Fuel Thermal Conductivity

NE 591

Housekeeping

- You all should have received graded exams in your email
- Exam 2 key is posted on moodle site
- Any questions, please let me know via email or during office hours tomorrow

- 3rd and final exam tentatively scheduled for April 23
  - Will be open book and timed via moodle
- Go into moodle, there is a an example assignment called “Upload test”
- Upload a document into this Upload test assignment so that we can all make sure we are capable of using the moodle system

Last time

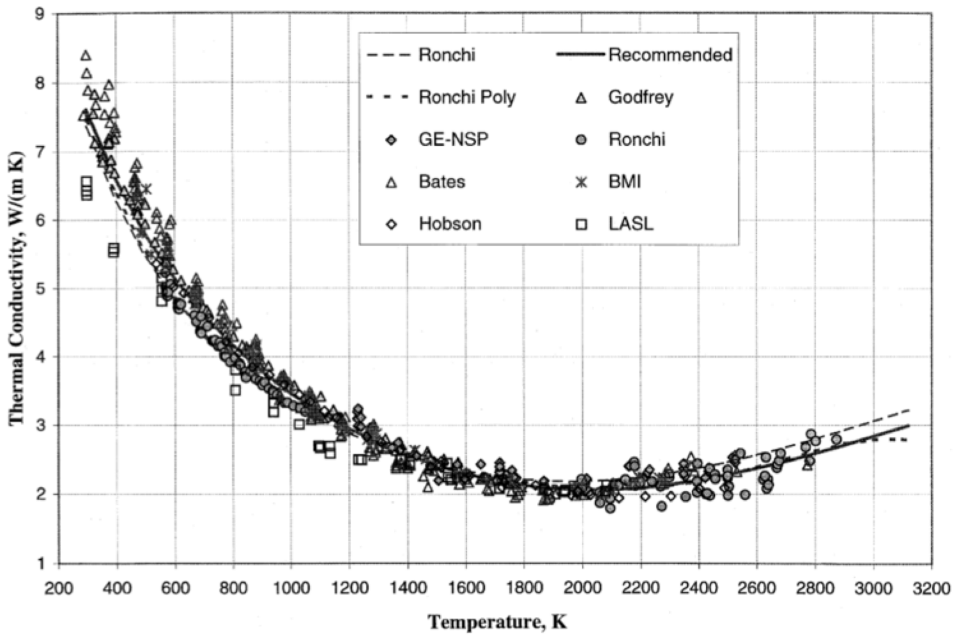
- Many materials models for fuel are empirical and correlated to burnup
- Fuel pellets change shape due to
  - Thermal expansion
  - Densification
  - Swelling
  - Creep
- Fracture also decreases the gap, as fractures pieces shift outward
- At high burnup but mid to low temperature the fuel restructures to have a small grain size and large bubbles
  - The structure is called High Burnup Structures (HBS)
  - HBS may actually improve many fuel properties

UO2 Thermal Conductivity

- We have established correlations for thermal conductivity of fresh UO2 fuel as a function of temperature

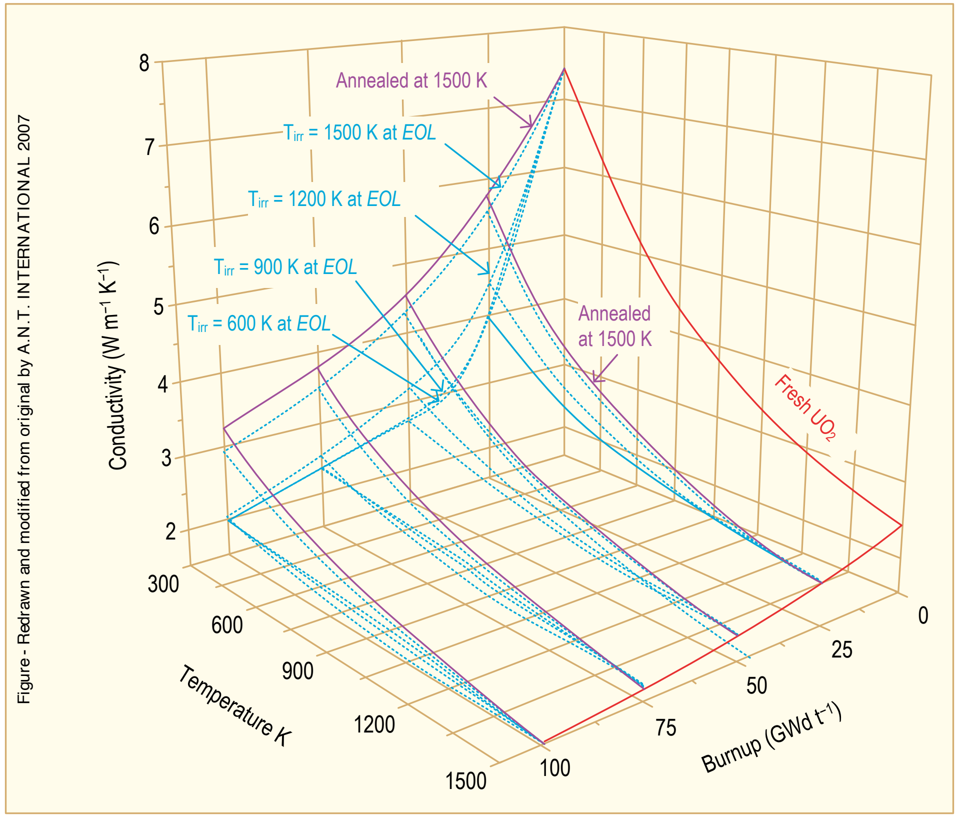
$$k_0 = \frac{100}{7.5408 + 17.629t + 3.6142t^2} + \frac{6400}{t^{5/2}} \exp\left(\frac{-16.35}{t}\right)$$

