INL/MIS-18-51680-Revision-0

Case Studies in Meso-scale Research to Improve Engineering-Scale Predictions

Jason D Hales, Kyle A Gamble, Sudipta Biswas, Andrea M Jokisaari

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Jason D. Hales
Idaho National Laboratory

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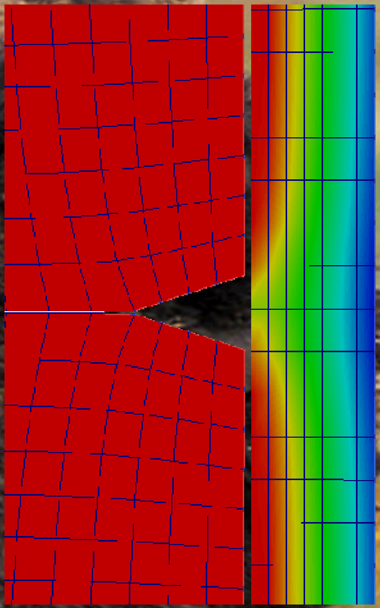
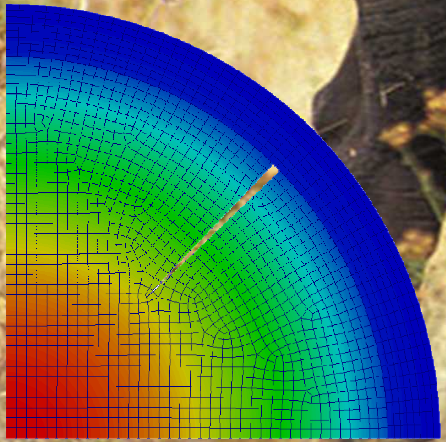
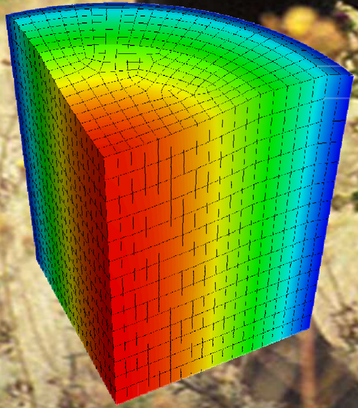
Bison: What is it?

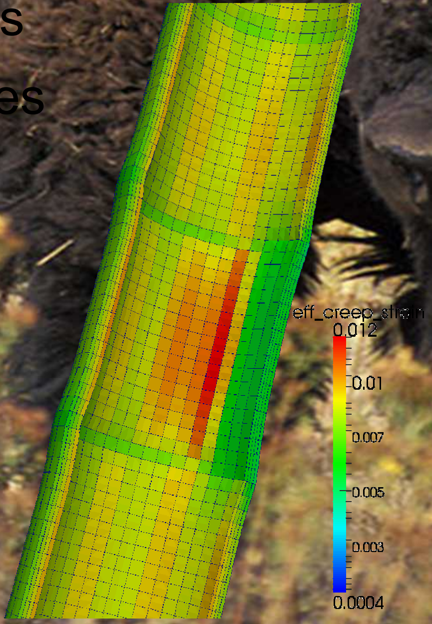
A finite element, thermo-mechanics code with material models and other customizations to analyze nuclear fuel

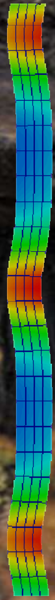
- Accepts user-defined meshes/geometries
  - 1D, 2D, or 3D
- Runs on one processor or many
- Analyzes a variety of fuel types
- Couples to other analysis codes

