Nuclear Fuel Performance

NE-591-010

Spring 2021

Last time

- Fission products change the fuel behavior
- Fission gas is released in three stages
  1. Fission gas production and diffusion to grain boundaries
  2. Grain boundary bubble nucleation, growth, and interconnection
  3. Gas transport through interconnected bubbles to free surfaces
- Fission gas release is measured using post-irradiation annealing and in pile experiments
- Fission gas release models are used to understand fission gas experiments and to predict gas release for fuel performance codes
- Spherical grain models predict a fraction of gas release for post-irradiation annealing or for in-pile gas release
- Fission gas diffusivity behavior changes with temperature and fission rate

Fuel Swelling/Dimensional Change

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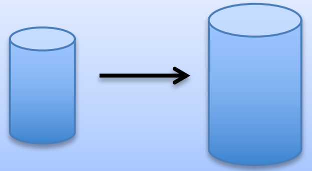
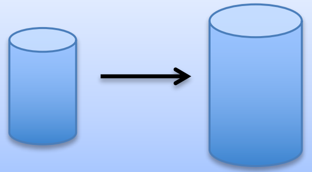
Fuel changes size and shape under reactor operation

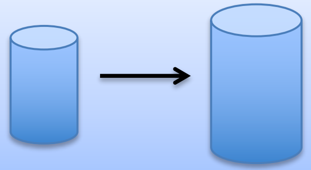
Thermal Expansion
- Increase in volume
- Decrease in density
- Caused by increasing temperature



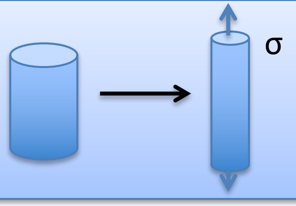
Densification
- Decrease in volume
- Increase in density
- Caused by shrinking of porosity left after sintering



Swelling
- Increase in volume
- Decrease in density
- Caused by fission products



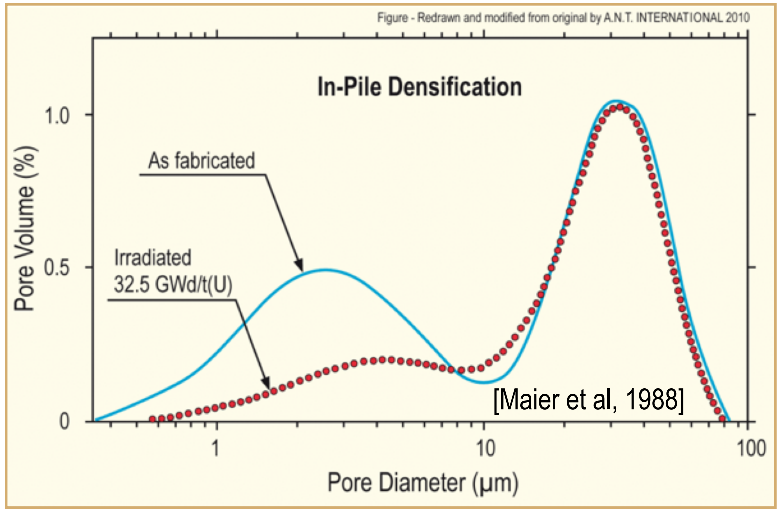
Irradiation Creep
- Change in shape
- Constant density
- Occurs under stress with $\sigma < \sigma_y$

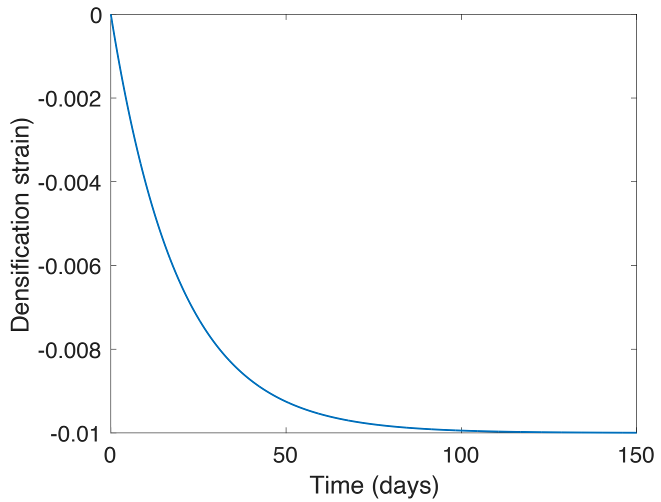


Densification

- Densification takes place during initial 5 - 10 MWd/kgU
  - Small, as-built pores close due to effects of fission spikes and vacancy diffusion
  - Large pores stable (in absence of large hydrostatic stress)
- Empirical correlation for densification is a function of
  - β - Burnup (in FIMA)
  - $\Delta\rho_0$ – Total densification that can occur (a common value is 0.01)
  - β_D – Burnup at which densification stops (a common value is 5 MWD/kgU)
  - C_D = 7.235 − 0.0086 (T(° C) − 25) for T < 750° C and CD = 1 for T ≥ 750 ° C

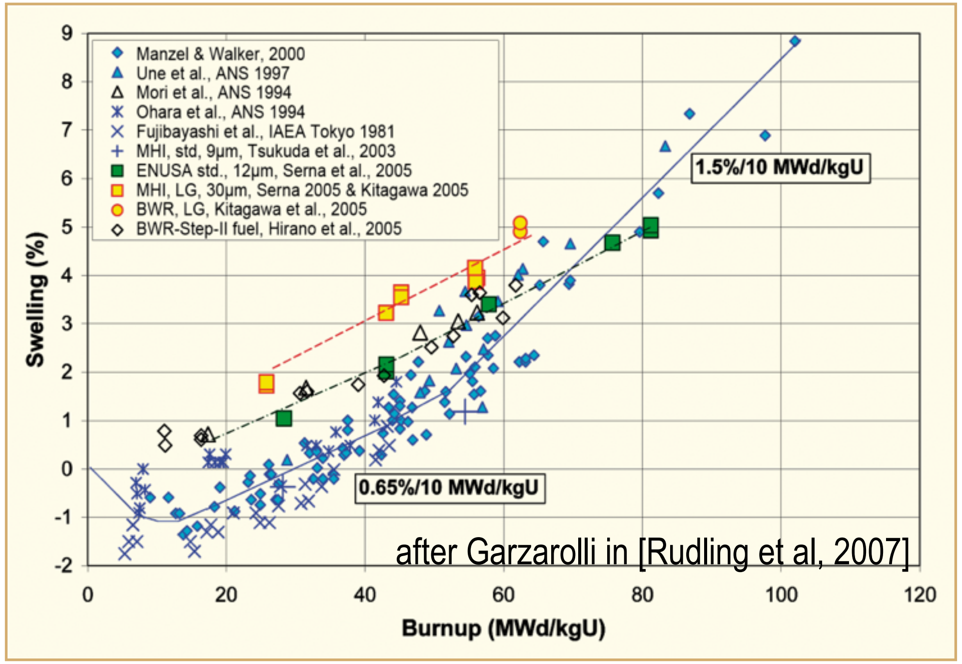
$$\epsilon_D = \Delta\rho_0 \left(e^{\frac{\beta \ln 0.01}{C_D \beta_D}} - 1 \right)$$





