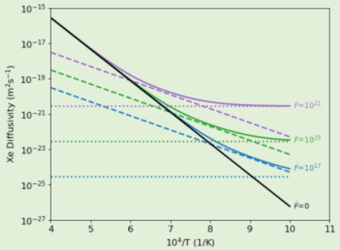
Increasing gap between point defect concentrations

Recrystallization?

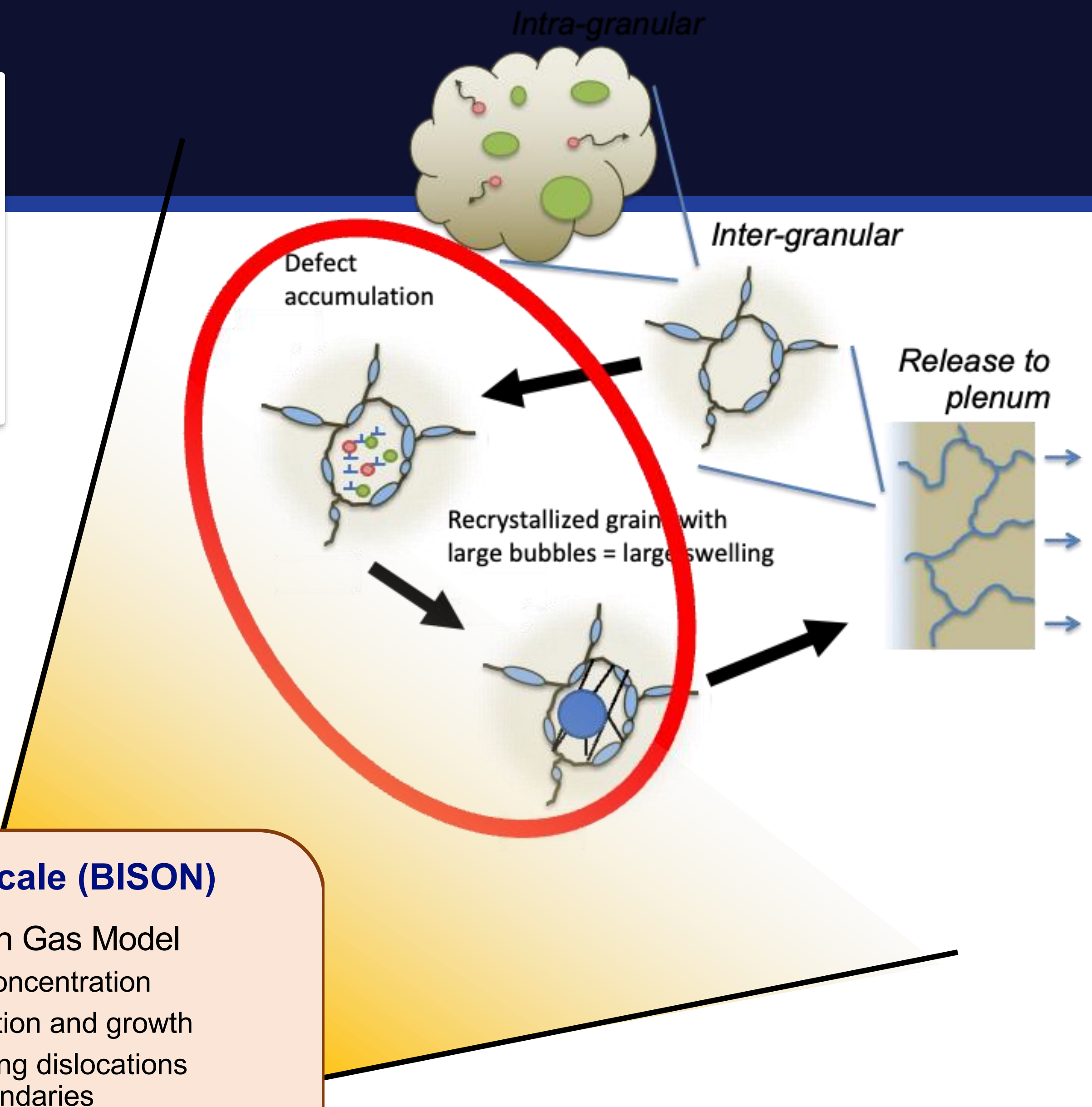
- The accumulation of extended defects makes it energetically favorable to form new grain boundaries
- Grain boundaries trap gas atoms and grow larger bubbles



Diffusion mechanism transition?