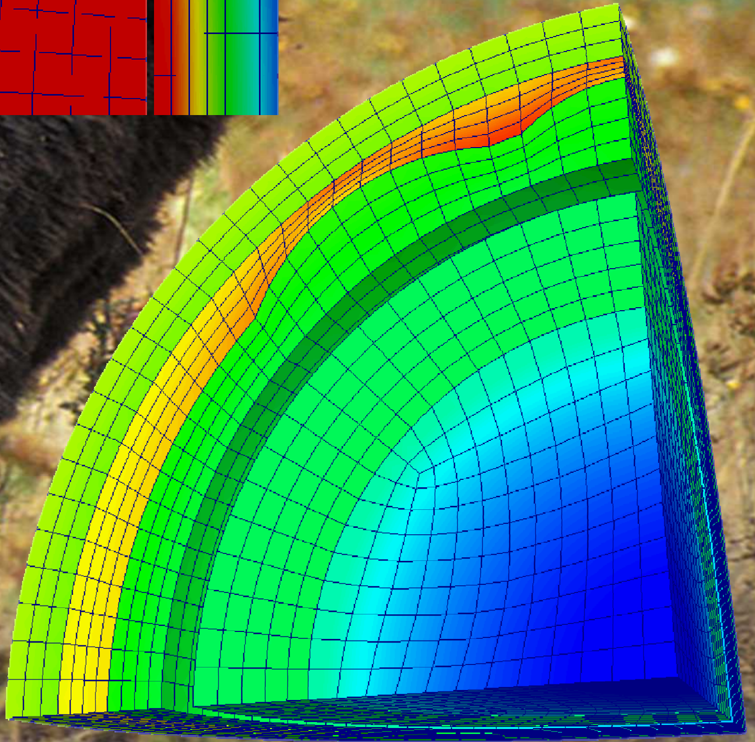








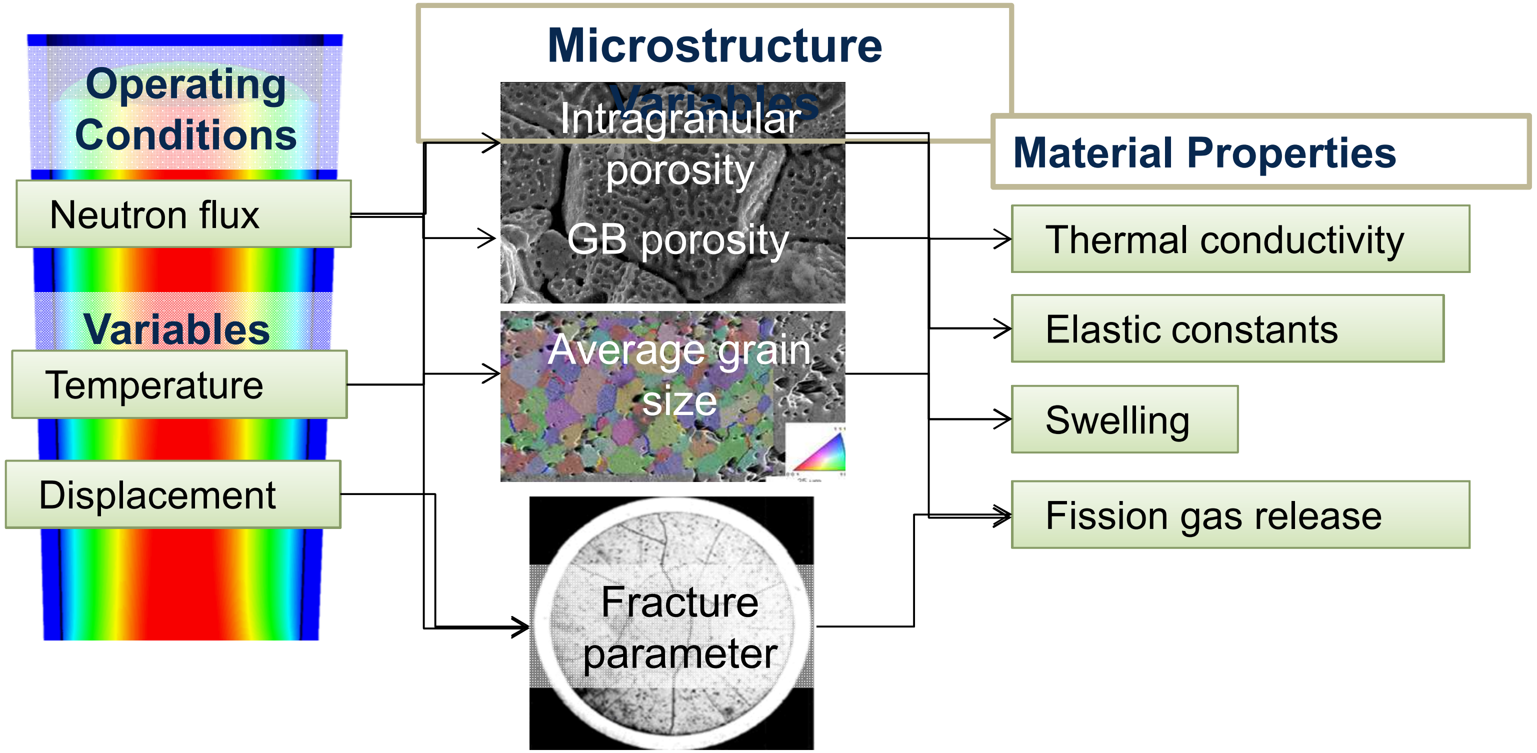




Typical Bison Swelling Correlations

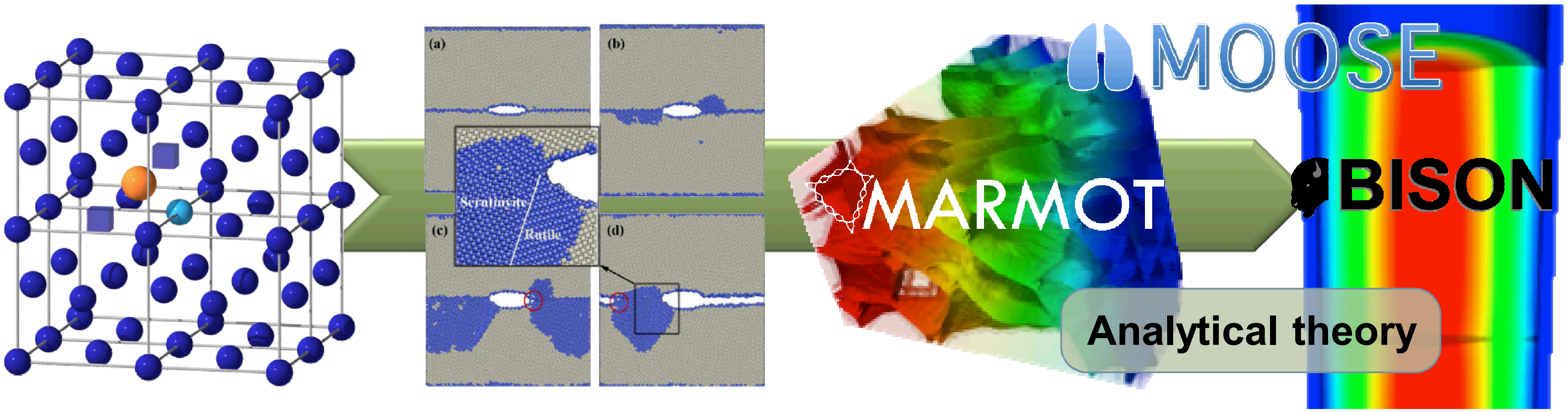
$$\Delta\varepsilon_{sw-s} = 5.577 \times 10^{-5}\rho\Delta Bu$$

$$\Delta\varepsilon_{sw-g} = 1.96 \times 10^{-31}\rho\Delta Bu(2800 - T)^{11.73}e^{-0.0162(2800-T)}e^{-0.0178\rho Bu}$$



Multiscale Material Model Development for ATF Concepts

- Atomistic simulations provide a means to identify mechanisms and properties for materials without significant experimental data available.
- Marmot simulations will provide basis to begin developing material models for Bison for ATF materials



- Thermal conductivity degradation, fission gas behavior, and swelling of U3Si2 are largely unknown at LWR temperatures
- This is an opportunity to apply our multi-scale approach
- We are also looking into the nonlinear behavior of FeCrAl (creep, hardening, burst behavior)

Accident Tolerant Fuel

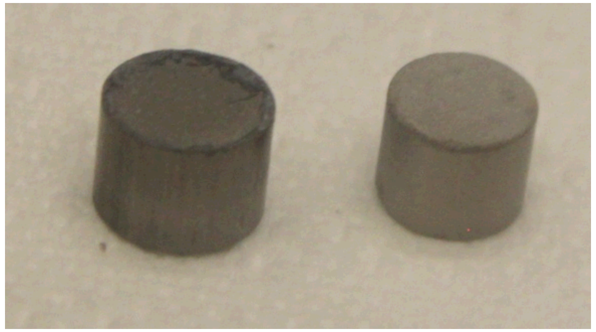
Understanding the swelling behavior of U_3Si_2

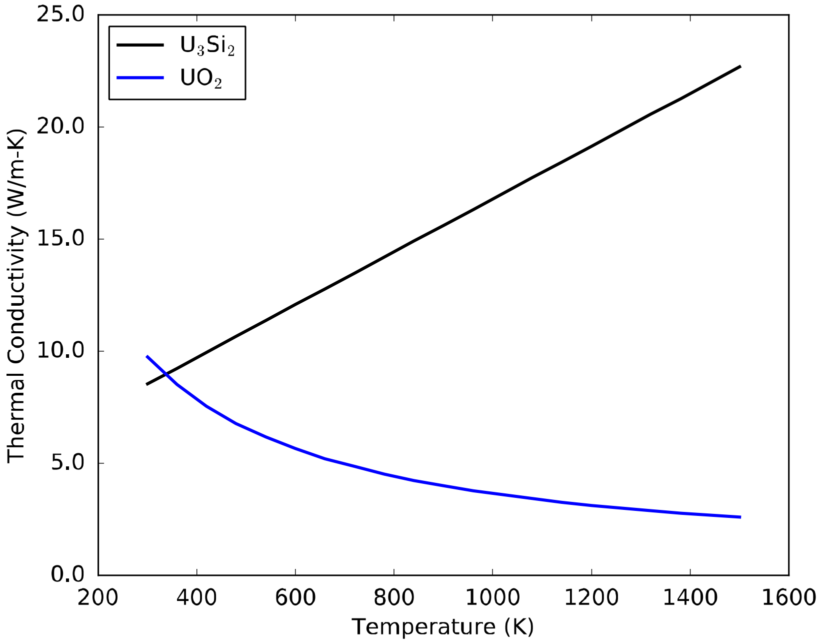
Kyle A. Gamble
Idaho National Laboratory

Uranium Silicide as a fuel in LWRs

- Uranium Silicide (U_3Si_2) is being considered as a replacement for UO_2 in LWR fuel rods. It is of interest because of its considerably higher thermal conductivity and uranium density compared to UO_2.
  - A higher thermal conductivity is expected to lead to less fuel cracking and fission gas release.

- Potential concerns with U_3Si_2 include a significantly lower melting temperature (~1938 K) and the possibility of rapid gaseous fission product swelling.

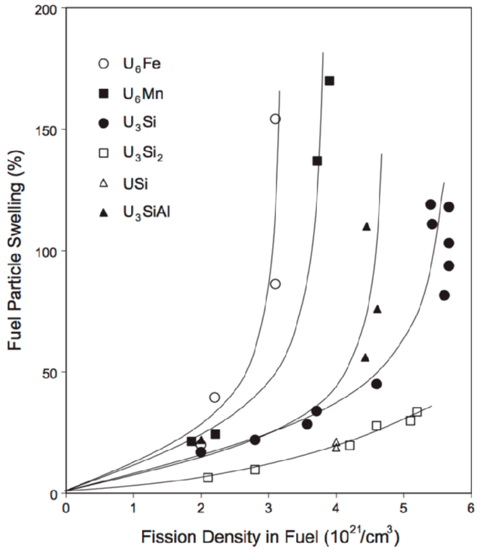




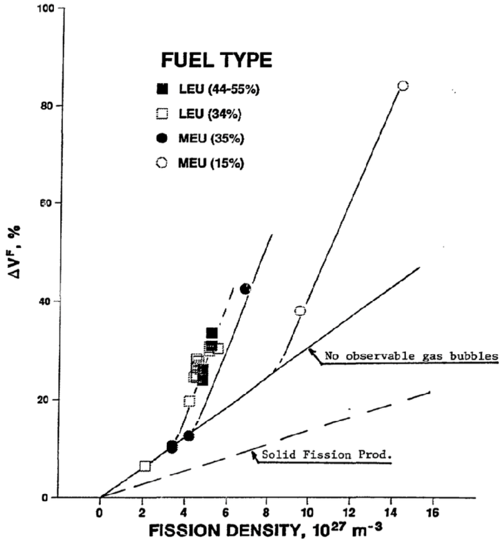
Unirradiated Thermal Conductivity

Empirical Gaseous Swelling Model

- Existing swelling data is from low temperature research reactors and a preliminary swelling model was developed.
- Fission density in the fuel was converted to burnup in FIMA using a conversion factor of: 3.63457×10^{-23}.
- Subtraction of the linear solid swelling based upon data of Hoffman and Ryu (1989) from the total given by the data of Finlay et al. (2004) gives the gaseous component.