Fission product induced swelling

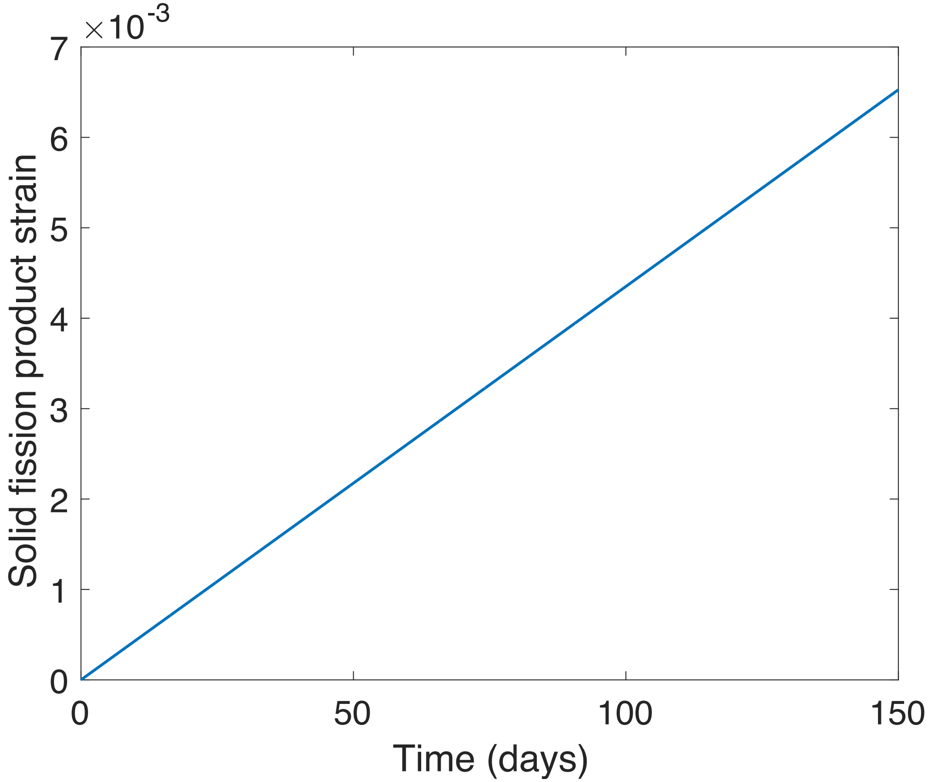
- Fission product swelling results from three changes in the fuel microstructure
  - Solid swelling: Accumulation of soluble and insoluble fission products in fuel matrix
  - Gaseous swelling: Accumulation of gaseous and volatile fission products in intragranular and intergranular pores
  - High burnup swelling: Restructuring of pellet rim with the accumulation of fission gas in a large number of small pores



Solid fission product swelling

- The solid fission product swelling model is a function of:
  - B – Burnup (in FIMA)
  - ρ – Initial UO_2 density (g/cm^3)

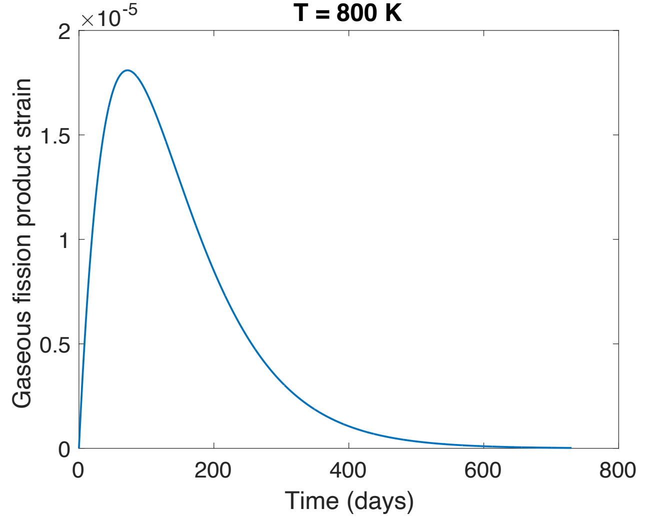
$$\epsilon_{sfp} = 5.577 \times 10^{-2} \rho \beta$$

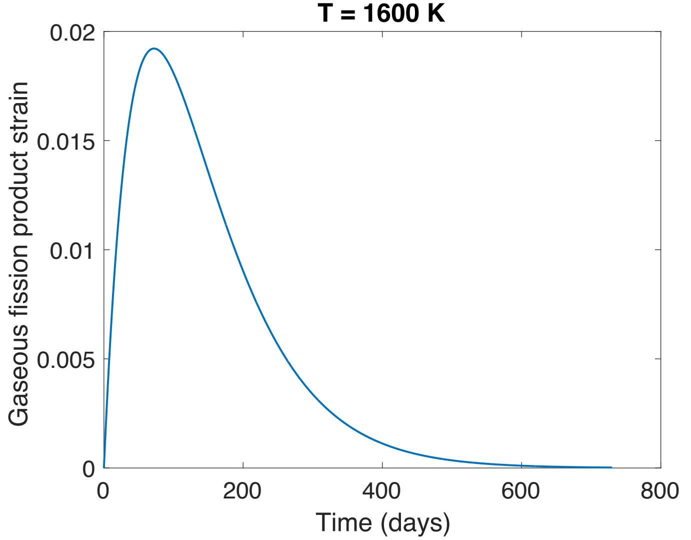


Gaseous fission product swelling

- Gaseous swelling varies strongly with temperature, fission rate and stress
- T < 1000K
  - Fission gas atoms remain in fuel matrix or collect in small, isolated, intragranular pores (<1 nm)
  - Intragranular pore size limited by fission spikes that drive gas back into fuel matrix
  - Gaseous swelling constrained by fission gas release
- T = 1000 to 1700 K
  - Swelling takes place at hot interior of pellet
  - Gas atoms in fuel matrix diffuse to grain boundaries and collect in pores
  - Gas pressure causes bubbles to increase in size and to coalesce into larger pores
  - Gaseous swelling opposed by applied stress
  - Gaseous swelling also constrained by fission gas release

$$\epsilon_{gfp} = 1.96 \times 10^{-28} \rho\beta (2800 - T)^{11.73} e^{-0.0162(2800-T)} \, e^{-17.8\rho\beta}$$