Modeling plan:
- Start with UO_2
- Adapt for UN



Lower Length Scale (DFT & EP)

- Defect stability and kinetics
  - U_i, V_U
  - N_i, V_N
  - $\{2U_i\}$
  - $\{Xe:2V_U\}$
  - etc.

- Defect stability & mobility

Meso-Scale (Centipede)

- Free Energy Cluster Dynamics (FECD)
  - Defect concentrations (irradiation-enhanced)
  - Self-diffusivity
  - Gas atom diffusivity
  - Defect clusters
  - Perfect interstitial dislocation loops
- Sensitivity to temperature, chemistry, and irradiation

CALPHAD calculations

- Sink strength

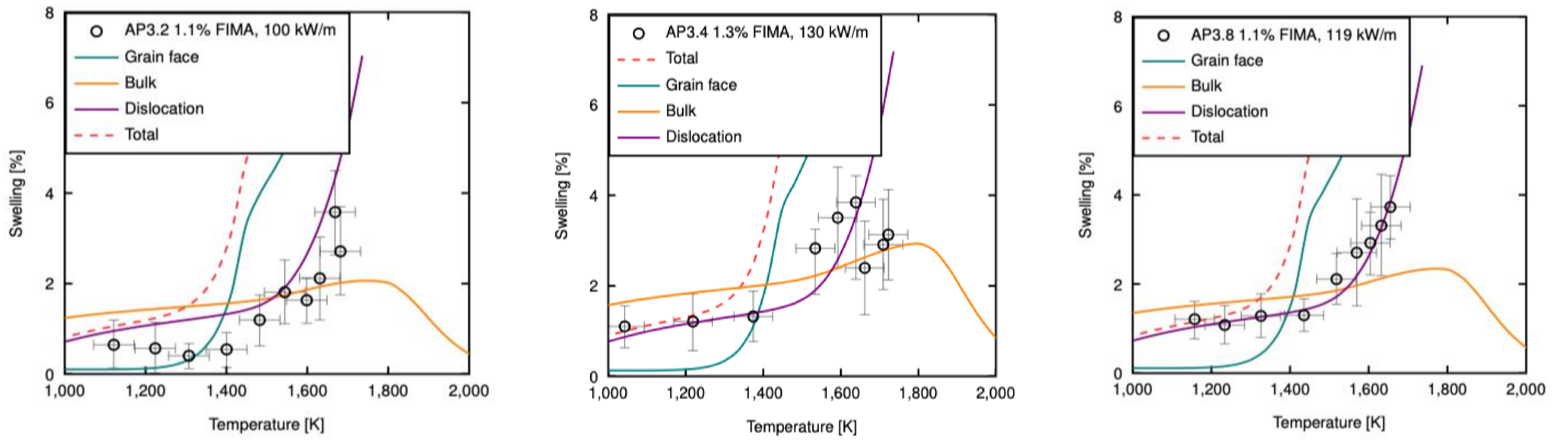
Engineering-Scale (BISON)

- SIFGRS: Fission Gas Model
  - Fission gas concentration
  - Bubble formation and growth
  - Collection along dislocations and grain boundaries
  - Fission gas release
  - Swelling

Mechanistic Model Results

- Quantitative Comparison to data with (almost) no calibration
- Upturn corresponds to self-diffusivity
- Constant dislocation density