M. R. Finlay et al., “Irradiation behaviour of uranium silicide compounds,”JNM, **325**, 2004, p. 118-128



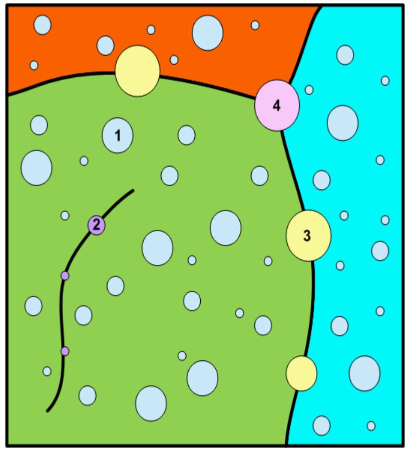
G. L. Hofman and W. S. Ryu, “Detailed Analysis of Uranium Silicide Dispersion Fuel Swelling,” Tech. Report CONF-8909141, ANL, 1989

$$\left(\frac{\Delta V}{V_o}\right)_{solid} = 0.34392Bu$$

$$\left(\frac{\Delta V}{V_o}\right)_{gaseous} = 3.8808Bu^2 + 0.45419Bu$$

A lower length scale informed model

- Since LWRs operate at higher temperatures, the empirical model may not be applicable
- A rate theory parameterization for study of U_3Si_2 in LWRs was based upon DFT calculations and research reactor PIE data
- Three temperature regimes
  - **T < 750 K**: dominated by small intragranular bubbles
  - **750 K ~ 1000 K**: dominated by bimodal-distributed intragranular bubbles
  - **T > 1000 K**: intergranular bubbles and gas release

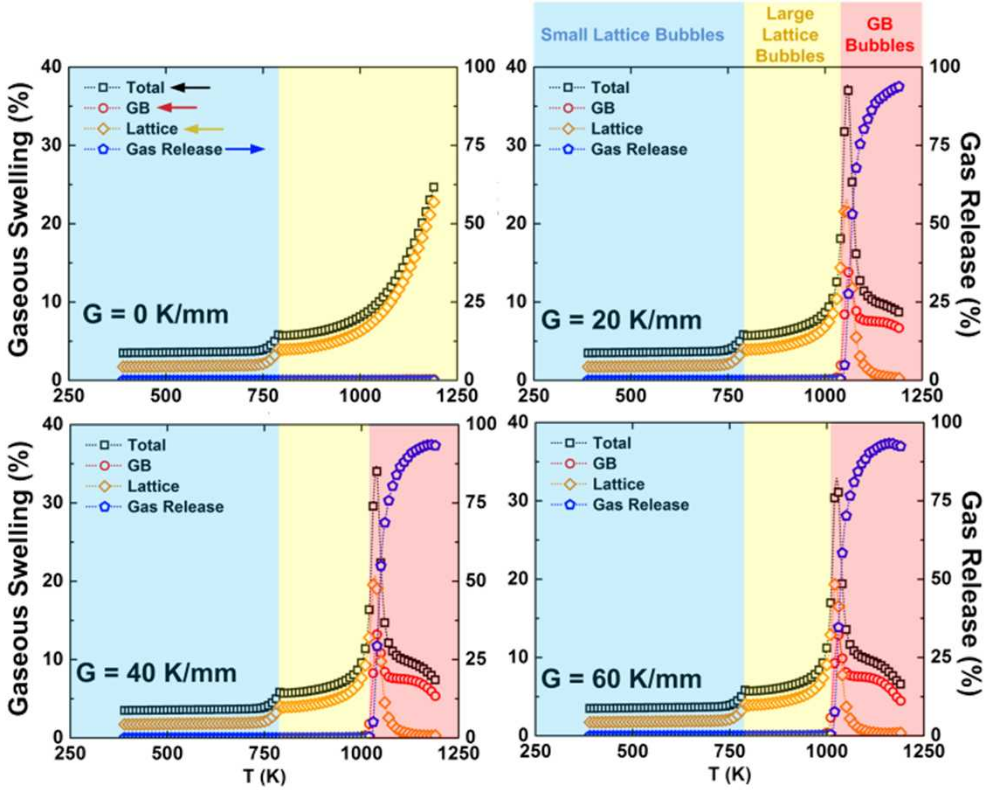


4 types of fission gas bubbles considered in rate theory modeling: (1) lattice (2) dislocation (3) grain face (4) grain edge

Y. Miao et al., "Gaseous swelling of U_3Si_2 during steady-state LWR Operation: A rate theory investigation," NED, **322**, 2017, p. 336-344.

Gaseous Swelling: Rate Theory

- A three factor model was developed using rate theory calculations at ANL for gaseous swelling and thermal conductivity degradation.
  - Temperature (T): 390 – 1190 K
  - Temperature gradient (G): 0 – 160 K/mm
  - Fission density (f): 0 - 2×10^{21} f/cm^3
- Tricubic interpolation is used for better continuity.
- Thermal conductivity degradation models taking into account intragranular and intergranular bubbles are multiplied by the intrinsic thermal conductivity.

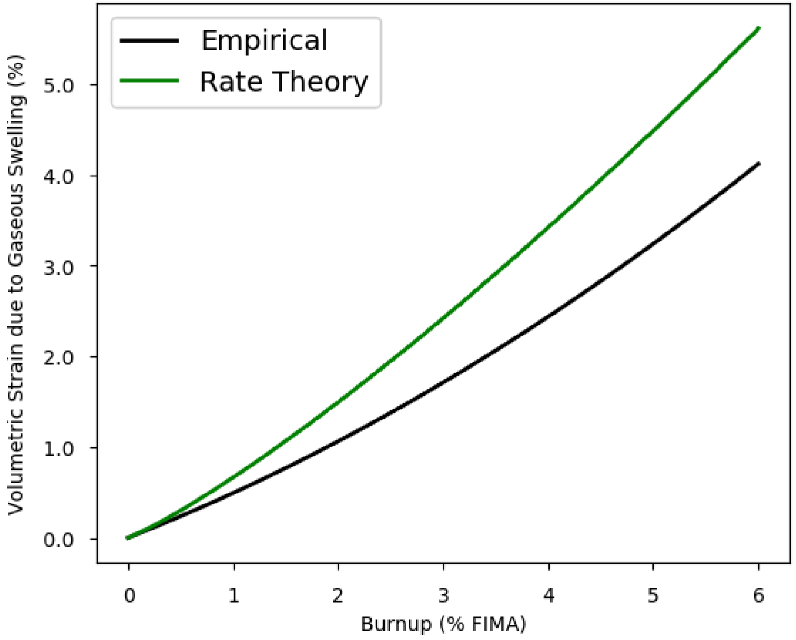


Temperature and Temperature gradient dependence on gaseous swelling at 1.3×10^{21}fiss/cm^3

Y. Miao et al., "Gaseous swelling of U_3Si_2 during steady-state LWR Operation: A rate theory investigation," NED, **322**, 2017, p. 336-344.

Results

- The lower length scale rate theory model provides not only gaseous swelling information but estimates thermal conductivity degradation as well.