Total change in volume

- The total change in volume is found by adding all components of dimensional change
  - $\varepsilon_{tot} = \varepsilon_{th} + \varepsilon_{D} + \varepsilon_{sfp} + \varepsilon_{gfp}$
- Example:
  - fission rate = 2.5e13 f/(cm^3 s)
  - T(fuel) = 1400 K
  - T_{ref} = 300 K
  - For densification: $\Delta\rho_0$ = 0.01 and β_D = 5 MWD/kgU
  - Total time: 2 weeks

Change in Volume Example

- First, we need to calculate the burnup, enrich 5%, $\beta = \dot{F}t/N_U$
  - M_{UO2}=16*2+238*0.95+235*0.05=269.9 g/mol
  - $N_U = N_a \rho_U/M_U$ = 6.022e23*10.97/269.9 = 2.45e22 atoms of U/cm^3
  - β = 2.5e13*3600*24*7*2/2.45e22 = 0.0012 FIMA
- Next, we need to determine the strain from thermal expansion
  - $\varepsilon_{th} = \alpha\Delta T$ = 11e-6*(1400 – 300) = 0.0121
- Then, we consider densification, $\epsilon_D = \Delta\rho_0 \left(e^{\frac{\beta \ln 0.01}{C_D \beta_D}} - 1 \right)$
  - We need to calculate C_D, but because we are higher than 750C, C_D = 1
  - We need to convert the burnup to FIMA, β_D = 5 MWD/kgU/950 = 0.0053 FIMA
  - ε_D = 0.01*(exp(0.0012*log(0.01)/(1*0.0053)) – 1) = -0.0065

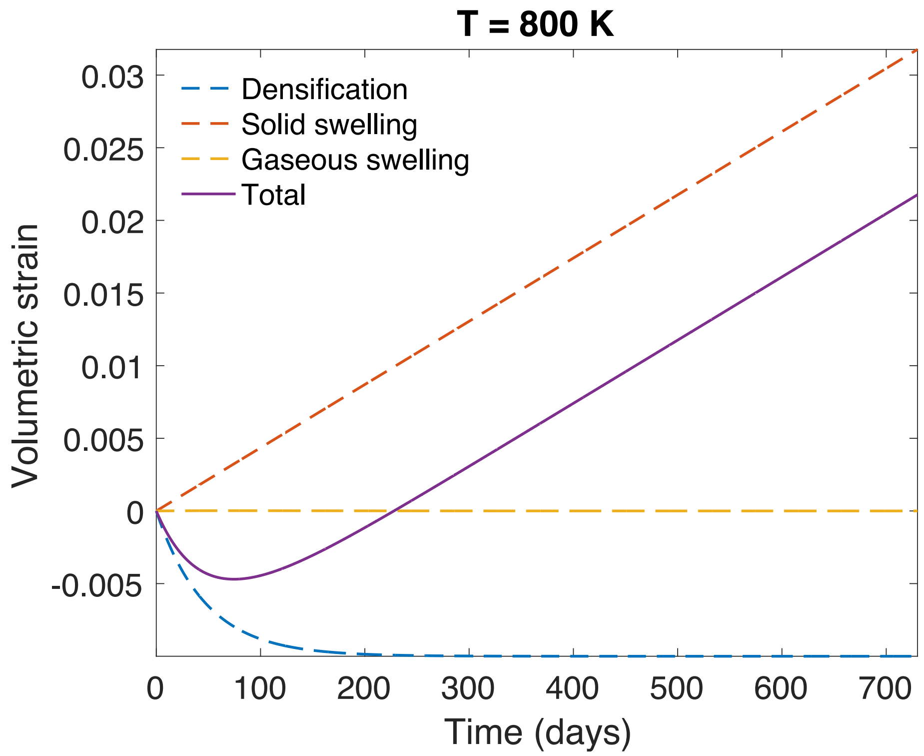
Change in Volume Example

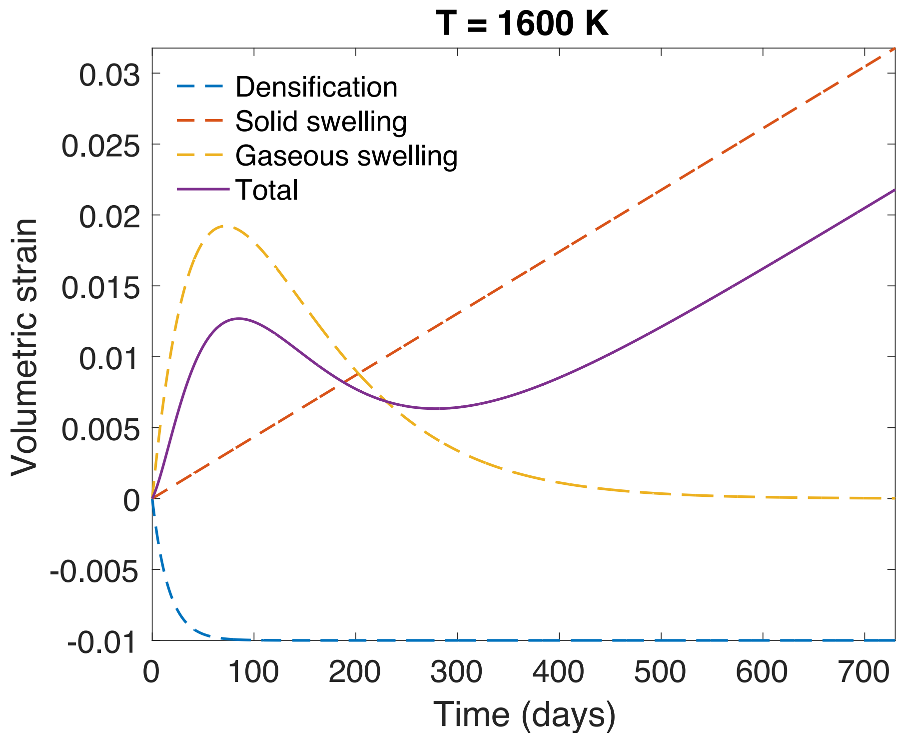
- For solid fission product swelling, $\epsilon_{sfp} = 5.577 \times 10^{-2} \rho\beta$
  - For the density of UO_2, ρ = 10.97 g/cm^3
  - ε_{sfp} = 5.577e-2*10.97*0.0012 = 7.34e-4
- Finally, gaseous fission product swelling

$$\epsilon_{gfp} = 1.96 \times 10^{-28} \rho\beta (2800 - T)^{11.73} e^{-0.0162(2800-T)}\, e^{-17.8\rho\beta}$$