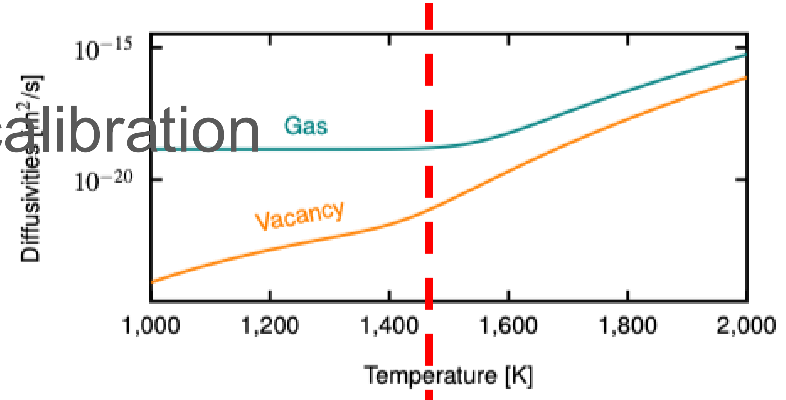
~1% FIMA



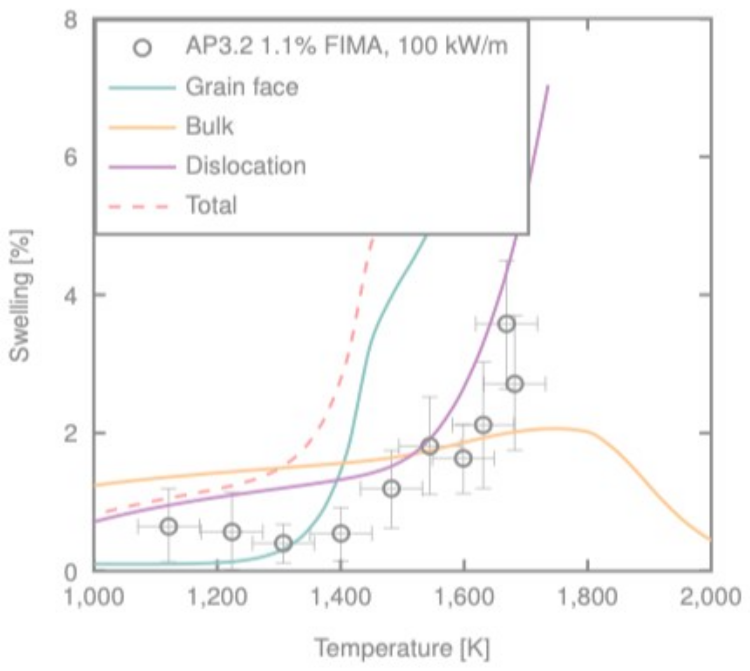
Mechanistic Model Results

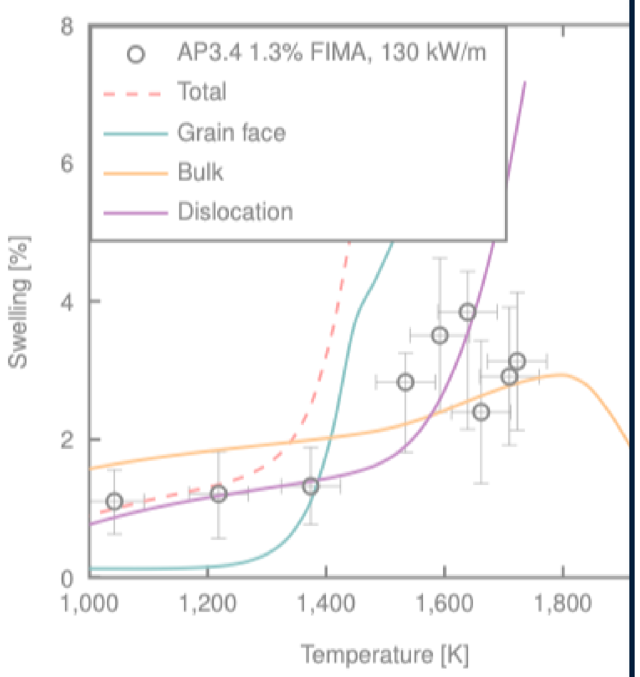
- Quantitative Comparison to data with (almost) no calibration
- Upturn corresponds to self-diffusivity
- Constant dislocation density