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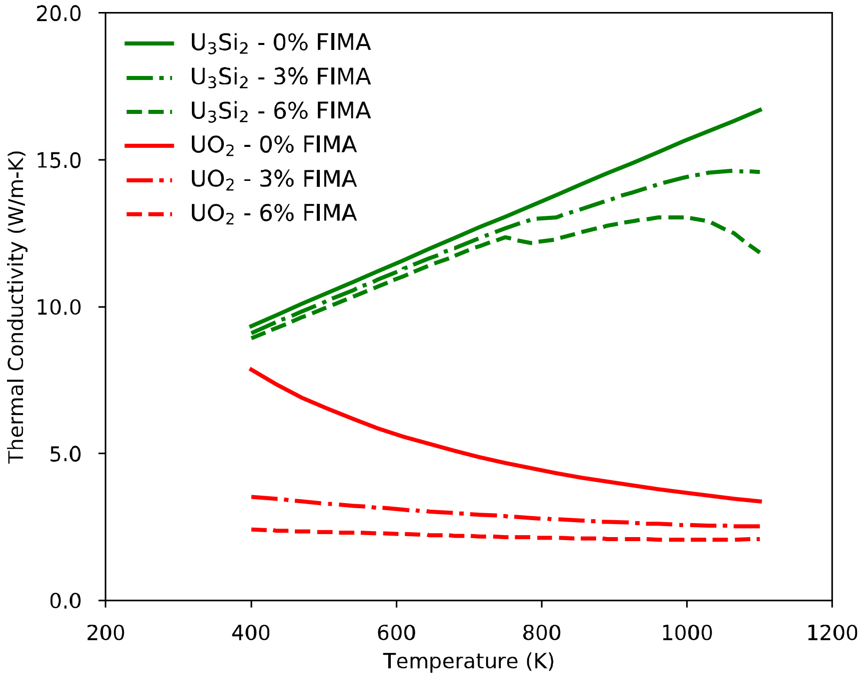


Degraded thermal conductivity comparisons between U_3Si_2 and UO_2 for a temperatures varying from 400 to 1100 K.

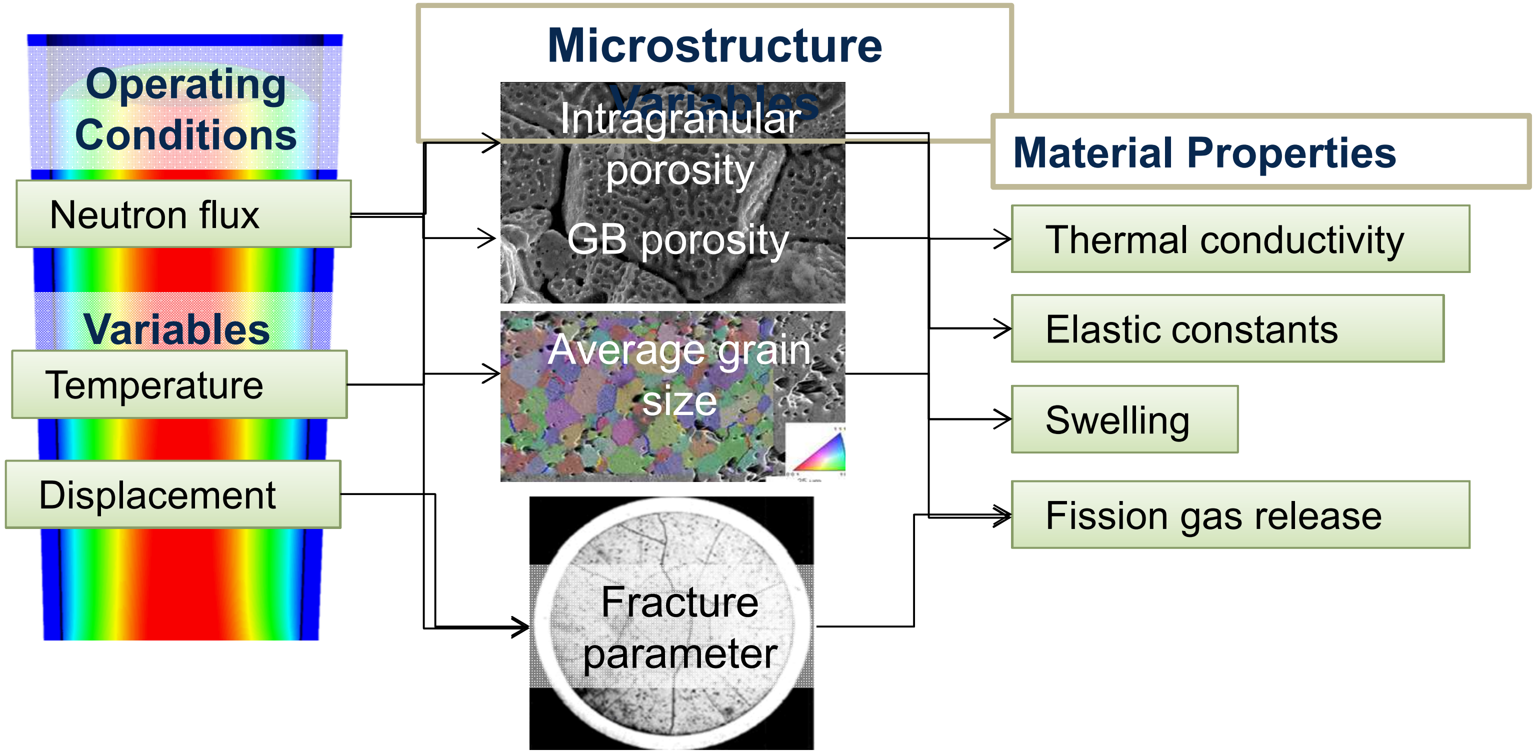
LWR Fuel

Understanding the grain growth of UO_2

Sudipta Biswas
Idaho National Laboratory

Motivation

- Grain size impacts thermal/mechanical properties and eventually the performance of the material
- Grain size varies over time depending on the temperature, burnup, porosity, bubble size, etc.
- Transient grain size evaluation is required to evaluate the material behavior under irradiation



Microstructural Analysis

- Grain growth is affected by presence of second-phase-particles/pores/gas-bubbles
- At lower temperature, immobile particles exert drag, limit grain growth
- At higher temperature, high surface diffusions renders particles mobile
- Grain growth rate increases with increase in particle mobility

Time: 0.000

Particle Free

Time: 0.000

Immobile Particles

Time: 0.000

Mobile Particle

Engineering-Scale Model

Model I: Empirical formulation used for engineering scale analysis

$$\frac{dD}{dt} = k\left(\frac{1}{D} - \frac{1}{D_m}\right)$$ *(Bison Manual)*

Grain size is limited based on temperature and not actual porosity

Model II: Pinning effect due to immobile pores

$$\frac{dD}{dt} = M_{GB}\left(F_g - N_p F_p\right)$$ *(Tonks et al, MSMScEng 2015)*

Exerts excess drag and arrests grain growth

Model III: GB mobility is modified considering presence of particles

$$\frac{dD}{dt} = M_{eff} F_g = \frac{M_{GB}\, M_p/N_p}{M_p/N_p + M_{GB}} F_g = \frac{M_{GB}\, M_p}{M_p + M_{GB}\, N_p} F_g = \frac{M_{GB}}{1 + \frac{M_{GB}\, N_p}{M_p}} F_g$$

Particle/pore driven grain growth exerting drag for low particle mobility $\left(\frac{M_{GB}\, N_p}{M_p} \gg 1.0\right)$