  - ε_{gfp} = 1.96e-28*10.97*0.0012*(2800 – 1400)^11.73* exp(-0.0162*(2800 – 1400))*exp(-17.8*10.97*0.0012) = 0.0023
- Total:
  - $\varepsilon_{tot} = \varepsilon_{th} + \varepsilon_{D} + \varepsilon_{sfp} + \varepsilon_{gfp}$ = 0.0121 – 0.0065 + 7.34e-4 + 0.0023 = 0.0086

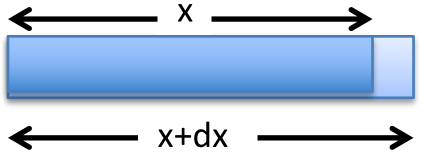
The overall swelling behavior depends on temperature



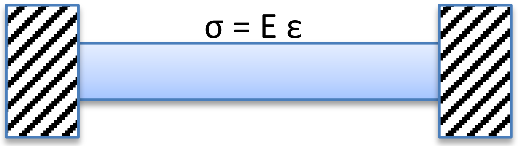


Creep

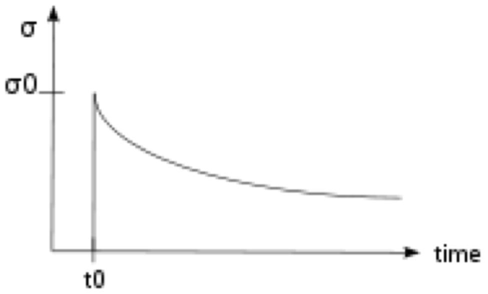
- Creep is a general mechanism for plastic deformation that occurs over time when $\sigma < \sigma_y$
- Consider a heated metal beam so it expands some distance dx



- We then fix it between two walls and let it cool down
- Because $\sigma < \sigma_y$, that stress remains constant



- In creep, defect diffusion is induced by the stress to cause permanent deformation and reduce the stress
- Therefore, creep
  - Occurs over time
  - Increases with increasing number of diffusing defects
    - High temperature (**thermal creep**)
    - Irradiation (**irradiation creep**)