Diffusivities

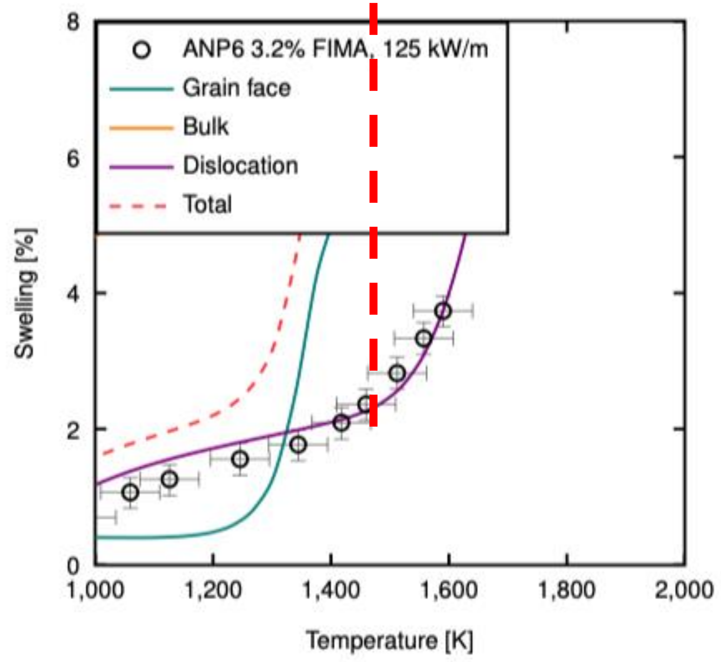


~1% FIMA





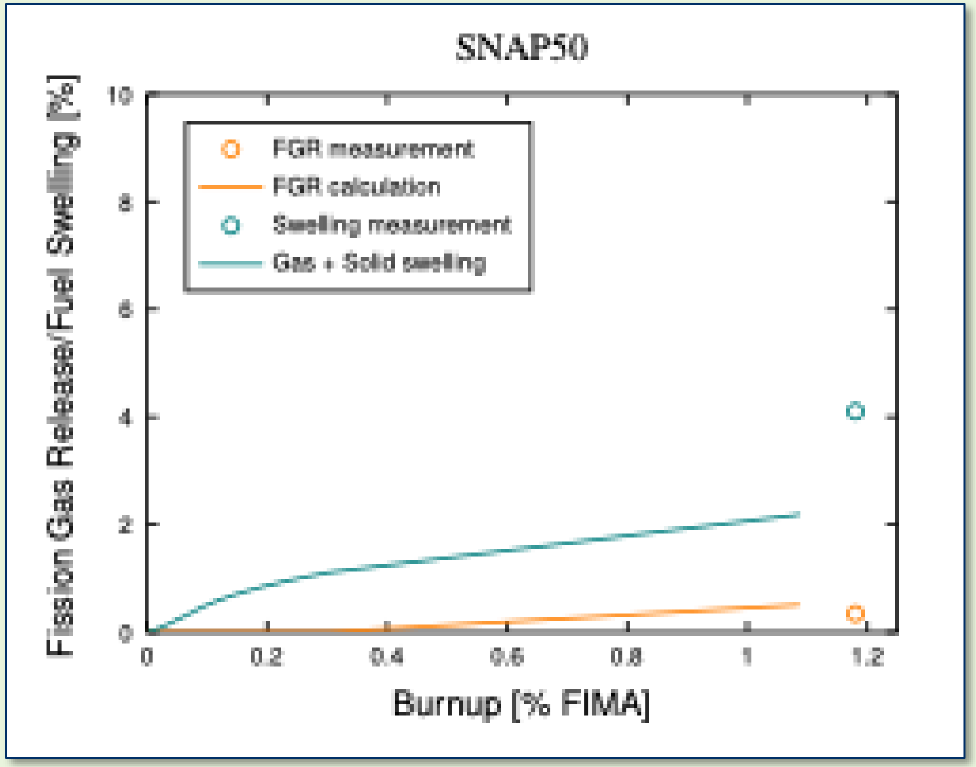
~3% FIMA



Integral experiments: Combined assessments with same parameters

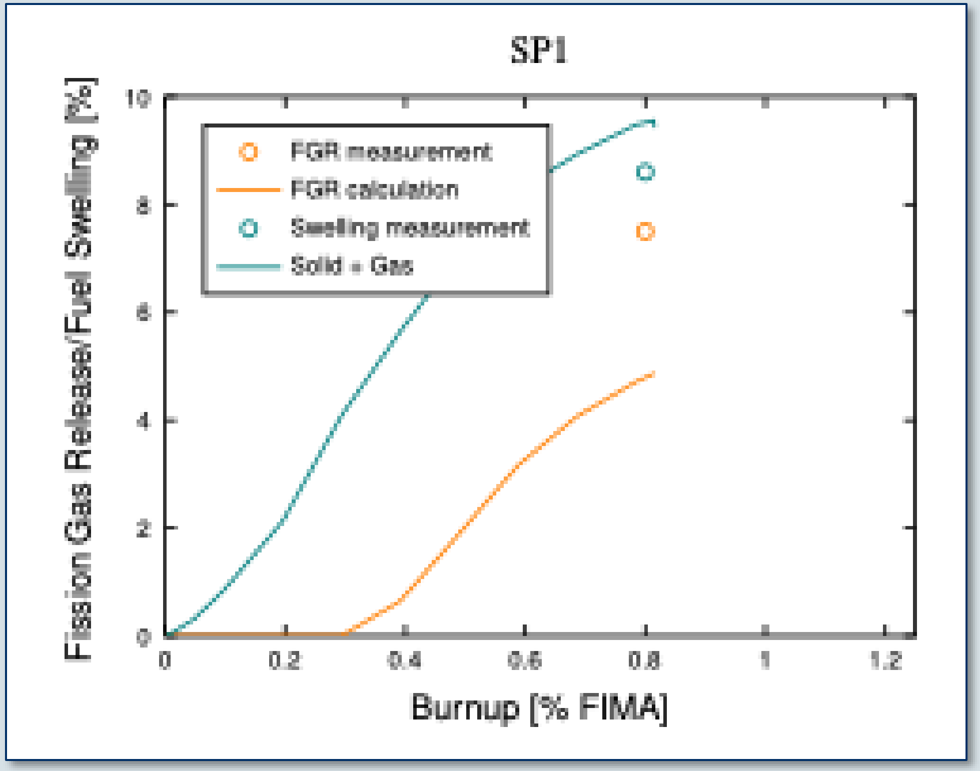
SNAP50-57-672 (MTR)

- Model with best historical data