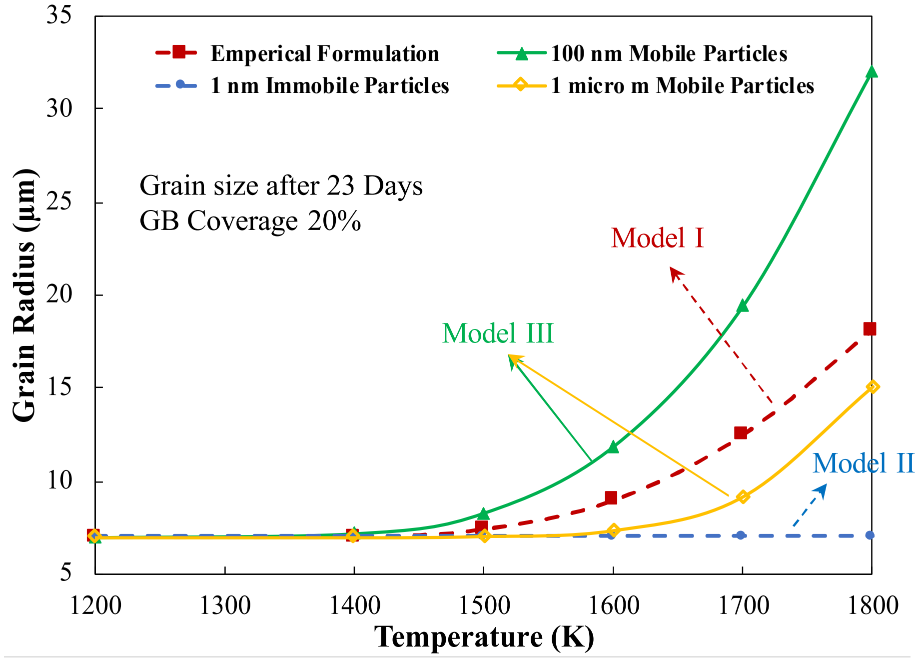
GB driven grain growth at higher particle mobility $\left(\frac{M_{GB}\, N_p}{M_p} \ll 1.0\right)$

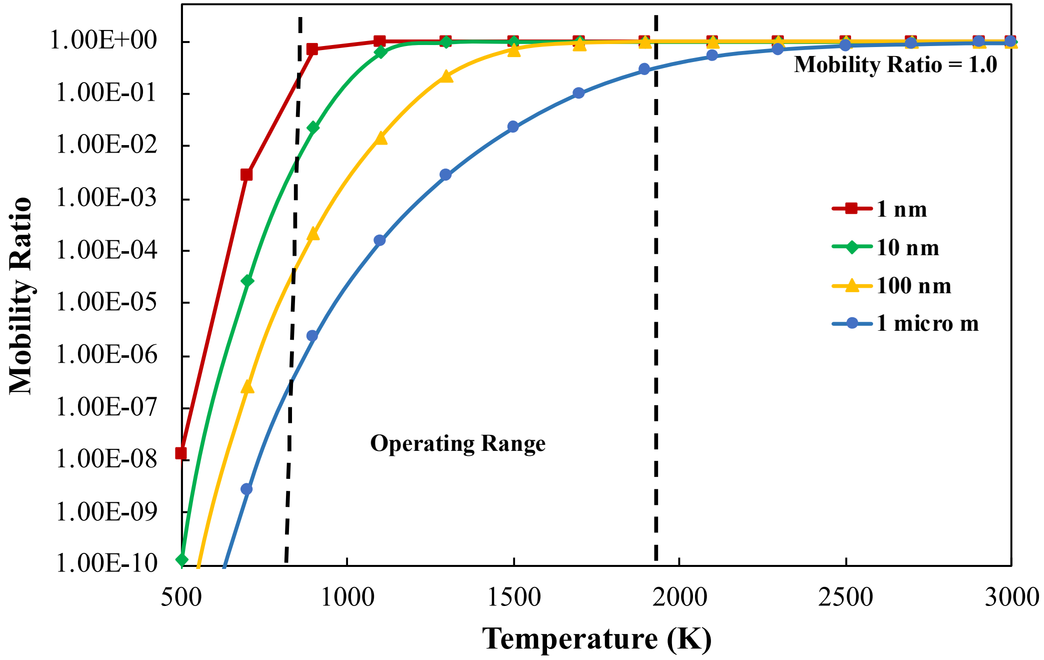
(Ahmed et al, CMS 2017)

D	Grain Size
D_m	Limiting grain size
M_{GB}	GB mobility
F_g	Driving force for the curvature driven grain growth
N_p	No. of particles
M_p	Particle mobility
F_p	Driving force for particles

Grain Size Evaluation

- Engineering-scale model is updated based on meso-scale analysis
- Even mobile particles may exert significant drag at lower temperature
- Particle mobility increases with temperature and varies with pore/particle size
- At operating temperature, grain size is determined based on surface diffusion, particle size, and GB coverage





Mobility ratio, $M_r = \frac{M_p}{M_p + M_{GB}\, N_p}$

GB Coverage 20%

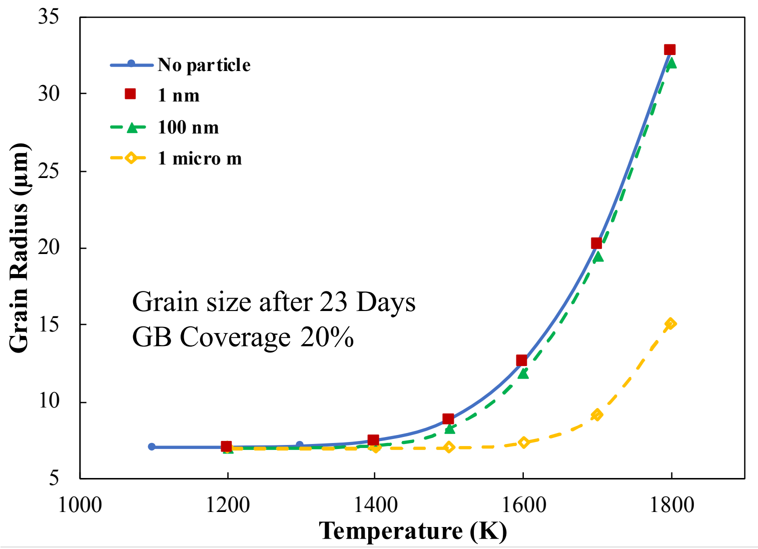
Effect of Porosity

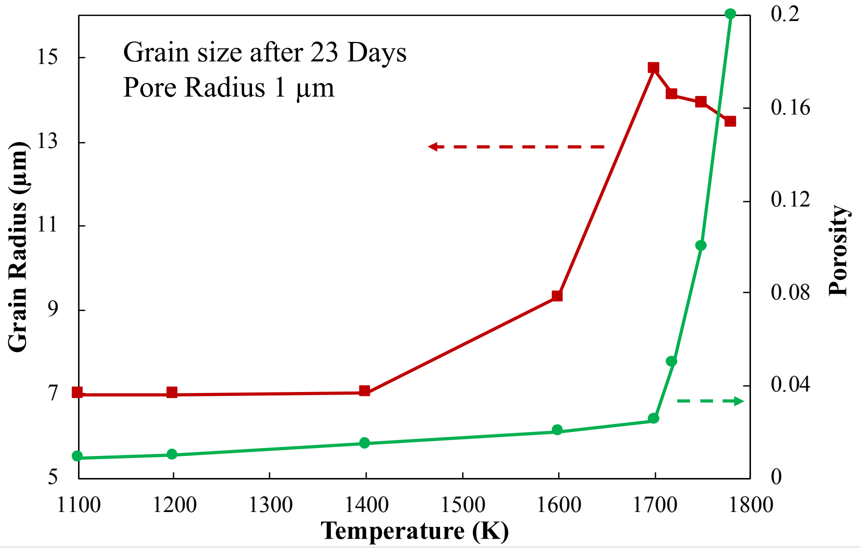
Assumptions:

- All the pores in the system are located on the GBs

Observations:

- Presence of second-phase particle exerts a drag force and reduces the grain-growth rate
- At high temperature, higher porosity may lead to reduction in grain size





Future Scope

- Not all particles are mobile and have the same velocity. A generic formulation needs to be developed considering both mobile and immobile particles.

- Further 3D meso-scale grain size evaluation is needed for validating the model, alleviating some assumptions.

- Porosity calculation needs to be updated with the fission rate model for fuel operating conditions.

- Radial variation of porosity and corresponding grain sizes are to be predicted for performance evaluation of the fuel rods.

