Nuclear Fuel Performance

NE-533

Spring 2025

Last Time

- Talked through numerical thermomechanics
- All fuel performance codes: a) Numerically model the temperature in the fuel, b) Numerically model the stress in the cladding, c) Consider gap pressure, closure, and heat transfer
- Some multiphysics fuel performance codes
  - FRAPCON/FRAPTRAN
  - BISON
- Intro into material property evolution

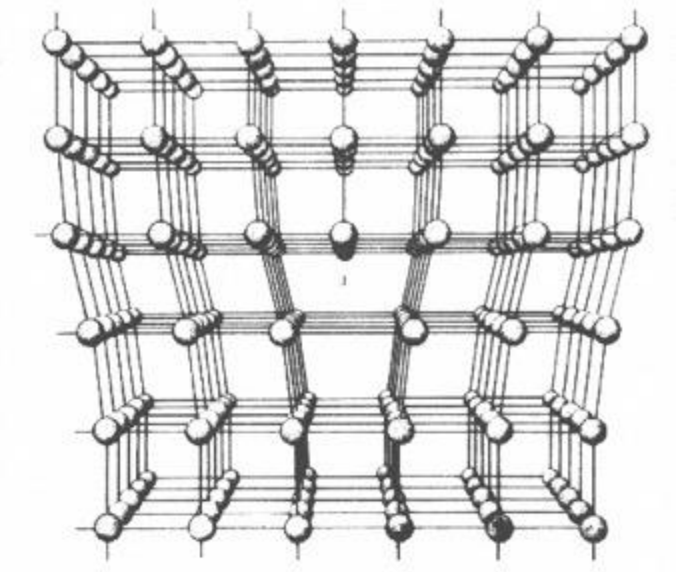
Paper Project

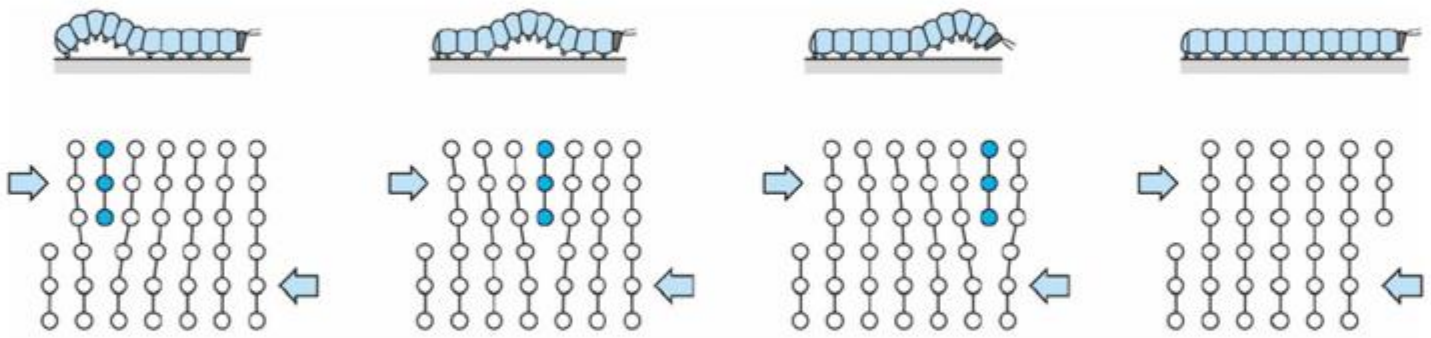
- Assigned papers uploaded to moodle with your name as a prefix
- This will be a critical review of the paper, similar to what we do for QE2, but much shorter
- Contextualize, summarize, and analyze
- 15-minute presentation that summarizes what was done in the paper, provides context on why it was done, and reviews what could or should have been done, or could be done next
- All presentations will be submitted via moodle, due by end of the day on Mar. 3
- Distance students will submit slides and a recording of their presentation
- Presentations will take place in-class on Mar. 4 and Mar. 6

MATERIAL PROPERTY EVOLUTION

Dislocations are imperfections associated with a line of lattice sites (1D defect)

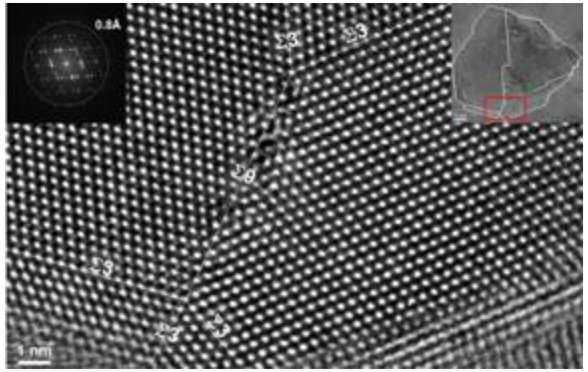
- In a dislocation, an extra half plane of atoms is inserted into the lattice
- When it moves, only a small number of bonds are broken at a time
- Dislocation motion controls the plastic (permanent) deformation of crystalline materials