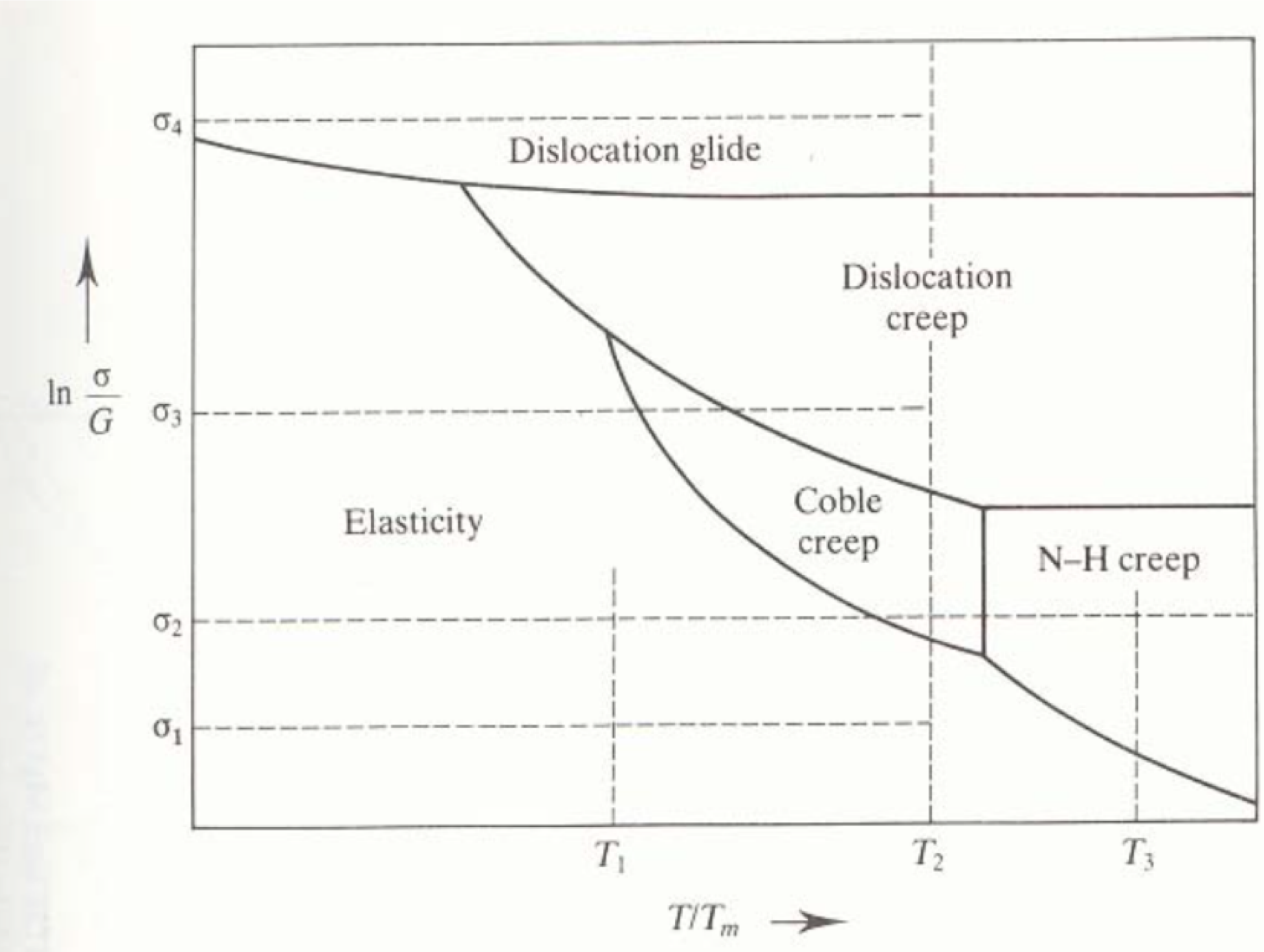


Creep

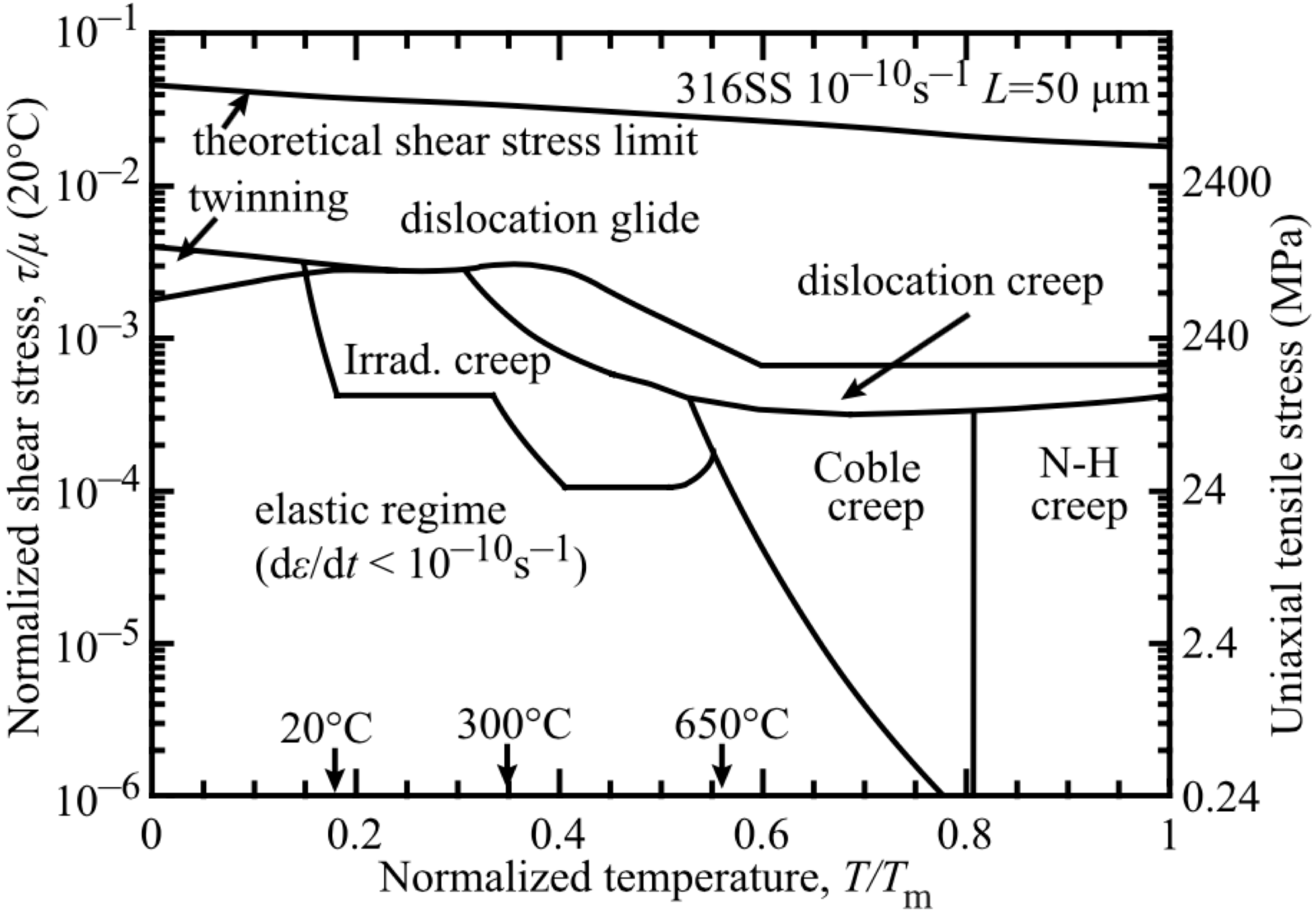
- General creep equation: $$\dot{\epsilon} = \frac{C\sigma^m}{D_{gr}^b} e^{\frac{-Q}{k_b T}}$$

- Creep can be caused by various microstructural mechanisms
- Bulk Diffusion (Nabarro-Herring creep)
  – Atoms diffuse (high T), causing grains to elongate along the stress axis
  – Q = Q(self diffusion), m = 1, and b = 2
- Grain boundary diffusion (Coble creep)
  – Atoms diffuse along grain boundaries to elongate the grains along the stress axis
  – Q = Q(grain boundary diffusion), m = 1, and b = 3
- Dislocation creep
  – Dislocations glide under a high stress
  – Dislocations climb due to defects to avoid obstacles
  – Q = Q(self diffusion), m = 4–6, and b = 0

Different creep mechanisms are active for different combinations of stress and temperature