  - Where t = T/1000
  - The first part of the equation describes the phonon interactions
  - The second part describes electronic transport which becomes significant at high temperature



UO2 Thermal Conductivity

- UO_2 thermal conductivity is low and decreases more during reactor operation
- The thermal conductivity has been collected after various amounts of burnup to make empirical fits



$$\lambda_{95} = \frac{1}{A(x) + aG + B(x)T + f_1(Bu) + f_2(Bu)g(Bu)h(T)} + \frac{C}{T^2}\exp\left(\frac{-D}{T}\right)$$

UO2 Thermal Conductivity

- The primary empirical model used in BISON is the NFIR model
- The model is a function of the temperature T (in °C) and the burnup β (in MWD/kgU

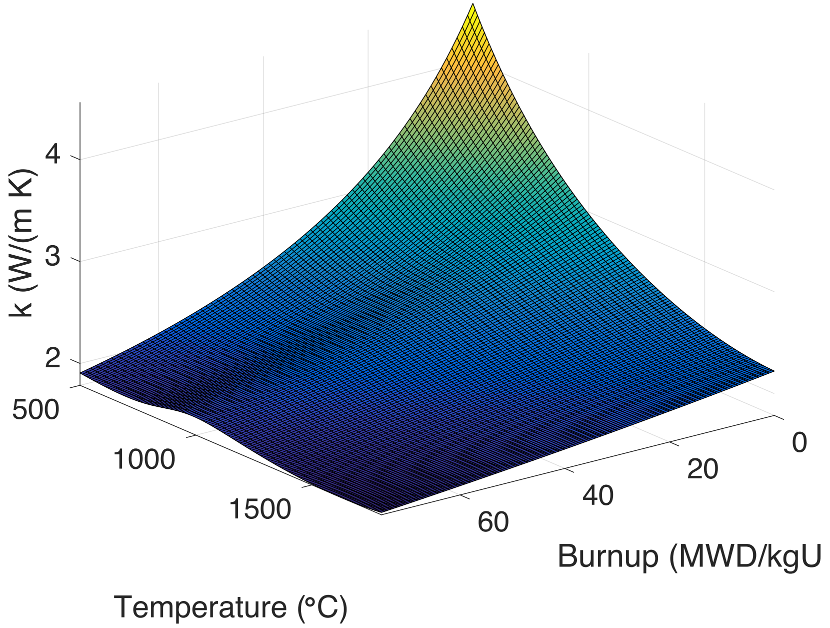
$$k = (1 - R_f(T))k_{ph1}(T,\beta) + R_f(T)k_{ph2}(T,\beta) + k_{el}(T)$$

$$R_f(T) = \frac{1}{2}\left(1 + \tanh\left(\frac{T-900}{150}\right)\right)$$

$$k_{ph1} = \frac{1}{(9.592 \times 10^{-2} + 6.14 \times 10^{-3}\beta - 1.4 \times 10^{-5}\beta^2 + (2.5 \times 10^{-4} - 1.81 \times 10^{-6}\beta)T}$$

$$k_{ph2} = \frac{1}{(9.592 \times 10^{-2} + 2.6 \times 10^{-3} \cdot \beta + (2.5 \times 10^{-4} - 2.7 \times 10^{-7}\beta)T}$$

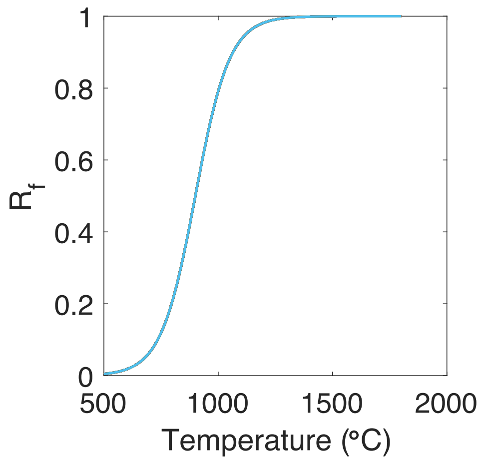
$$k_{el} = 1.32 \times 10^{-2}\, e^{1.88 \times 10^{-3} T}$$