- Effect of the updated grain size model on Bison’s fission gas release, thermal transport, creep and other mechanical behavior models need to be evaluated.

Metallic Fuels

Understanding the initial development of porosity in the α-uranium phase

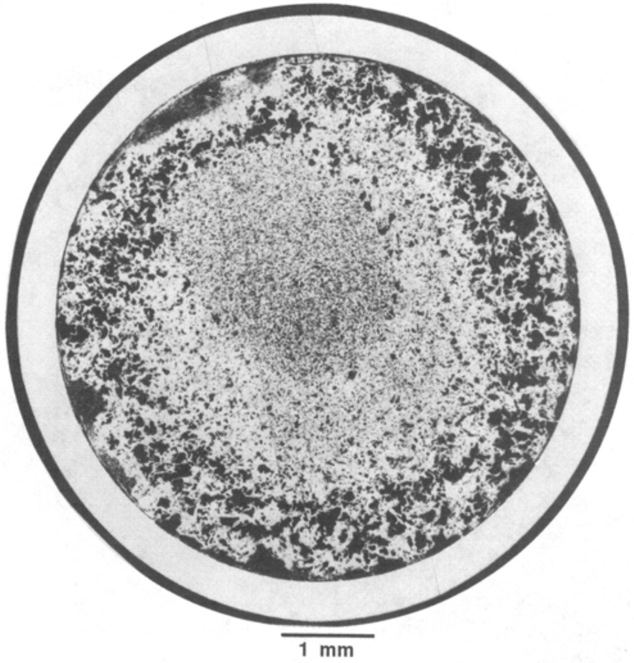
Andrea M. Jokisaari
Idaho National Laboratory

A. Rezwan
The Pennsylvania State University

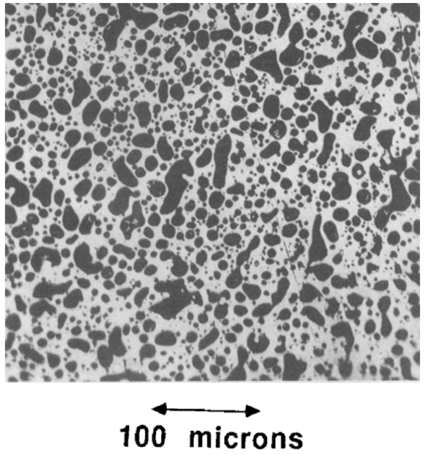
M. Tonks
University of Florida

Introduction and background

- **Metallic fuels** are proposed for **Gen IV** reactor designs
- Metallic fuels exhibit **different, and much greater, swelling** than oxide fuels
  - Swelling impacts fuel performance by changing thermal conductivity, can also lead to cladding failure
  - Experimental evidence indicates that irradiated polycrystalline α**-uranium** forms cracks along grain boundaries, while γ**-uranium** forms bubbles
- Need to **understand the physical mechanisms governing fuel swelling** to **accelerate fuel design** and **inform engineering scale** fuel performance models
  - Study the **development of stress** within polycrystalline α-uranium during **irradiation** to understand observed microstructures in fuel
  - **Predict** how and when **porosity** develops
  - **Assess available** materials **information**



α-U cavitation at 10% burnup [1]

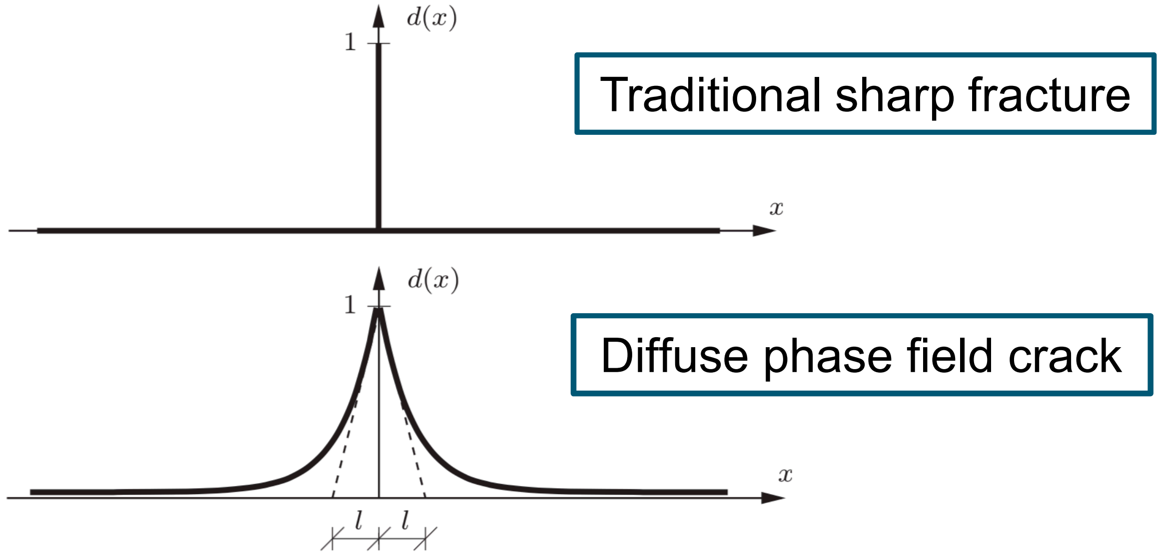


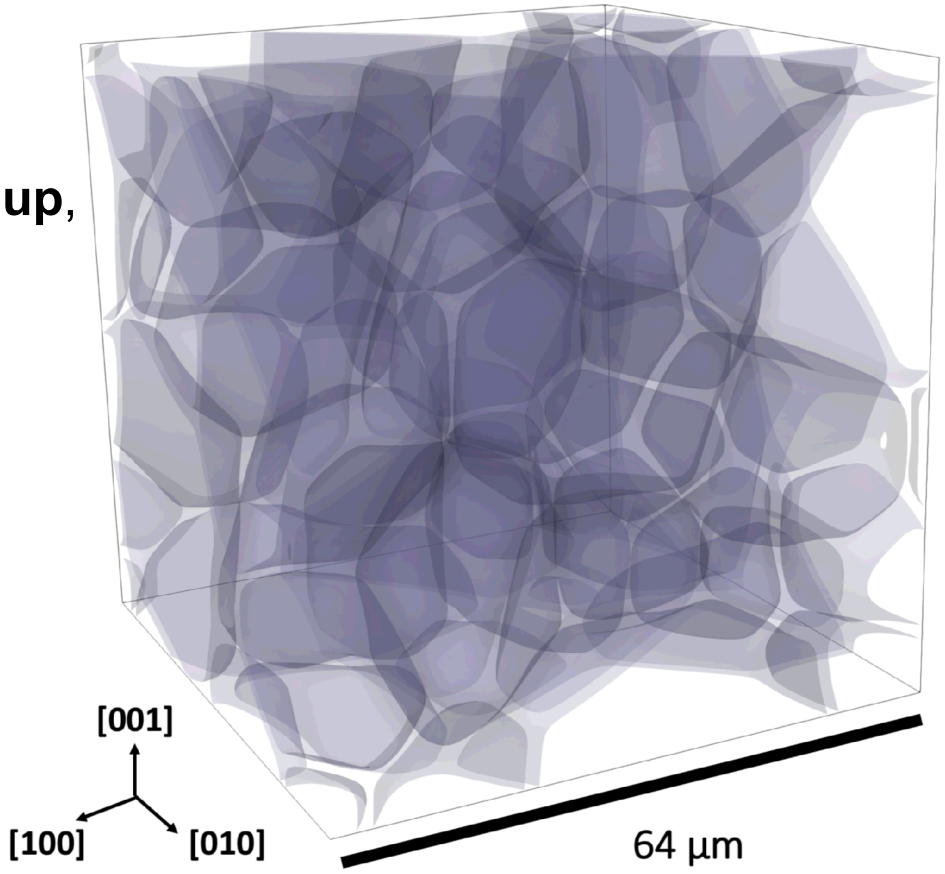
γ-U bubbles at 2% burnup [1]