The behavior of creep changes in irradiated materials

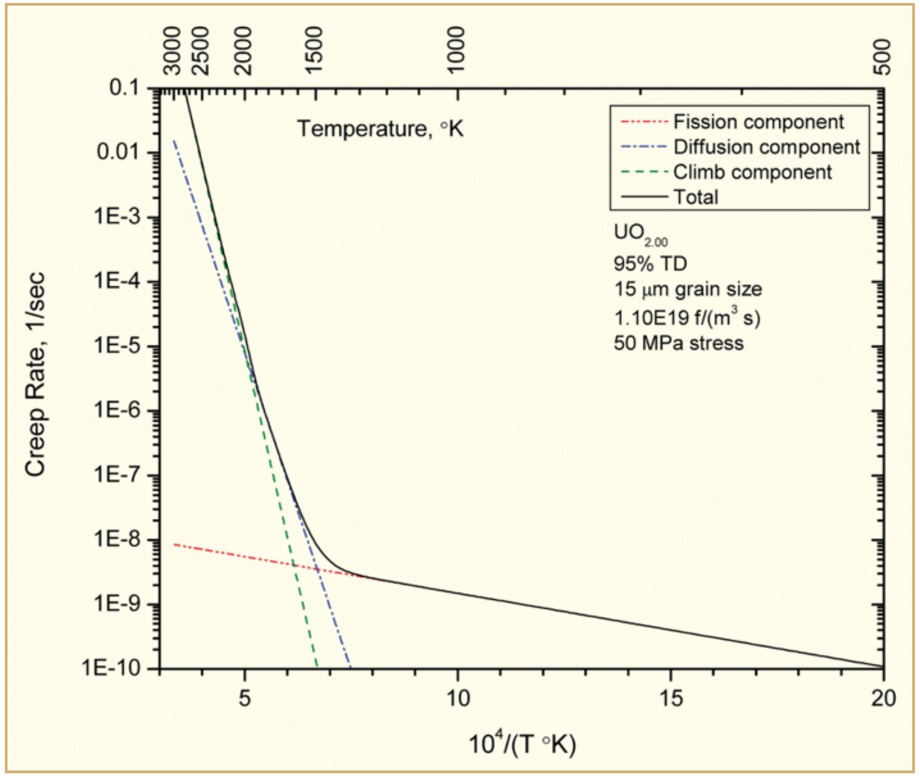


Irradiation and Creep

- Irradiation accelerates creep, causing it to be significant at lower temperatures
- Irradiation has little effect on diffusional creep, but it accelerates dislocation creep in cubic materials
- The dislocation creep rate can be written as $\dot{\varepsilon} = \rho_d^m b \mathrm{v}_d$
  - $\rho_d{}^m$ is the density of mobile dislocations
  - b is the burgers vector
  - v_d is the dislocation velocity
- Gliding dislocations quickly get pinned by obstacles
- As the dislocations absorb defects created by irradiation, they climb to different slip planes to avoid the obstacles
- More interstitials are absorbed than vacancies due to the higher sink strength for interstitials

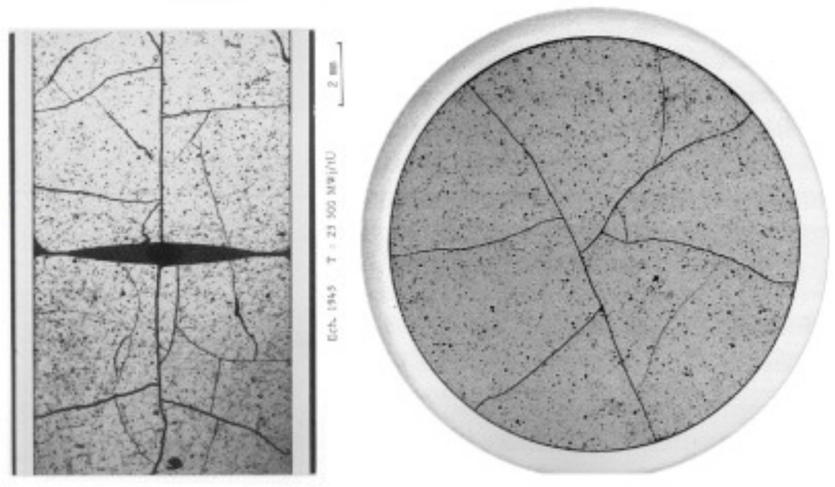
Fuel Creep

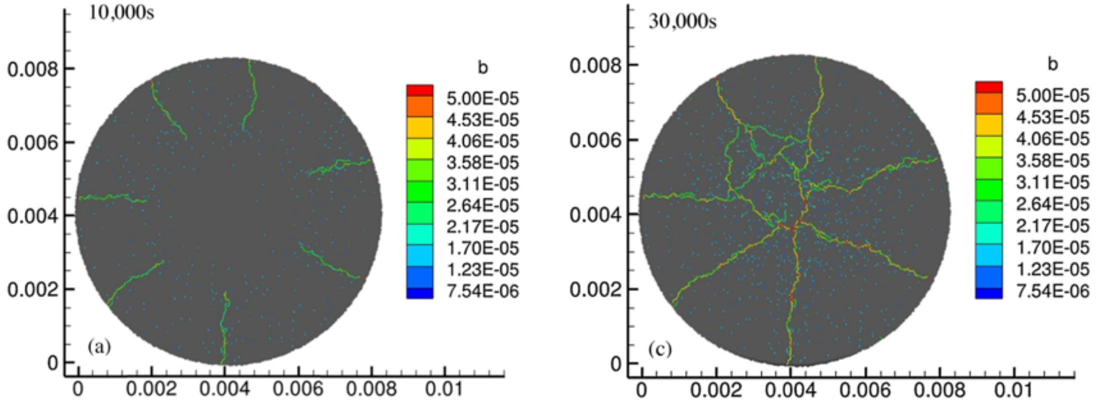
- Like other materials, the fuel also undergoes creep
- The fuel creep (In UO2) is a combination of diffusion creep and irradiation creep
- It is expected that fuel creep plays a major role in dimensional change in metallic fuels, largely via N-H and Coble creep, but still unproven experimentally and no good creep models exist for metallic fuels



Fracture

- UO_2 pellets fracture during changes in temperature due to large thermal stresses
- Fracture results in:
  - Increased gap reduction
  - Reduced thermal conductivity
  - Increased avenues for fission gas release
- Fracture has been typically modeled in two ways:
  - Empirical relocation model that is a function of burnup
  - Semi-empirical smeared cracking model
- Modern methods provide means of modeling discrete cracks

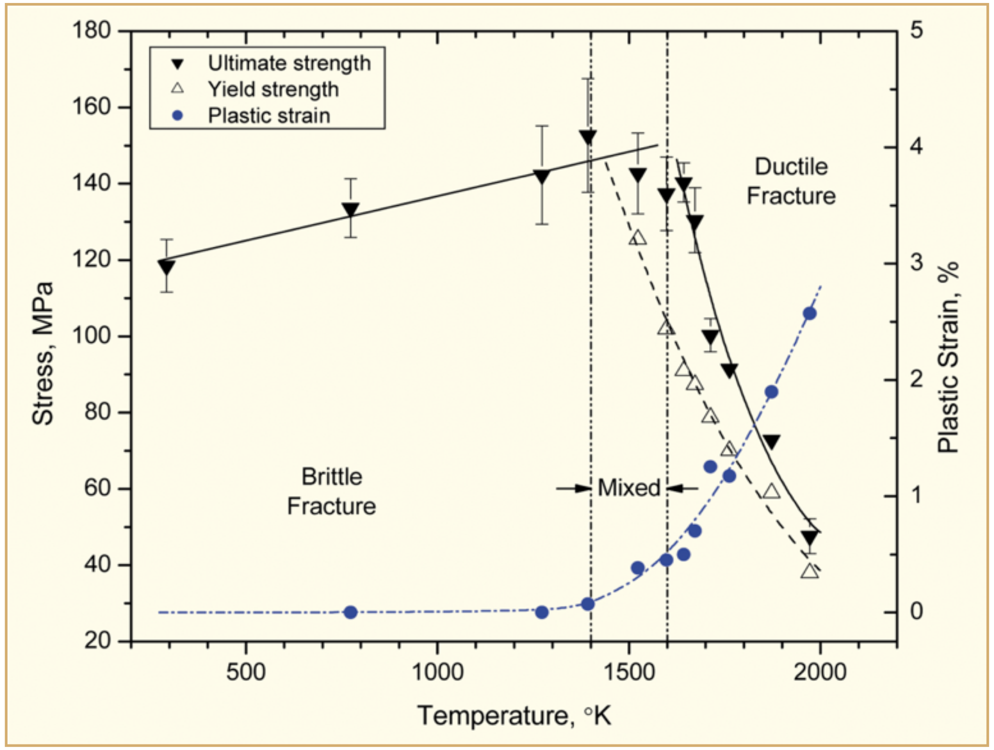




- Radial cracks partially penetrate the pellet during temperature increase
- Full cracking occurs when the temperature decreases