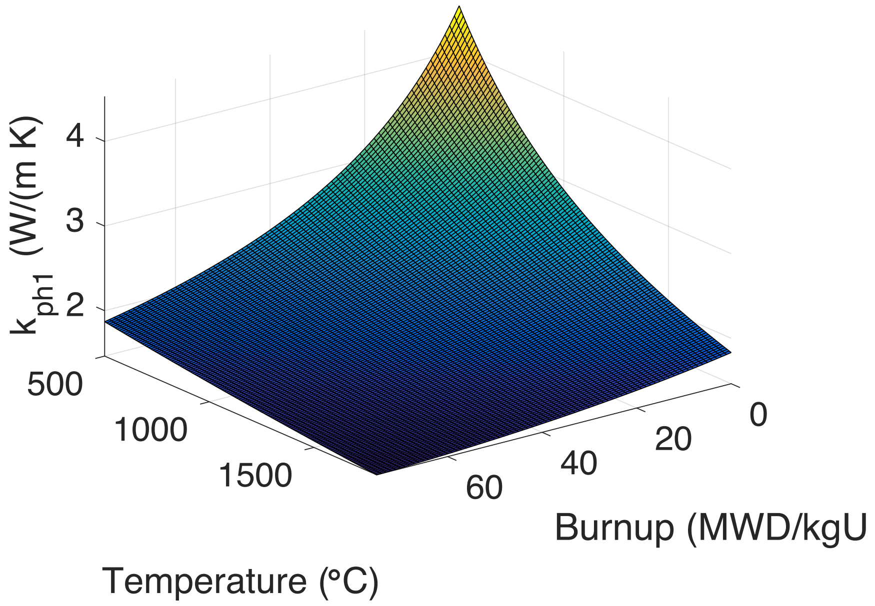


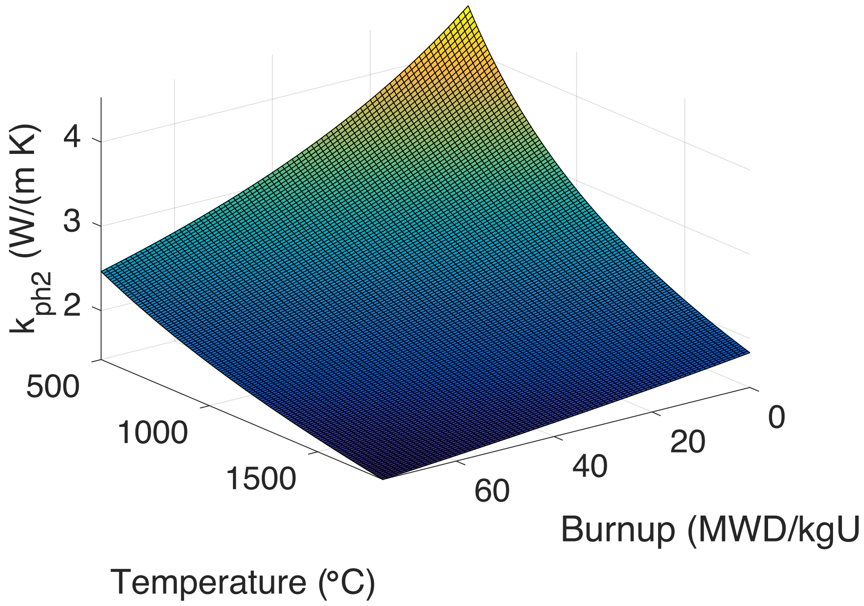
UO2 Thermal Conductivity

- The R_f function switches between two k_{ph} functions

$$R_f(T) = \frac{1}{2}\left(1 + \tanh\left(\frac{T - 900}{150}\right)\right)$$







UO2 Thermal Conductivity Example

- What is the thermal conductivity of a fuel predicted by the NFIR model at a temperature of 1200 K and a burnup of 5% FIMA?
- First, we need to convert T to °C and burnup to MWD/kgU
  - T = 1200 K – 273.15 = 926.85 °C, β = 0.05 FIMA*950 = 47.5 MWD/kgU
- Next, we need to calculate R_f
  - R_f = 0.5*(1 + tanh((926.86 – 900)/150)) = 0.5886
- Now, we need k_{ph1}
  - k_{ph1} = 1/(9.592e-2 + 6.14e-3*47.5 – 1.4e-5*47.5^2 + (2.5e-4 – 1.81e-6*47.5)*926.85) = 1.9685 W/(m K)
- Then, k_{ph2}
  - k_{ph2} = 1/(9.592e-2 + 2.6e-3*47.5 + (2.5e-4 – 2.7e-7*47.5)*926.85) = 2.2766 W/(m K)
- Finally, k_{el}
  - k_{el} = 1.32e-2*exp(1.88e-3*926.85) = 0.0754 W/(m K)
- Then, we put it all together
  - k = (1 – 0.5886)*1.9685 + 0.5886*2.2766 + 0.0754 = 2.23 W/(m K)

$$R_f(T) = \frac{1}{2}\left(1 + \tanh\left(\frac{T - 900}{150}\right)\right)$$

$$k_{ph1} = \frac{1}{(9.592\times10^{-2} + 6.14\times10^{-3}\beta - 1.4\times10^{-5}\beta^2 + (2.5\times10^{-4} - 1.81\times10^{-6}\beta)T}$$

$$k_{ph2} = \frac{1}{(9.592\times10^{-2} + 2.6\times10^{-3}\cdot\beta + (2.5\times10^{-4} - 2.7\times10^{-7}\beta)T}$$