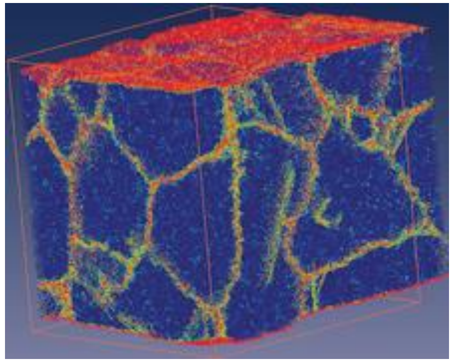


Grain boundaries

- Materials are typically composed of various regions where the crystal lattice is oriented differently. These regions are called **grains**
- When two grains meet, there is a plane of atoms that do not follow the crystal lattice called a **grain boundary (2-D defect)**
- Most crystalline materials are polycrystalline, not single crystal

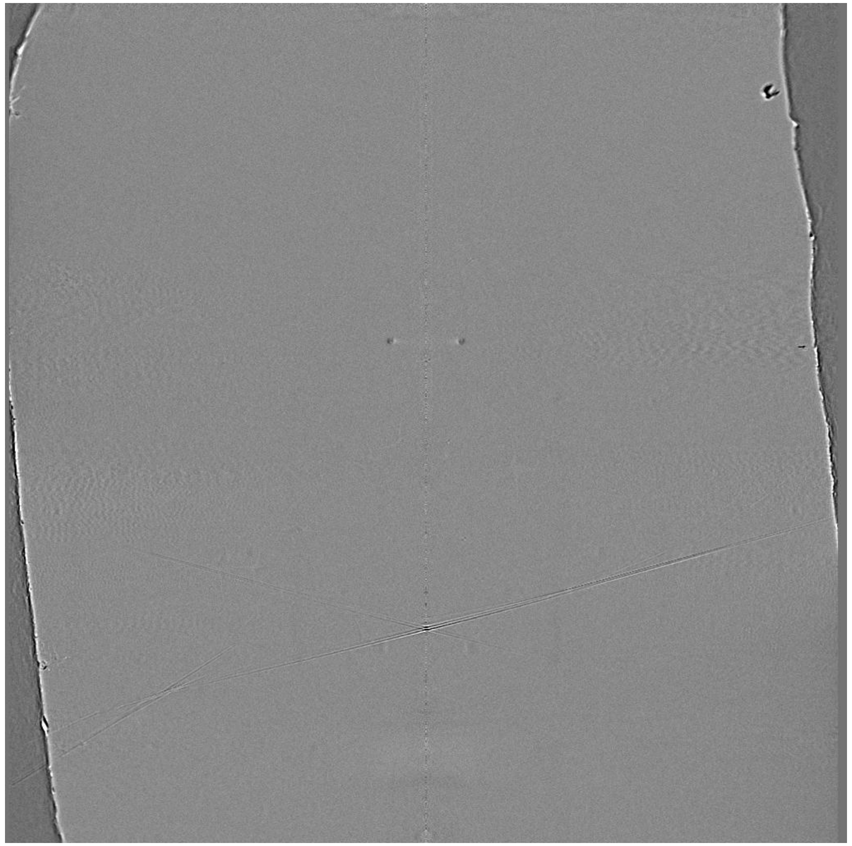


High-res transmission eleectron microscopy can also show individual atoms (palladium) *www.knmf.kit.edu/TEM.php*