- Temperatures [K]: 1430, 1500 (avg, max)
- Fsnrates [fsn/m^3/s]: 1-1.5x10^{19} (avg, max)



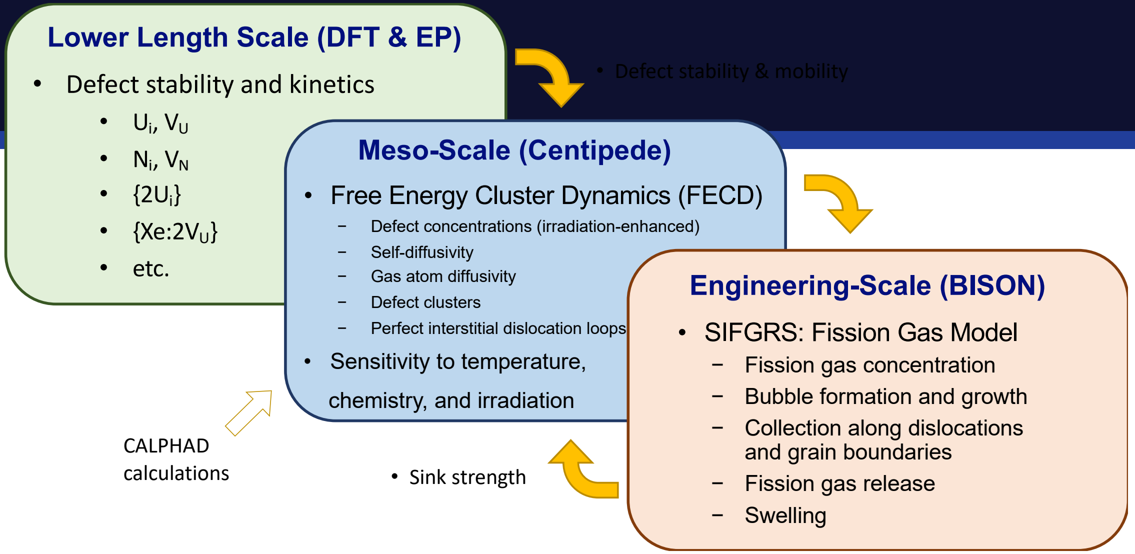
SP1 (EBR-II)

- Model with best historical data
- Temperatures [K]: 1800, 2050 (avg, max)
- Fsnrates [fsn/m^3/s]: 3-3.3x10^{19} (avg, max)