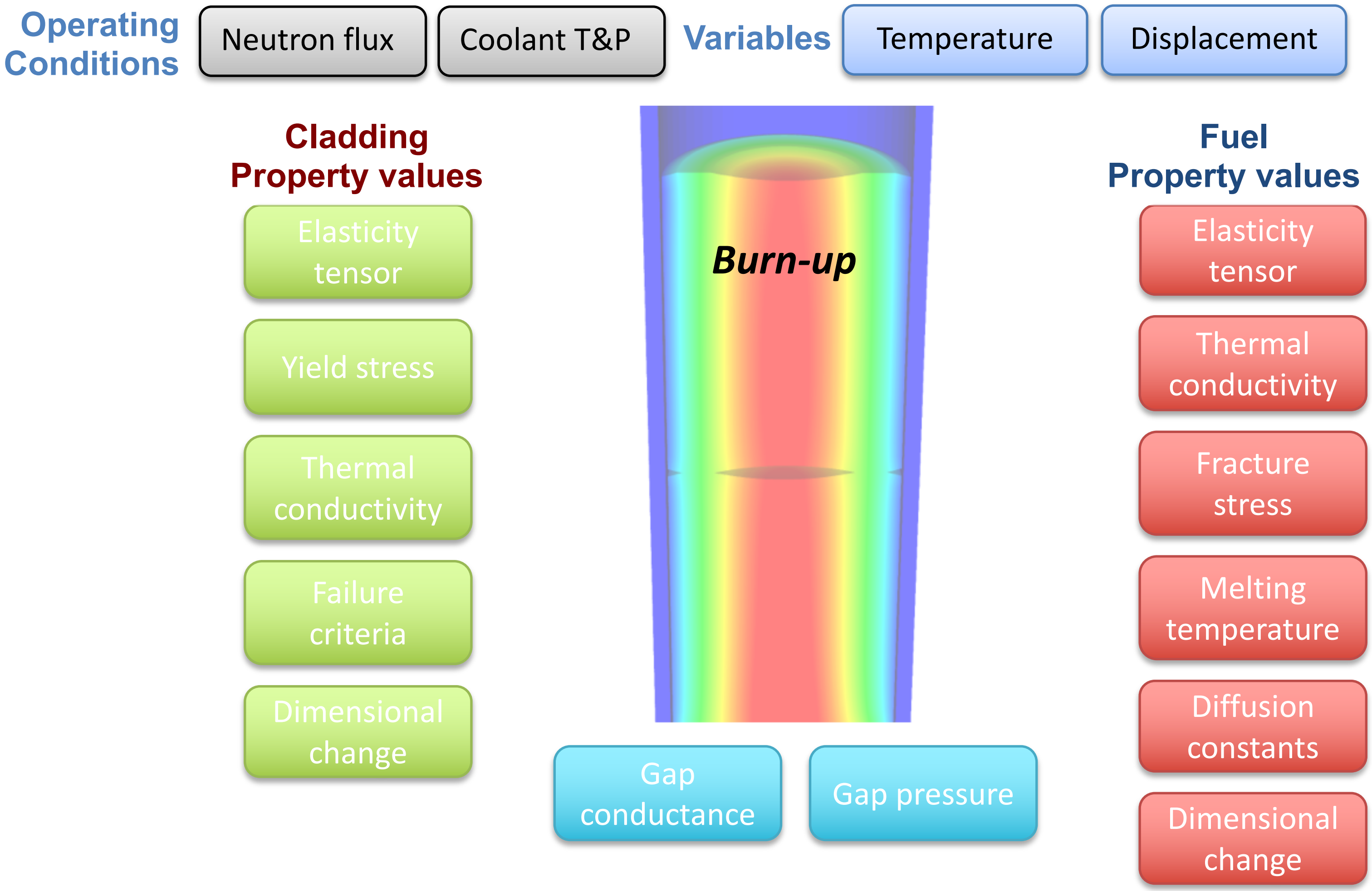
$$k_{el} = 1.32\times10^{-2}\, e^{1.88\times10^{-3}T}$$

$$k = (1 - R_f(T))k_{ph1}(T,\beta) + R_f(T)k_{ph2}(T,\beta) + k_{el}(T)$$

Going beyond burnup…

- Fuel performance codes historically rely on materials models correlated to temperature and burn-up

- Development has begun on models based on microstructure rather than burn-up

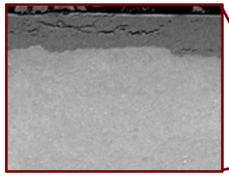


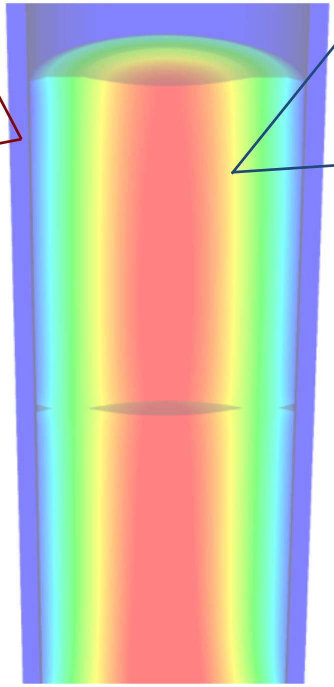
Microstructure-based fuel performance modeling

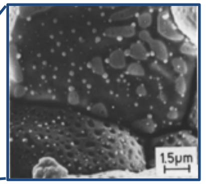
Structure/property relationships connect the microstructure variables to the property values

Operating Conditions: Neutron flux | Coolant T&P

Variables: Temperature | Displacement | Stoichiometry







Cladding Property values

- Elasticity tensor
- Yield stress
- Thermal conductivity
- Failure criteria
- Dimensional change

Microstructure evolution models (Cladding)

- Grain growth
- Plasticity
- Defect prod. & transport
- Hydrogen transport
- Loop evolution

Cladding Microstructure variables

- Average grain size
- Dislocation density
- H concentration
- Hydride fraction
- Point defect concentrations
- Loop density
- 2^{nd} phase particle fraction

Gap variable

- Gap fission gas concentration

Fuel Microstructure variables

- Average grain size
- Dislocation density
- U defect concentrations
- Pu concentration
- Fission product precipitate fractions
- Dissolved fission products
- Fission gas bubble fraction
- Grain boundary fission gas bubble coverage
- Crack parameter