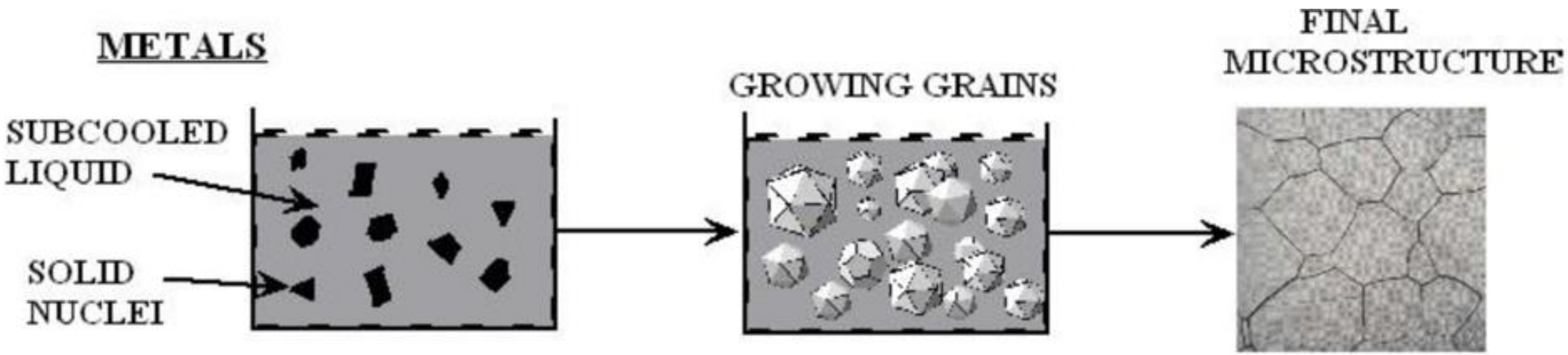
Atomistic simulation of grain boundaries in 3D

Metals are often cast, and polycrystals naturally form during casting



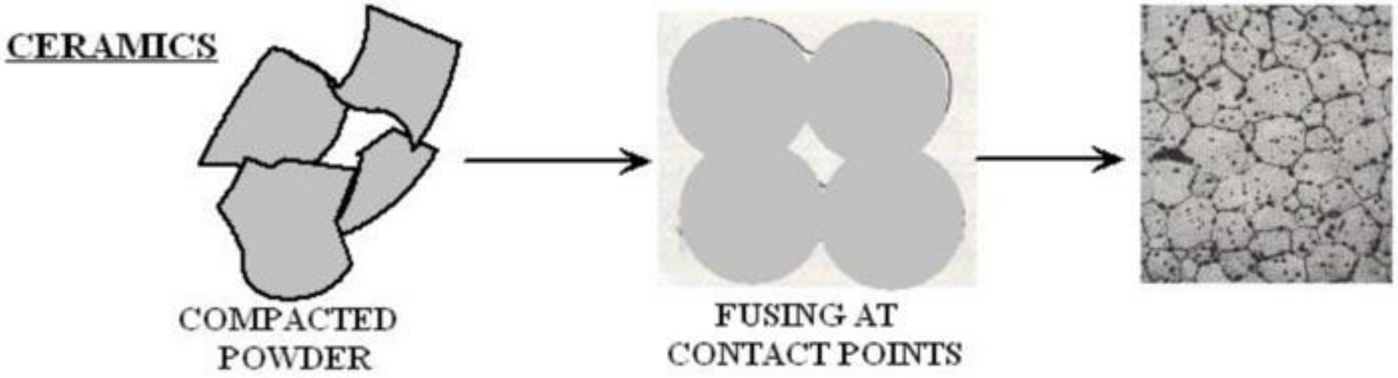
Polycrystals naturally form during casting

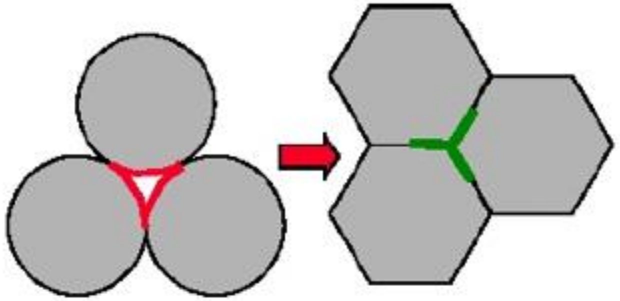
- Solidification begins in different regions of the melt, each with a different orientation
- Once the different regions meet, grain boundaries form between them

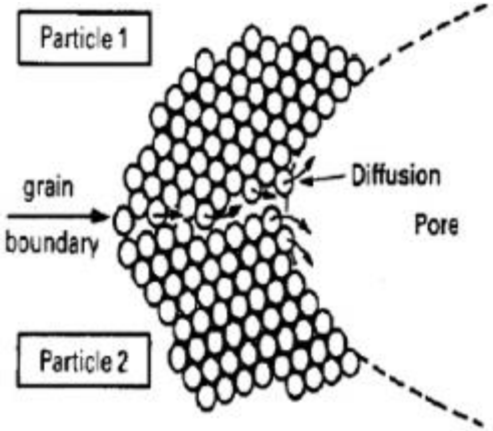


Ceramic sintering

- Ceramics are typically sintered, and polycrystals also naturally form from sintering
- In sintering, powders are compacted at high temperature
- The particles are each oriented differently, and as they fuse, grain boundaries form
- The differences between the grain orientations result in the grain boundary