Fracture

- The fracture behavior of the fuel is fairly complicated
- Fracture strength varies with grain size (G)
  - $\sigma_{frac} = G^{-m}\sigma_{frac, ref}$, m = 0.04 – 0.05 (vs. m ~ 0.5 for metal)
  - Increasing grain size from 10 μm to 100 μm reduces σ_{frac} by ~10%
- Ductility transition temperature is lower in-reactor than in thermal tests
- Fracture strength is ~10 × higher in compression than in tension
- Load-deformation behavior strongly affected by creep under in-reactor conditions



Summary

- Many materials models for fuel are empirical and correlated to burnup
- Fuel pellets change shape due to
  – Thermal expansion (increase in volume)
  – Densification (decrease in volume)
  – Swelling (increase in volume)
  – Creep (volume stays the same)
- Fracture also decreases the gap, as fractures pieces shift outward

Fuel Thermal Conductivity

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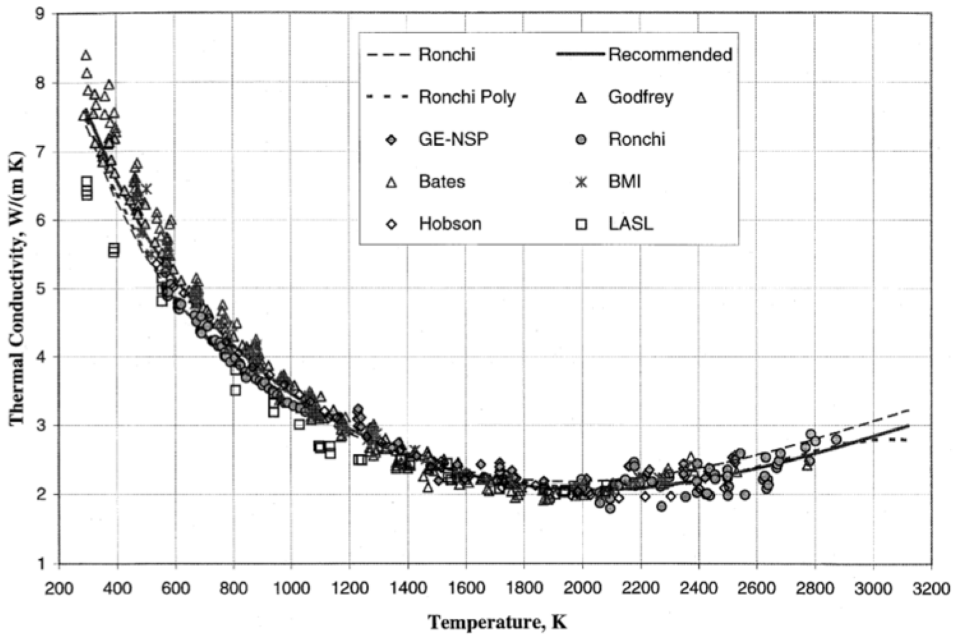
UO2 Thermal Conductivity

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

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

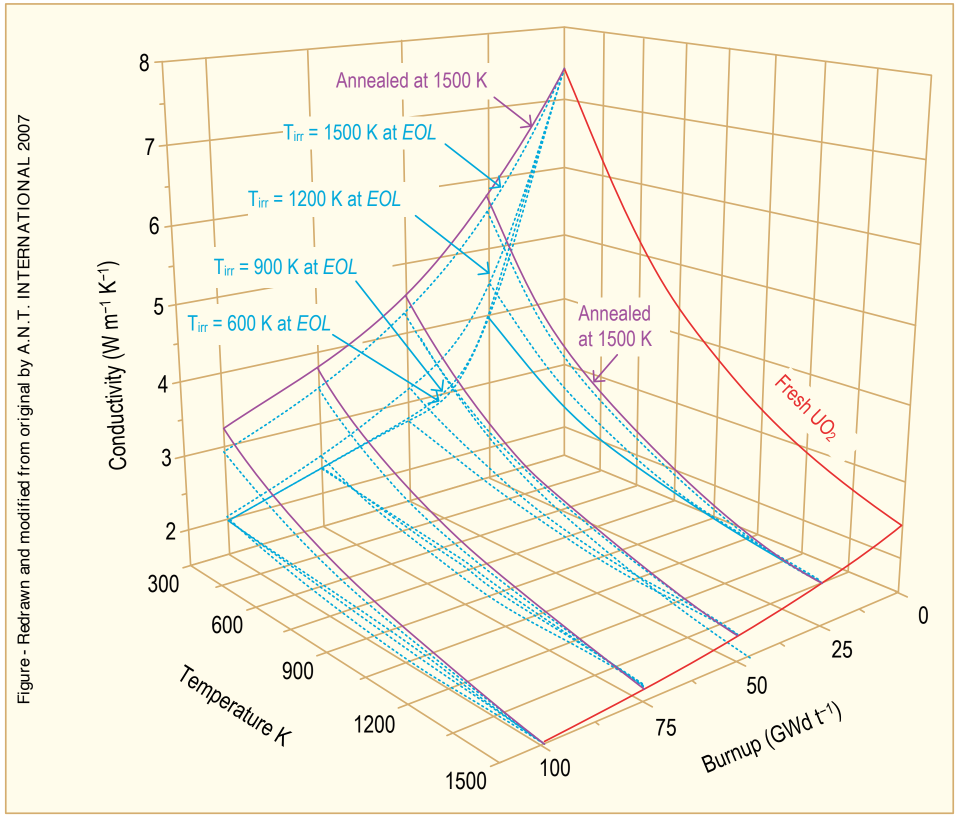
  - Where t = T/1000
  - The first part of the equation describes the phonon interactions
  - The second part describes electronic transport which becomes significant at high temperature