Microstructure evolution models (Fuel)

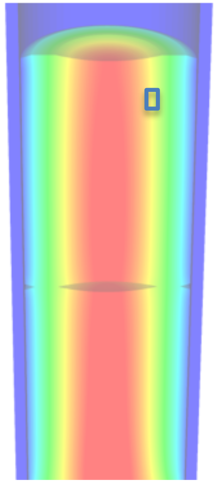
- Grain growth
- Plasticity
- Defect prod. & transport
- Fission gas behavior
- Densification
- Fracture

Fuel Property values

- Elasticity tensor
- Thermal conductivity
- Fracture stress
- Melting temperature
- Diffusion constants
- Dimensional change

Example: fission gas behavior in the fuel

- Take into account a finite set of variables to describe the state of the material
- Utilize a mechanistic model of fission gas behavior to predict the evolution of the microstructure
- Utilize this updated microstructure to inform a number of structure/property relationships

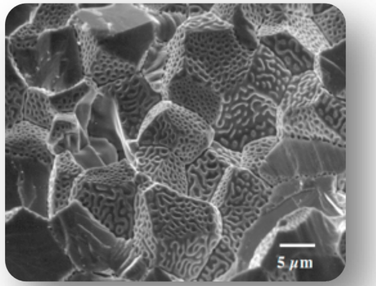


Variables

Temperature

Displacement

Stoichiometry



Model of fission gas behavior

- Dissolved fission products
- Fission gas bubble fraction
- Grain boundary fission gas bubble coverage
- Gap fission gas concentration

Structure/property relationships

Elasticity tensor

Thermal conductivity

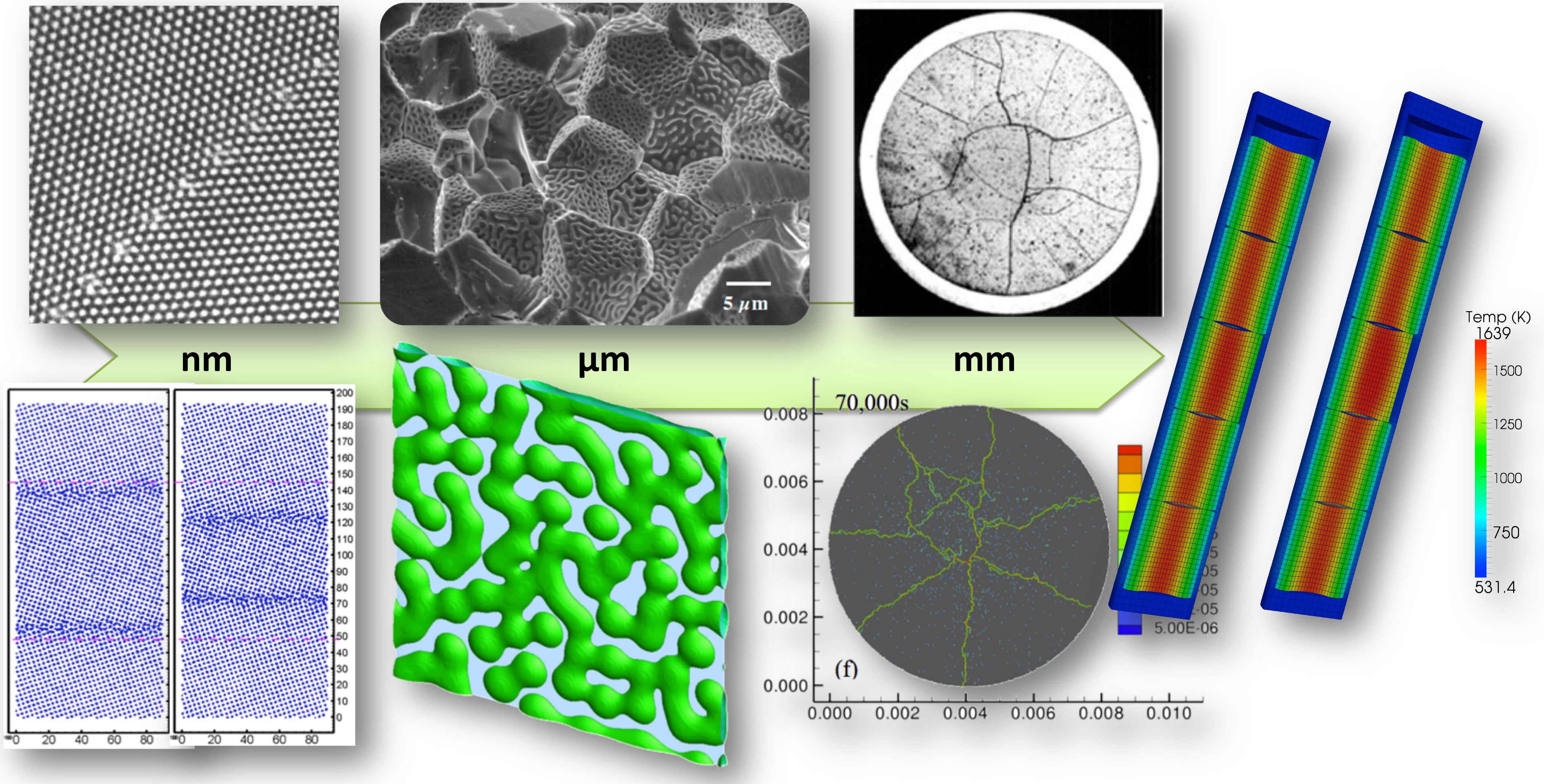
Fracture stress

Dimensional change

Gap conductance

Gap pressure

Multiscale separate effects experiments and simulations inform the development of the models