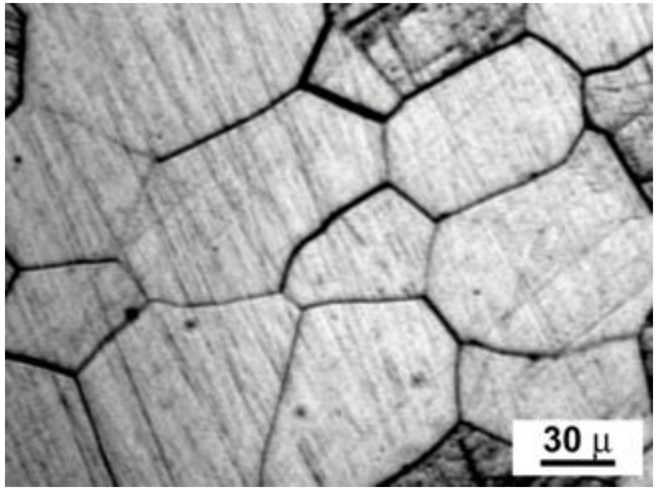


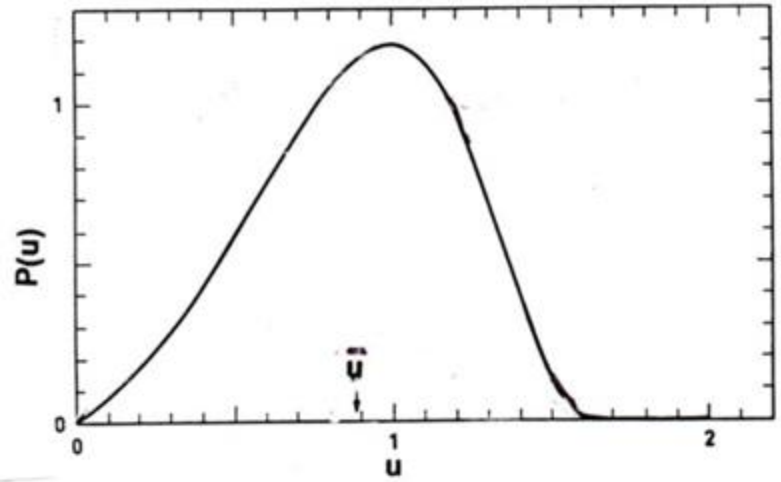


Distribution of grain sizes

- In a polycrystal, there is also a distribution of grain sizes
- Therefore, we commonly refer to the grain size distribution and the **average grain size**
- The Hillert distribution is an analytical distribution for grain size
- Real materials often vary from this behavior

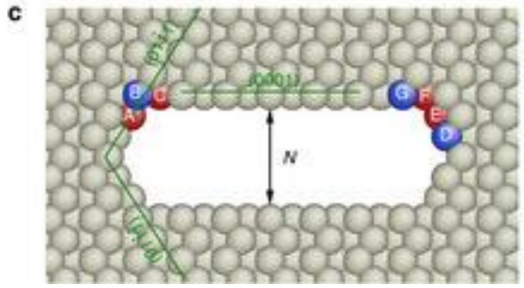
$$P(u) = (2e)^{\beta} \cdot \frac{\beta u}{(2-u)^{2+\beta}} \cdot \exp \frac{-2\beta}{2-u}$$

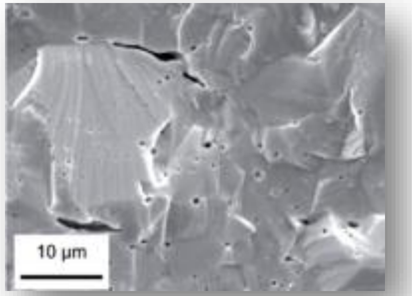


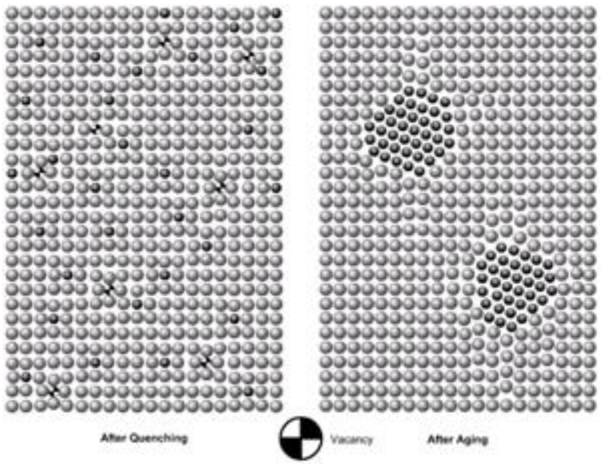


3D Defects

- When point defects cluster, they form three dimensional defects
- The energy of a point defect is reduced when several point defects cluster together
- Larger clusters of vacancies are called **voids**
- Clusters of impurity atoms are called **precipitates**