[1] R. G. Pahl et al., Met. Trans. A 21A (1990) 1863-1870

Model and analysis approach

- **Mesoscale** formulation examining effect of **irradiation-induced dimensional changes** on polycrystalline material
  - **Simplified to α-U**
  - **Burnup-dependent misfit strain**
- Model 1: study the development of the **hydrostatic** stress, **von Mises** stress, and **elastic energy** as a function of **burnup**, **applied stress**, and **grain size**
- Model 2: Include **phase field cracking** and **J2 plasticity**

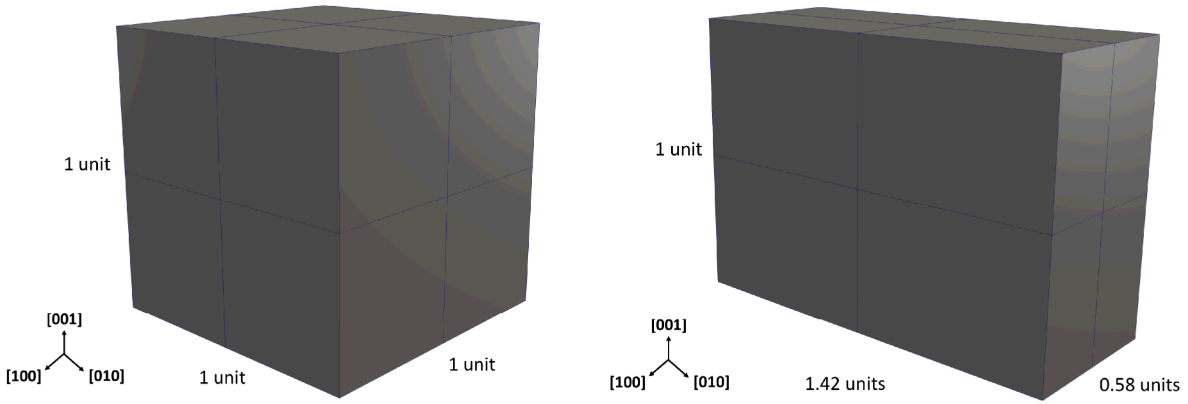


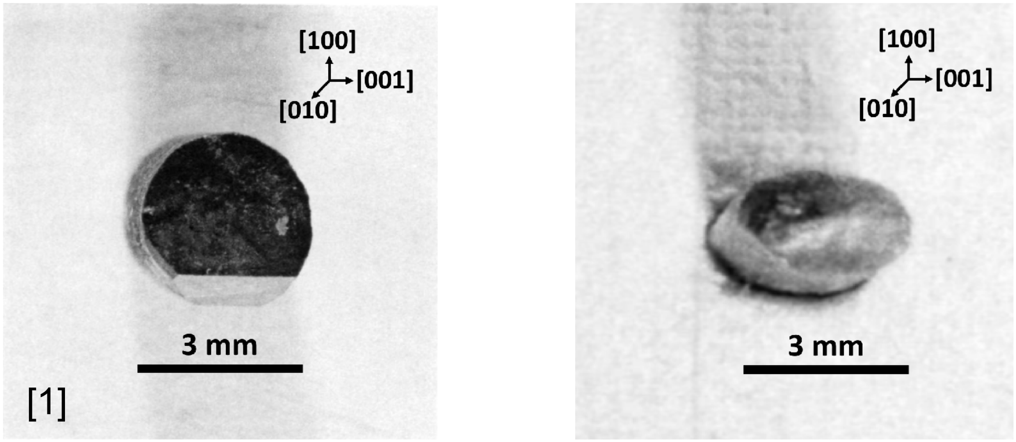


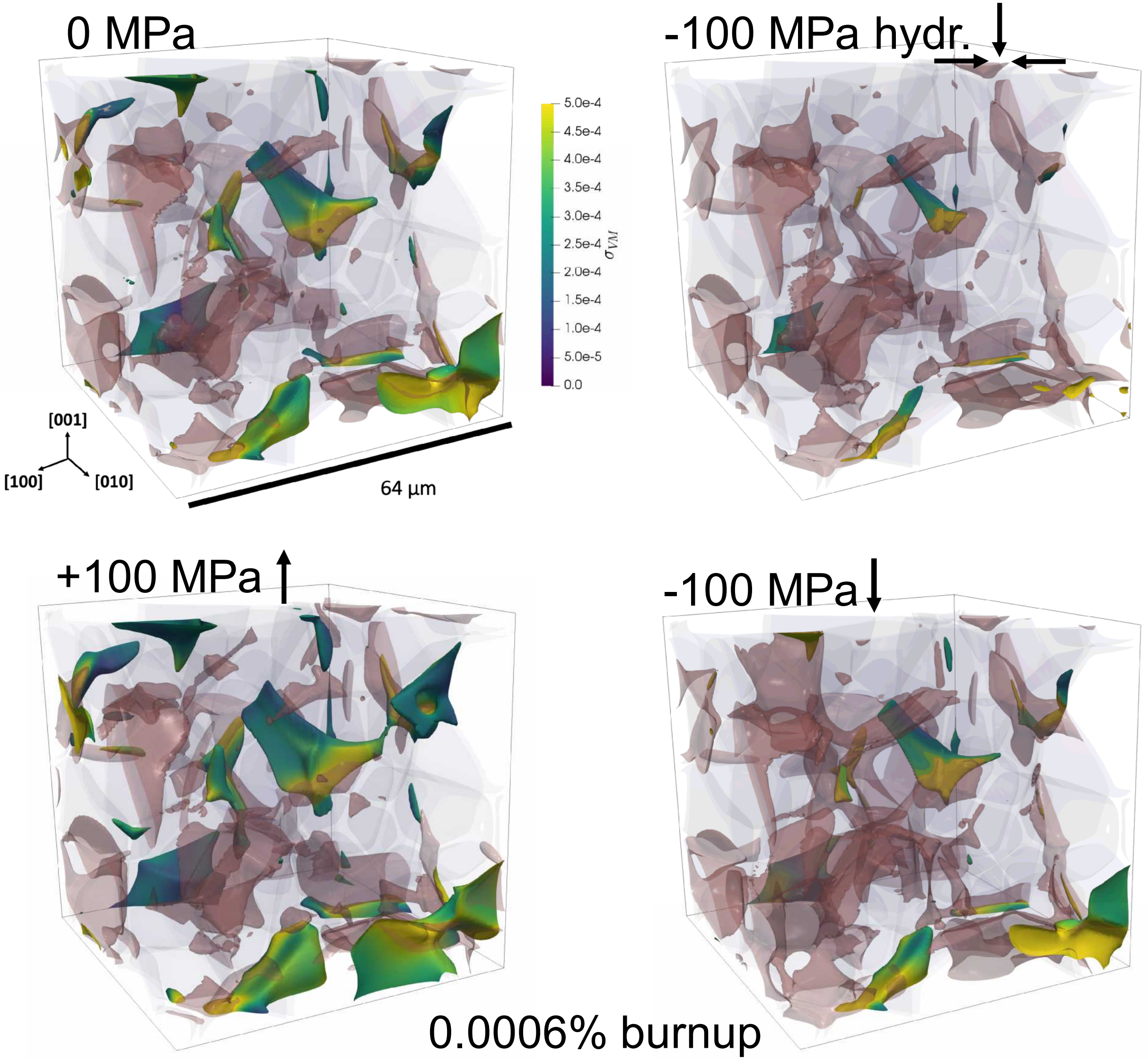
Results – Single crystal and polycrystal deformation