Microstructure-based models

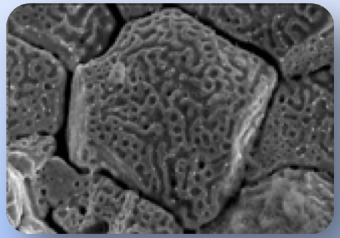
- Can provide a structure/property relationship to replace the existing burnup dependent model
- For example, thermal conductivity, taking into account microstructural features and their evolution

Grain boundary and bubbles

Intragranular porosity

Precipitated fission products

$$k = \frac{\kappa_{GB}\kappa_p\kappa_{pr}}{A + BT + CT^2 + C_v c_v + C_i c_i + C_g c_g}$$



Bulk conductivity

Vacancies and interstitials

Fission gas

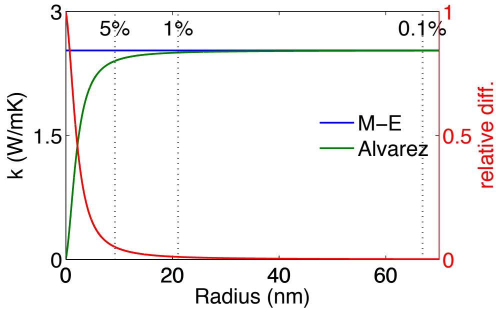
Parametrizing the mechanistic model

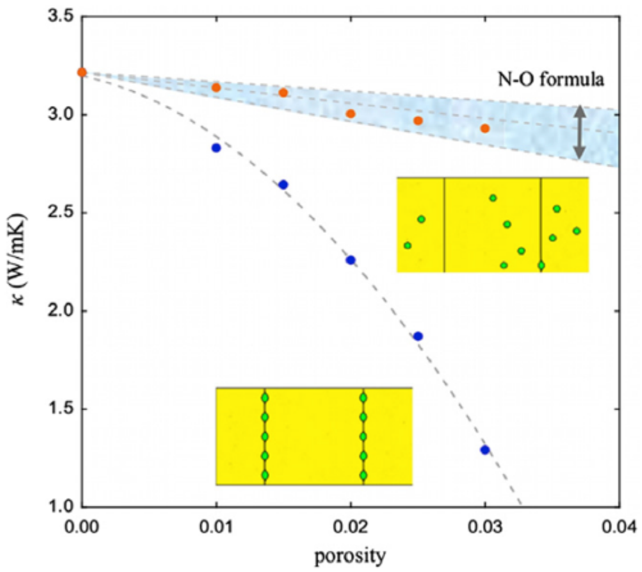
- We employ multiscale modeling and simulation to determine the various parameters for the model
- MD simulations conducted at LANL have been used to determine the coefficients for various point defects
- MD simulations have shown that phonon scattering must be accounted for to accurately represent small bubbles
- Mesoscale simulations have shown that GB bubbles have a larger impact on the thermal conductivity

Defect	a_i	Defect	a_i
O interstital	12.63	Xe atom	33.9
O vacancy	21.74	La atom	3.97
U interstital	29.98	Zr atom	2.23
U vacancy	23.78	Pu atom	0.08

Maxwell-Eucken (no phonon scattering)

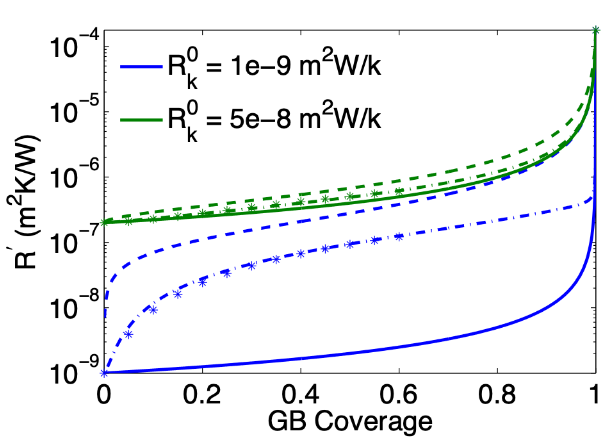
$$\kappa_{ME} = \frac{1-p}{1+p/2}$$



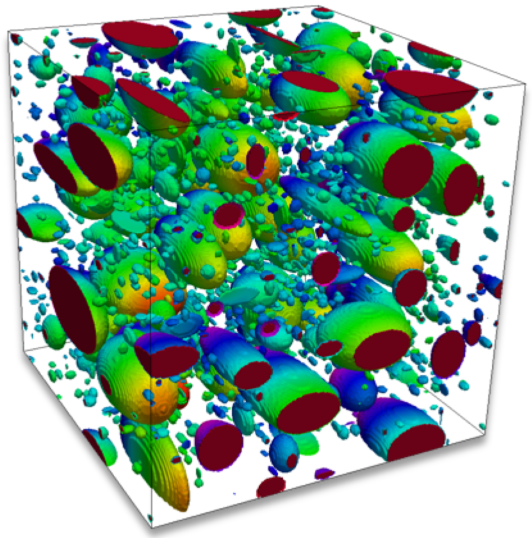


Parametrizing the mechanistic model

- A thermal resistor model is created to describe the impact of GB bubbles on the thermal conductivity