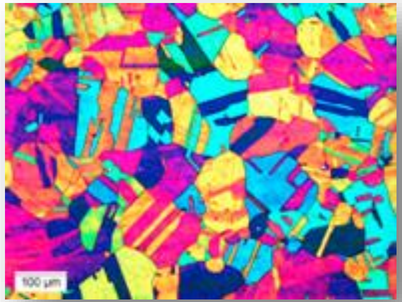






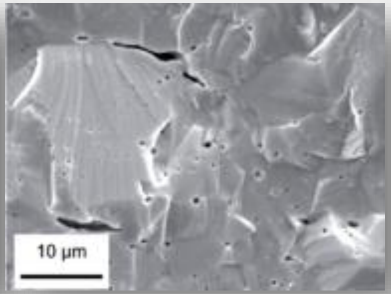
Microstructure

- Material microstructure is the structure observable with 25x magnification
- The microstructure includes grain structure, secondary phases, porosity, and more
- The microstructure can strongly influence physical properties such as strength, toughness, ductility, hardness, corrosion resistance, high/low temperature behavior or wear resistance.
- These properties in turn govern the application of these materials in industrial practice

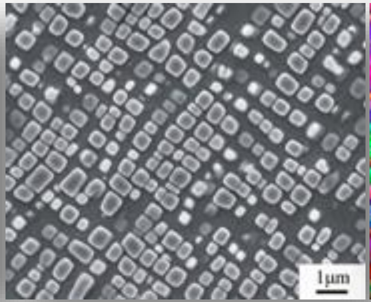


Annealed Stainless Steel

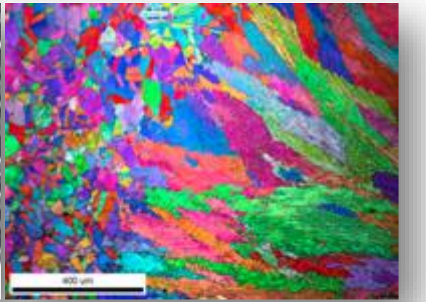
Cast Bronze



Sintered UO2

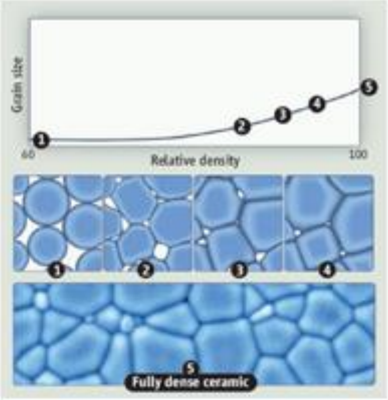


Co-Al-W Superalloy



Friction stir welded stainless steel

Material processing



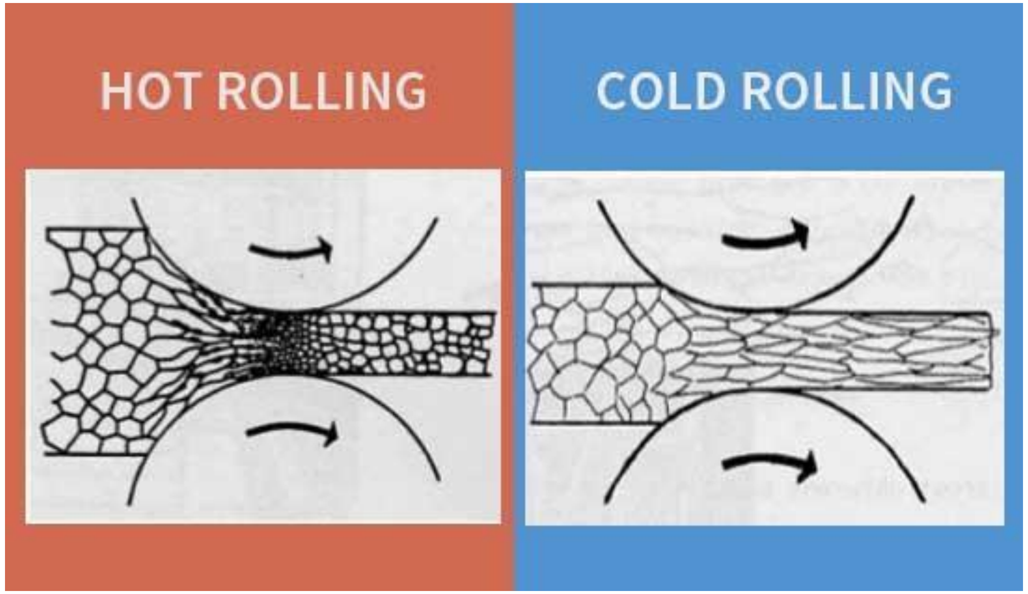
- The processes we use to make a material have a huge impact on its microstructure and properties
- **Casting** – manufacturing process in which a liquid material is poured into a mold and then allowed to solidify
  - Can be used to make complex shapes
  - The solidified microstructure typically has properties that are far from ideal
- **Sintering** – Forming a solid from a powder using heat and/or pressure without melting the material
  - Applicable to metals and ceramics
  - Difficult to obtain a material that is fully dense
  - Used to make fuel pellets
- **Post-fabrication processing**
  - **heat treatment**
  - **working**