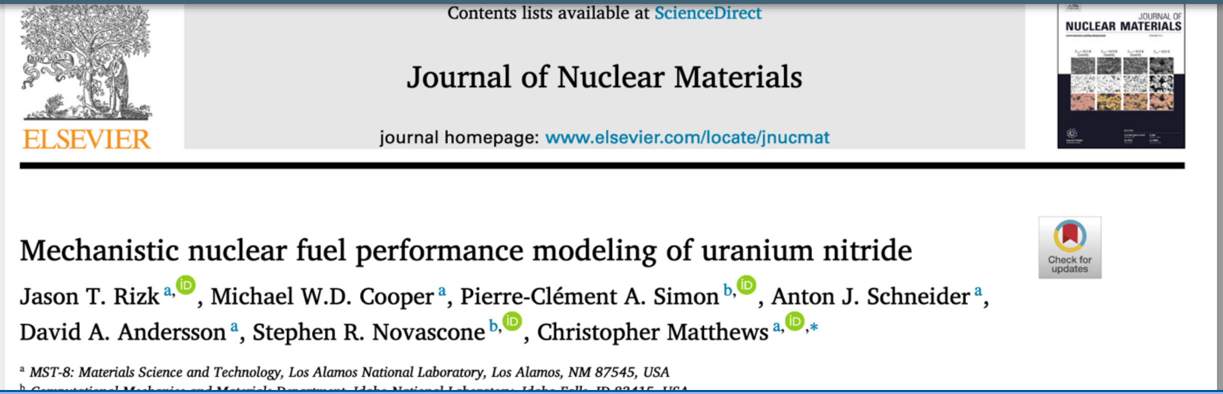


Uranium Nitride: Recent Accomplishments

- Developed first-of-a-kind mechanistic model for UN fission gas release and swelling
  - Revived dislocation model in BISON
  - Adapted lower-length scale UN parameters
- Quantitatively capturing swelling behavior in UN
- Expanded assessment data base and high burnup extension forthcoming in FY25



Uranium nitride capable BISON ready for external users


Contents lists available at ScienceDirect

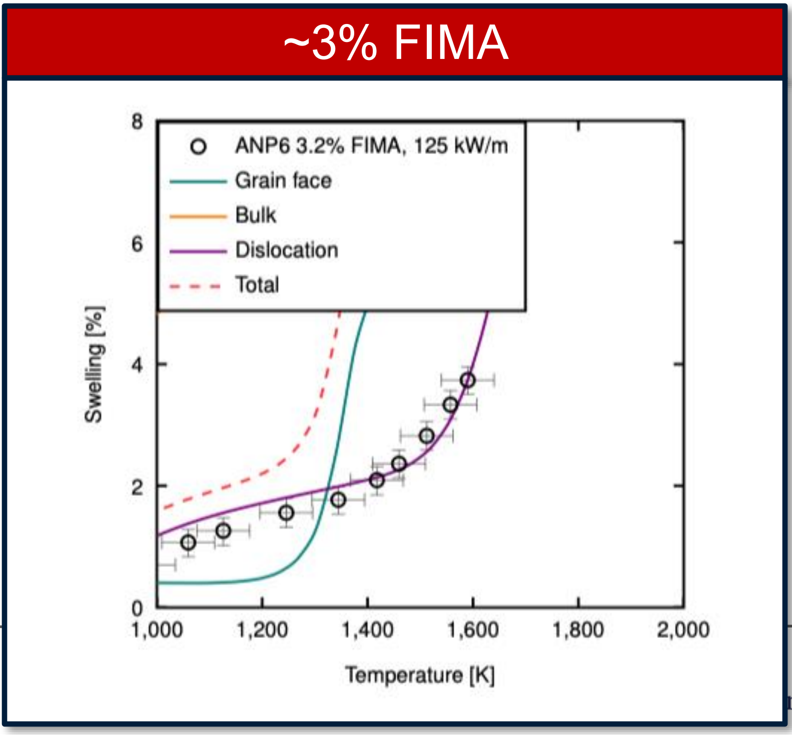
Journal of Nuclear Materials

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

Mechanistic nuclear fuel performance modeling of uranium nitride

Jason T. Rizk [a], Michael W.D. Cooper [a], Pierre-Clément A. Simon [b], Anton J. Schneider [a], David A. Andersson [a], Stephen R. Novascone [b], Christopher Matthews [a,*]

[a] MST-8: Materials Science and Technology, Los Alamos National Laboratory, Los Alamos, NM 87545, USA



Continuing work focused on 1) chemistry dependence, 2) porosity dependence, and 3) application to TRISO