- MARMOT simulations are currently being used to inform the development of the precipitate multiplier



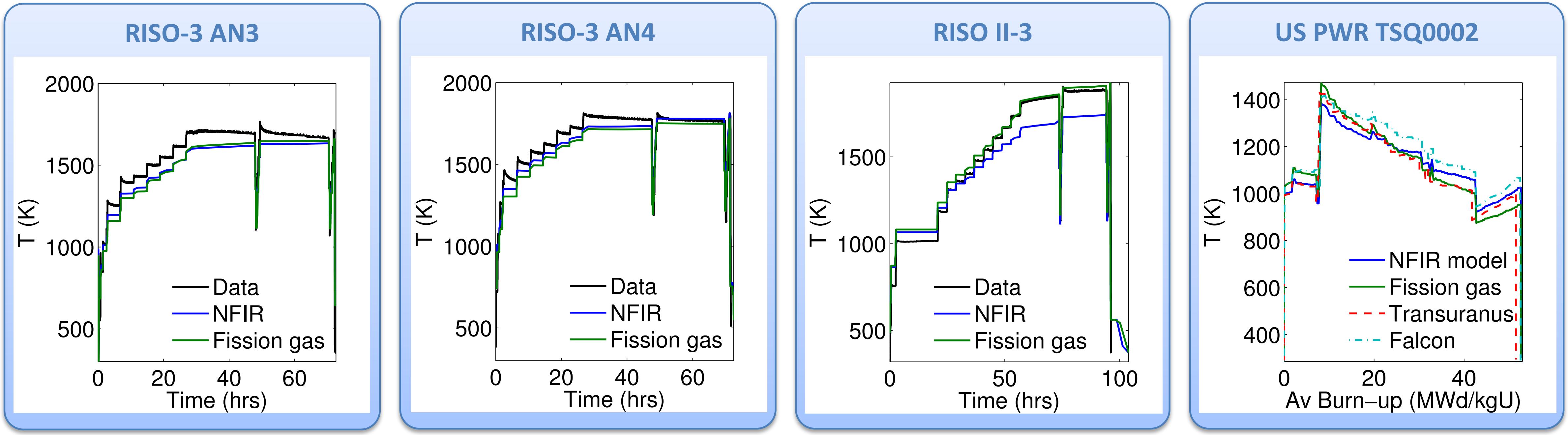
Parametrizing the mechanistic model

- Each term in the expression must be coupled to a corresponding state variable
- The full model calculates the thermal conductivity as a function of:
  - Temperature
  - Point defect concentrations
  - Intragranular bubble density and average radius
  - Fractional coverage of bubbles on GBs and average radius
  - Precipitate volume fractions and average sizes
- Currently effects of precipitates fission products and individual point defects are neglected in the model, as they are not tracked or predicted in BISON

$$k = \frac{\kappa_{GB}\kappa_p}{A + BT + CT^2 + C_g c_g}$$

Comparing with experiments…

- The model under-predicts the temperature in most cases, but not all
- Thus, the model is neglecting some resistive effects from the microstructure
- But generally performs as well, and in some cases better, than the burnup based model



Summary

- The fuel thermal conductivity decreases with burnup
- The NFIR model is a fairly accurate empirical model of the fuel thermal conductivity
- Researchers are working to develop materials models for the fuel and cladding that are mechanistic rather than empirical and that are based on the evolution of the microstructure rather than the burnup.

MOOSE Project

- We will be utilizing MOOSE for a project and we need to find a way to get it working for all
- Go to this site: https://www.mooseframework.org/getting_started/ and try to download and install MOOSE on your own/local machine
- Also, I am working on getting a functional MOOSE build on rdfmg cluster such that we don't require individual students to have sufficient computing capacity
- Once we all have MOOSE, we will do 1-2 lectures of training and examples

Presentation Project

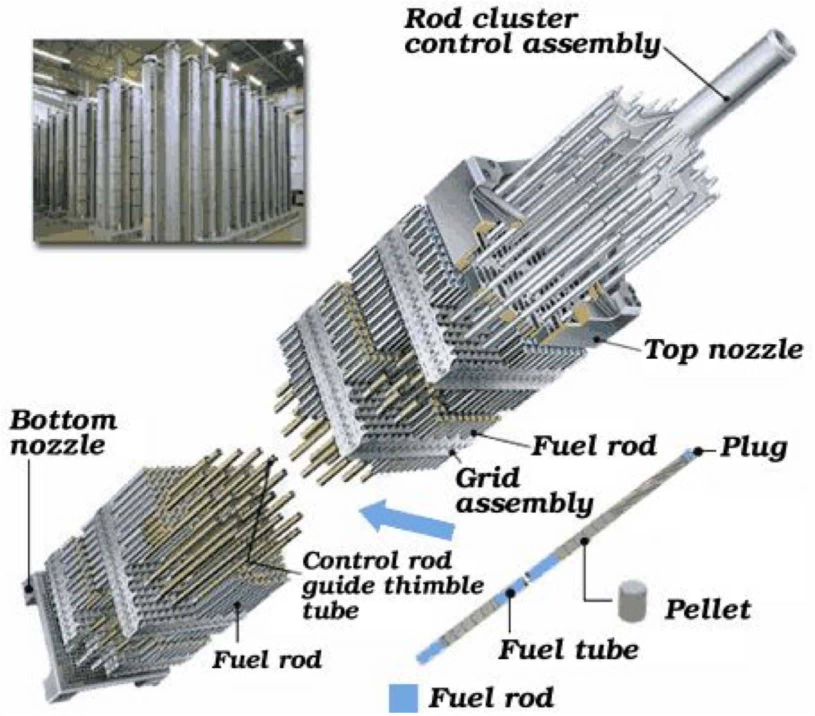
- Vedant: https://doi.org/10.1016/j.jnucmat.2019.151965
- Yuqing: https://doi.org/10.1016/j.jnucmat.2020.152069
- Khadija: https://doi.org/10.1016/j.jnucmat.2020.152050