Material processing

- Heat treatment: heating or cooling a material to extreme temperatures to get desired microstructure and properties
  - Used to control the rate of microstructure change, including diffusion, grain growth, or phase change
  - Annealing
    - heat and hold the material, which allows for any defects in the material to repair themselves
    - The metal is then allowed to cool back to room temperature at a slow pace to produce a more ductile crystalline structure
  - Quenching
    - heated to a temperature that transforms its internal structure, held at that temperature, then rapidly cooled
    - The quick cooling process locks in the high T structure, or forces phase transformation without the ability to relax stresses

Material processing

- Working: metalworking process that plastically deforms the alloy
- Cold working occurs below the recrystallization temperature, hot working occurs above
- By plastically deforming the material, we are increasing the number of dislocations and dislocation barriers, increasing the yield strength
- Main types of working processes:
  - Squeezing (rolling/extrusion/drawing)
  - Bending (shaping)
  - Shearing (slitting)



Summary

- Gap size changes due to thermal expansion, changing temperature profile
- Often have displacements instead of strains, and can solve for stress via displacements

- Fuel and pellet conditions change with time due to microstructure evolution
- Atoms in the fuel and cladding materials are arranged in a crystal lattice
- The crystal lattice is never perfect; it has defects
  - Point defects, dislocations, grain boundaries, voids and precipitates
- All materials have defects, radiation damage causes many more defects
- Microstructure can be tailored through processing, during fabrication or post-fabrication

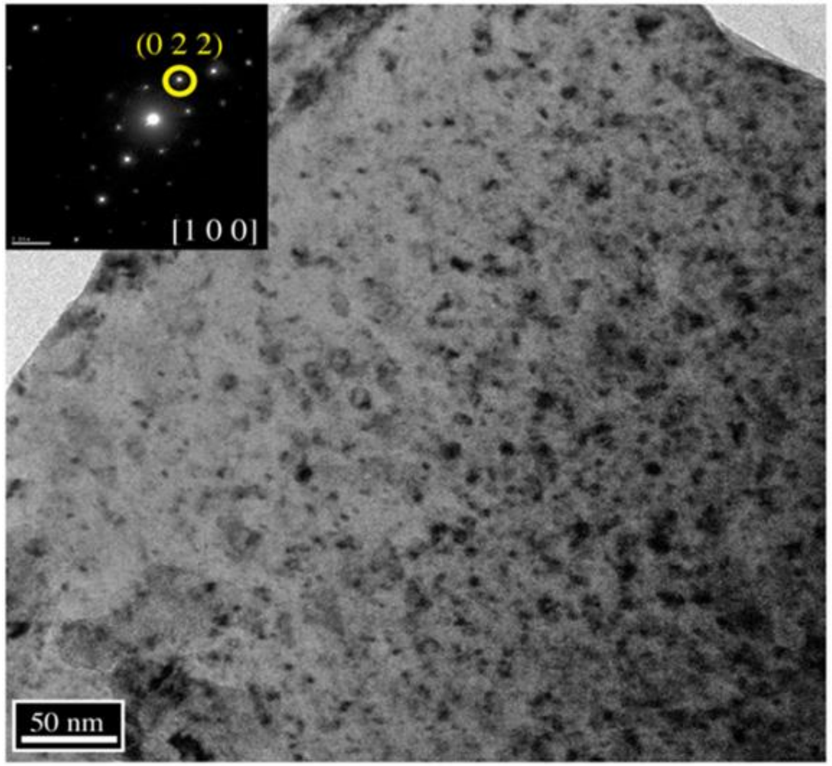
UO_2 RADIATION EFFECTS

Radiation Damage

- The macroscopic and observable results of exposure of solids to energetic particles are collectively known as radiation effects
- Heat production from the nuclear fuel to generate electricity ensues mostly from the slow down of the fission products by nuclear or electronic interactions
- As a direct consequence, there are also defects created along the path of the fission fragments leading to modification of the physical properties of the fuel
- Most Frenkel defects (interstitial-vacancy pair) are produced by secondary collision cascades
- Local charge neutrality prevents the formation of interstitials and vacancies as independent processes, as the cations and anions are charged species
- In UO2, two anion vacancies need to be created for each cation vacancy, forming a Schottky trio
- The dominant defect type is anion Frenkel pairs