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

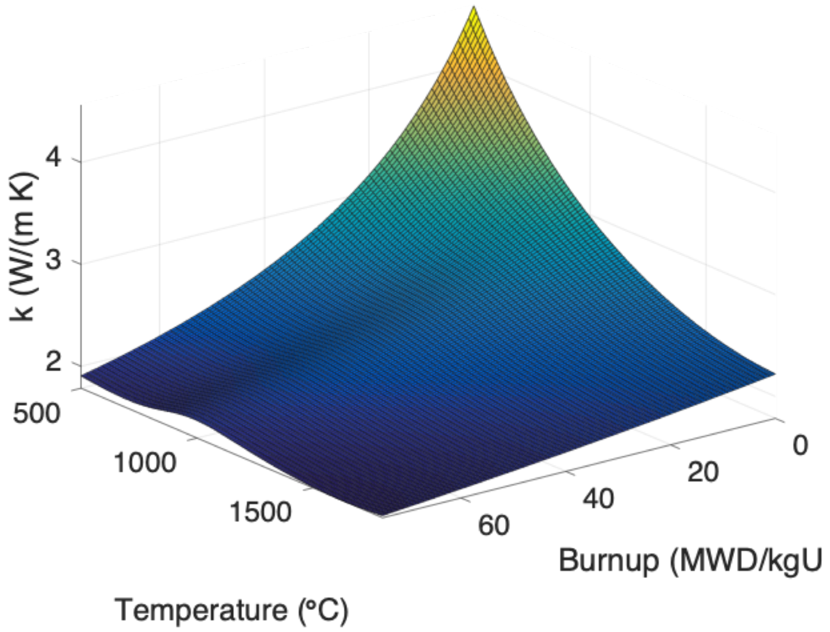
$$k = (1 - R_f(T))k_{ph1}(T,\beta) + R_f(T)k_{ph2}(T,\beta) + k_{el}(T)$$

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

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

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

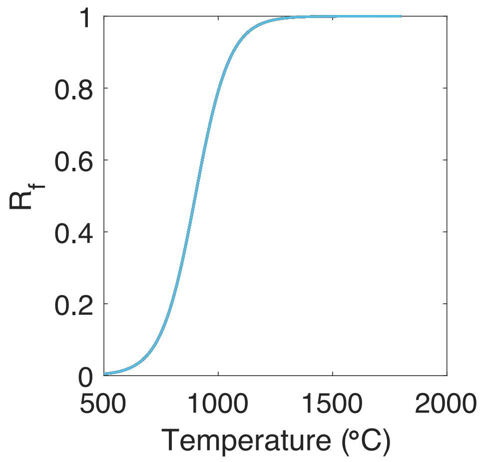
$$k_{el} = 1.32 \times 10^{-2}\, e^{1.88\times 10^{-3}T}$$

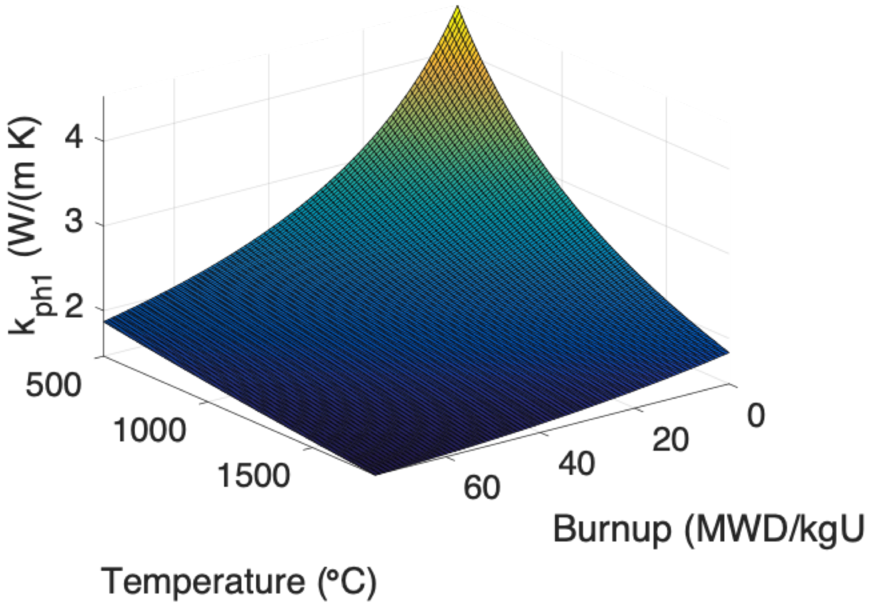


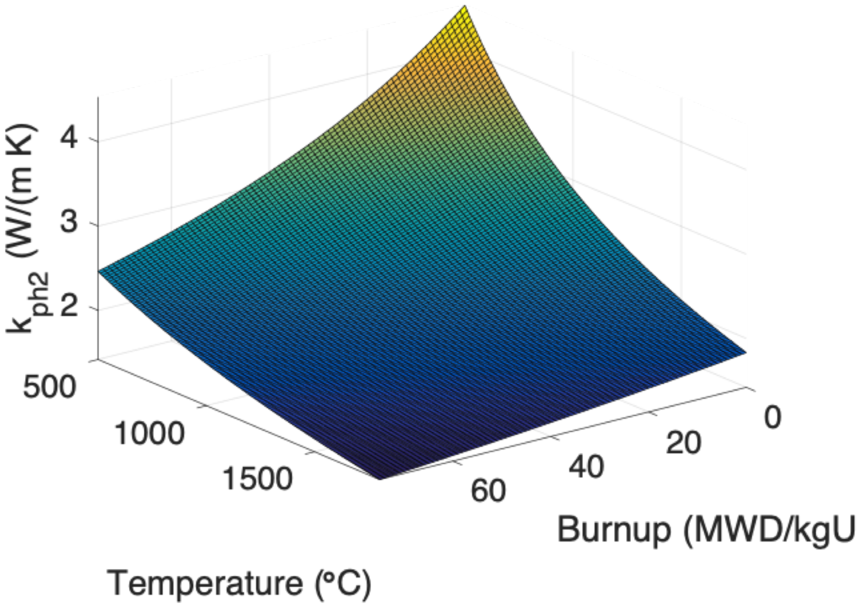
UO2 Thermal Conductivity

- 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)

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

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

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

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

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

Summary

- The fuel thermal conductivity decreases with burnup
- Empirical models take into account both phonon and electron based thermal transport
- BISON primarily utilizes the NFIR model to describe thermal conductivity
- The NFIR model is a fairly accurate empirical model of the fuel thermal conductivity