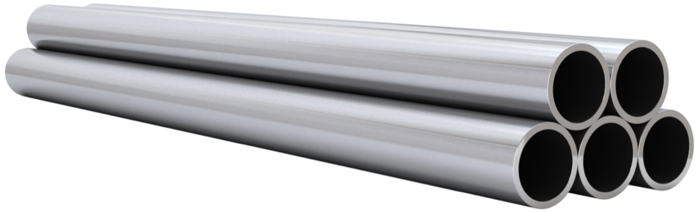
- Presentations will be conducted on ZOOM, Thursday, April 9
- Article overview, background, motivation, brief methods, results summary, critical analysis, potential future work

Zirconium Cladding

Cladding

- The purpose of the cladding is to
  - Hold the pellets together so that coolant can freely flow past
  - Transport heat from fuel to the coolant
  - Contain fission products
  - Contain fuel fragments
- We would also prefer if the cladding had little to no impact on the neutron transport in the reactor





Why Zirconium alloys?

Benefits

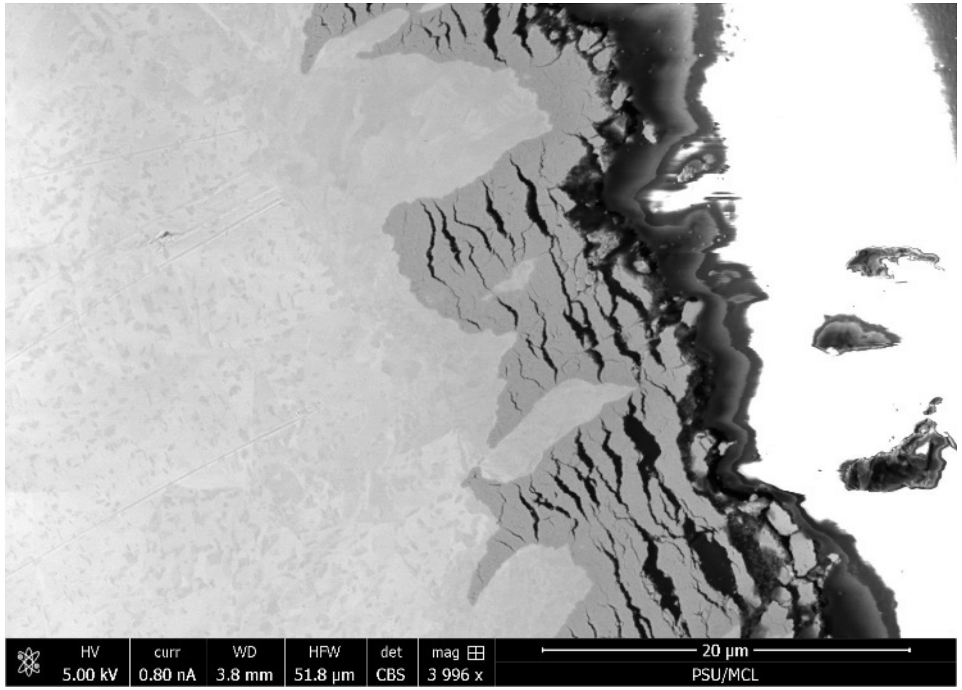
- Low neutron cross section
- Corrosion resistance in 300° C water
- Resistance to void swelling
- Adequate mechanical properties
- Good thermal conductivity
- Affordable cost
- Available in large quantities

Problems?

- Corrosion under high temperature steam
- Hydride embrittlement
- Anisotropic characteristics lead to creep and growth

Zirconium

- Pure zirconium was not acceptable due to its oxidation behavior
- Oxygen with water reacted to form an oxide layer
- The oxide layer is brittle and flakes off, allowing more oxidation to occur
- Zr alloys were developed to reduce corrosion resistance



Commercial Zr Alloys in PWRs

Alloy	Sn %	Nb %	Fe %	Cr %	Ni %	O %	Fuel Vendor
PWRs (structural components and fuel rods)							
Zircaloy-4 (SRA)	1.2-1.7	-	0.18-0.24	0.07-0.13	-	0.1-0.14	
ZIRLO (SRA)	1	1	0.1	-	-	0.12	W
Optimized ZIRLO (pRXA)	0.7	1	0.1	-	-	0.12	W
M5 (RXA)	-	0.8-1.2	0.015-0.06	-	-	0.09-0.12	AREVA
HPA-45 (SRA/RXA)	0.6	-	Fe+V	-	-	0.12	AREVA
NDA (SRA)	1	0.1	0.3	0.2		0.12	NFI
MDA (SRA)	0.8	0.5	0.2	0.1		0.12	MHI/MNF

Summary

- Zirconium alloys used as cladding
- Zirconium fabricated into an alloy to increase corrosion resistance
- There are a number of Zr alloys utilized in PWRs as cladding and structural materials