unirradiated

0.1% burnup



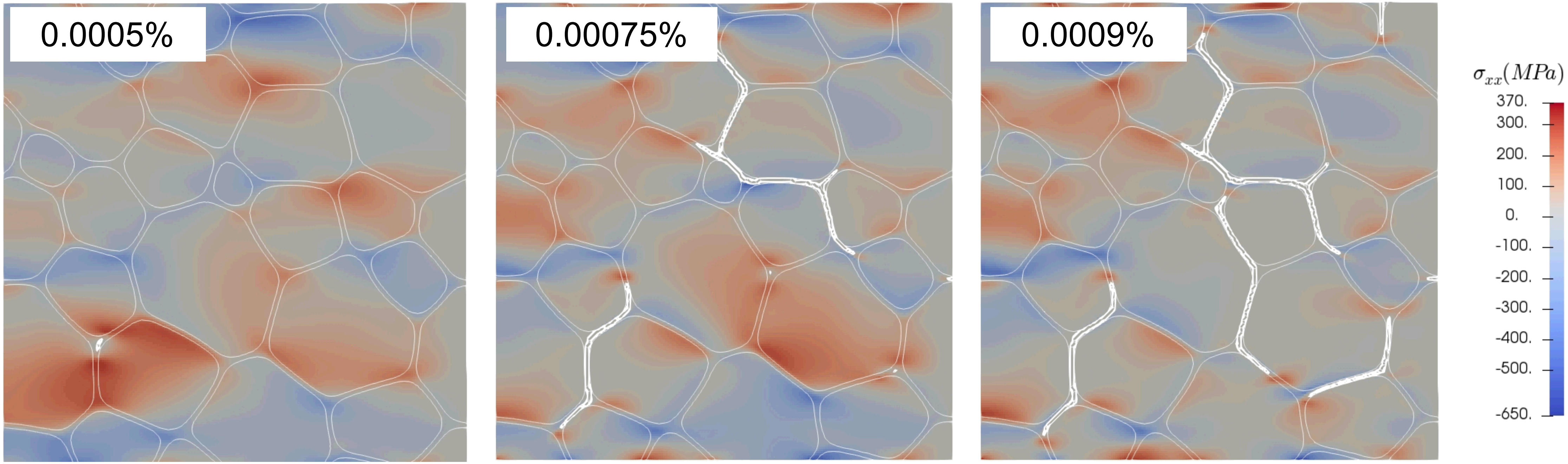




0.0006% burnup

[1] S. Paine, J. Kittel, ANL-5676, Argonne National Lab., Lemont, IL, 1958.

Results – crack nucleation and propagation



Cracking initiates as predicted in burnup model

Cracks propagate and blunt, new cracks form

Cracking continues along grain boundaries

Summary and what's next

- Knowing **when, where,** and **how** tearing occurs will inform **engineering-scale models** of **thermal conductivity** and **mechanical performance of the cladding**
  - Cracked volume, crack morphology & interconnectivity
  - Can supply parameters or reduced-order models to fuel swelling, FCCI and thermal conductivity models as a function of burnup, temperature, stress state
- Developed **mesoscale models** to study the development of **initial porosity** in polycrystalline **α-uranium** under **irradiation**
  - Predict the **initial formation** of porosity after approximately **0.0005% - 0.001% burnup**, equivalent to 1-2 hours under EBR-II conditions
  - Predict that crack formation occurs at triple points, grain boundaries, and exterior surfaces
  - Find that **applied stresses up to 100 MPa have no significant effect on internal stresses** after approximately 0.0005% burnup
- **Many basic material properties are poorly characterized or altogether missing**
- Potential **next steps** at the mesoscale:
  - Incorporate effect of δ-UZr_2, thermal strains and model plastic flow
  - Develop model for porosity formation in γ-uranium
  - Develop model for porosity fraction and connectivity that can be used in Bison and by fuel designers

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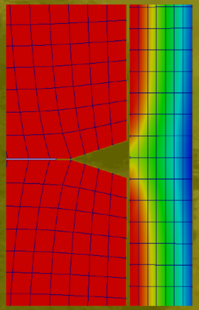
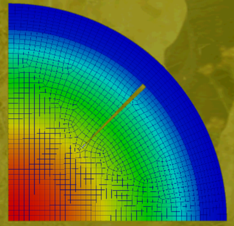
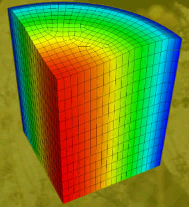
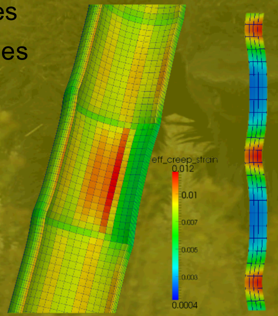

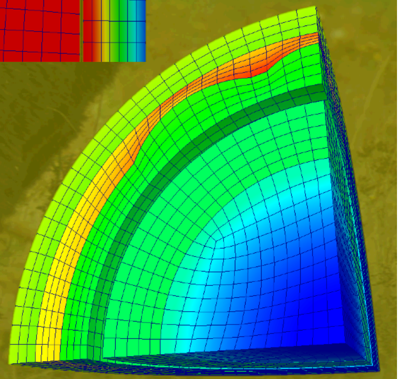

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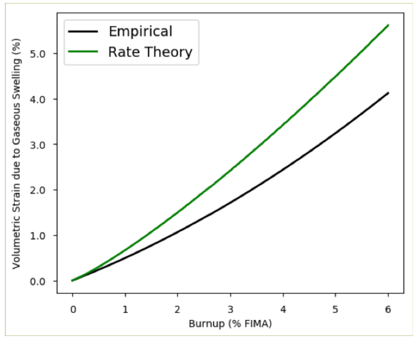

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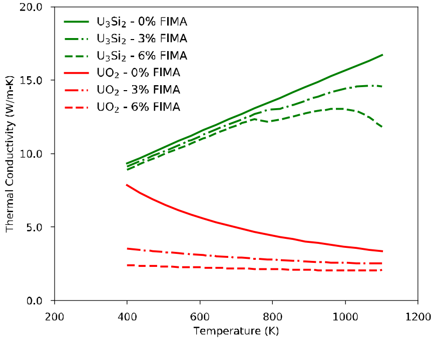

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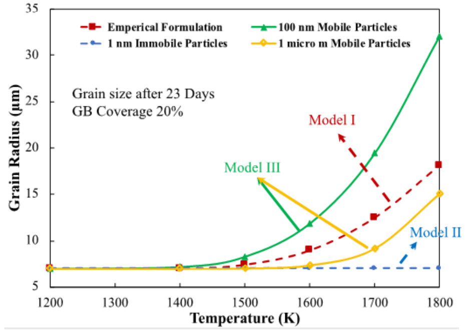

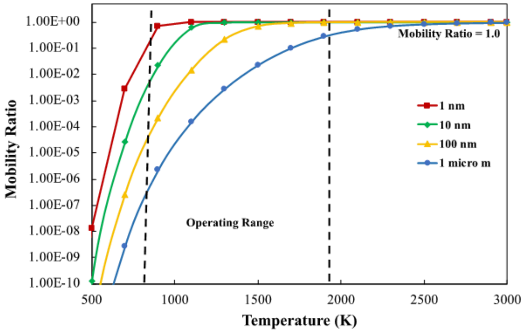

Mobility ratio, $M_r = \frac{M_p}{M_p + M_{GB} N_p}$

GB Coverage 20%

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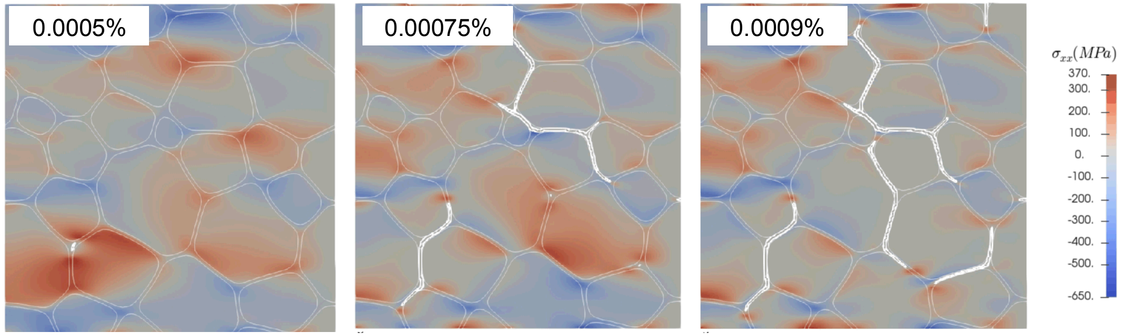
Results – crack nucleation and propagation



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