Loop Formation

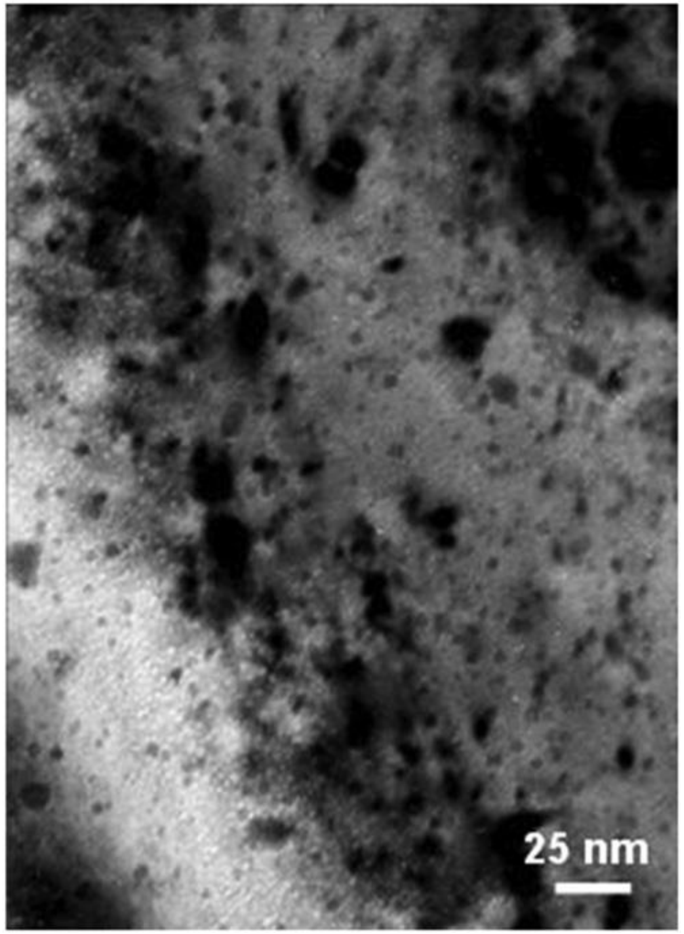
- Dislocations generally a mixture of screw and edge components in the shape of a loop
- The most important slip system in UO2 is the one which minimizes the electrostatic energy, the easy slip along {100}<110> tends to minimize the intense repulsive force between cations
- Prismatic loops are of interstitial type and consist of a disc-shaped layer of defects in a cluster
- This defect cluster is more energetically favorable than dispersed defects in the bulk
- Vacancy clusters will form into voids



Prismatic loops in UO2 from alpha particle irradiation

Voids

- Due to preferential absorption of interstitials at dislocations, we are left with a slight excess of vacancies in the bulk to nucleate and grow voids
- Void nucleation can occur homogeneously by the collection of vacancies in the matrix, or heterogeneously at structural features (precipitates, grain boundaries, etc.)
- The vacancy-rich radiation damage core is considered to be an important void nucleation mechanism in UO2
- Vacancy diffusion then allows void growth
- Gas atoms can often serve to stabilize small voids



Voids (bright spots) from alpha irradiation in UO2

Radiation Effects

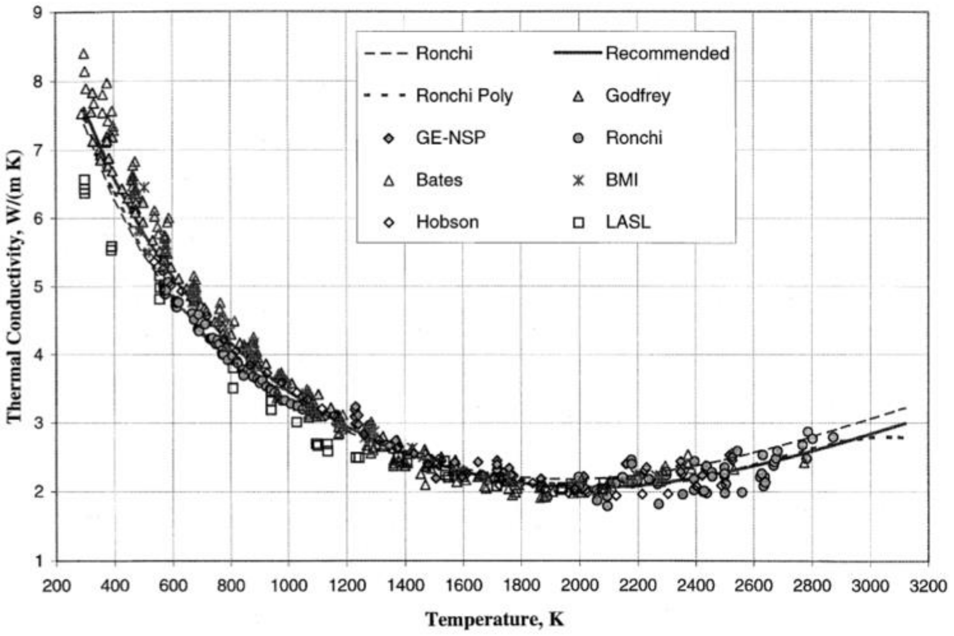
- Chemistry changes
  - two fission products are generated from each fission, resulting up to about 3% of the chemical species present at the end of life for commercial fuel
  - the amount of fission products change both chemical and physical properties
- Physical property changes
  - The physical effects caused by atomic displacements are rather complex and depend on the relative sink strengths of a given material for interstitials and vacancies and on the temperature
  - lattice parameter, thermal conductivity, elasticity, formation of the high burnup structure

Thermal Conductivity Degradation

- One of the major effects of defect formation is the degradation of thermal diffusivity, due to phonon scattering
- Results obtained on irradiated UO_2 show that the thermal conductivity is decreasing with increasing burn-up, and that at equal burn-up, samples with higher irradiation temperatures have higher thermal conductivity
- There are mesoscopic and atomistic features that affect the thermal conductivity
- The porosity existing in fresh fuels evolves during irradiation and has a strong impact on heat transport, because voids/bubbles have significantly lower kth than the lattice
- Precipitates are formed by fission products that are insoluble in the UO_2 lattice, forming oxide or metallic inclusions: can use composite theory to get effective thermal conductivities; typically, these precipitates INCREASE the thermal conductivity of the fuel

Thermal Conductivity Degradation

- Actinides, rare earths, and transition metals can form mixed oxides with UO2 (soluble fission products): these atoms act as phonon scattering centers as a result of the differences in bonding, radii, or mass, and thus decrease kth
- Volatile fission products/gases are partially in solution and partially in bubbles, where they act as phonon scatterers or as low kth composite fractions
- Point defects and extended defects contribute to the degradation of the thermal conductivity by scattering or limiting the mean free path of the phonons

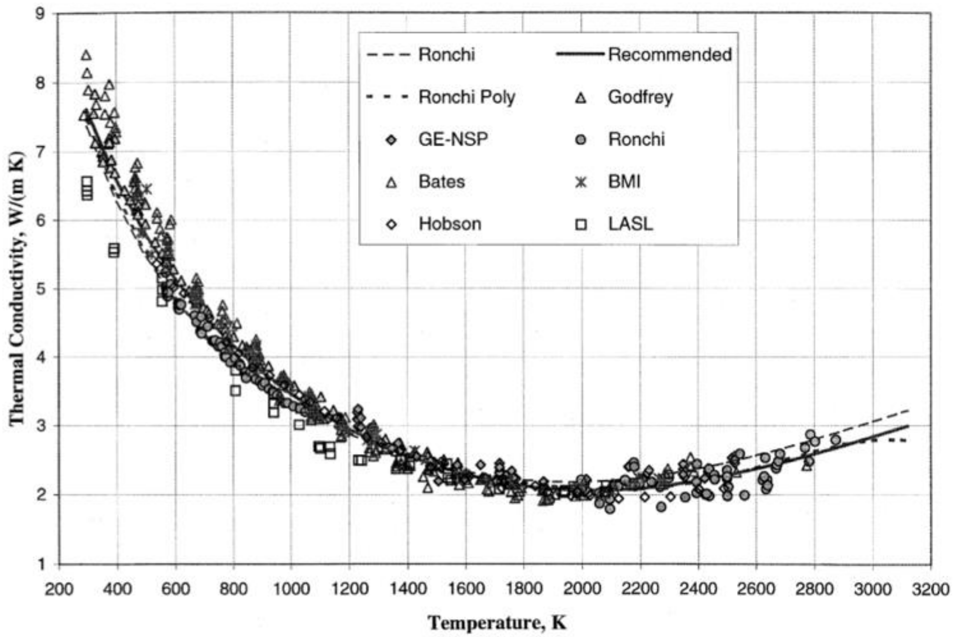


UO2 Thermal Conductivity

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

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

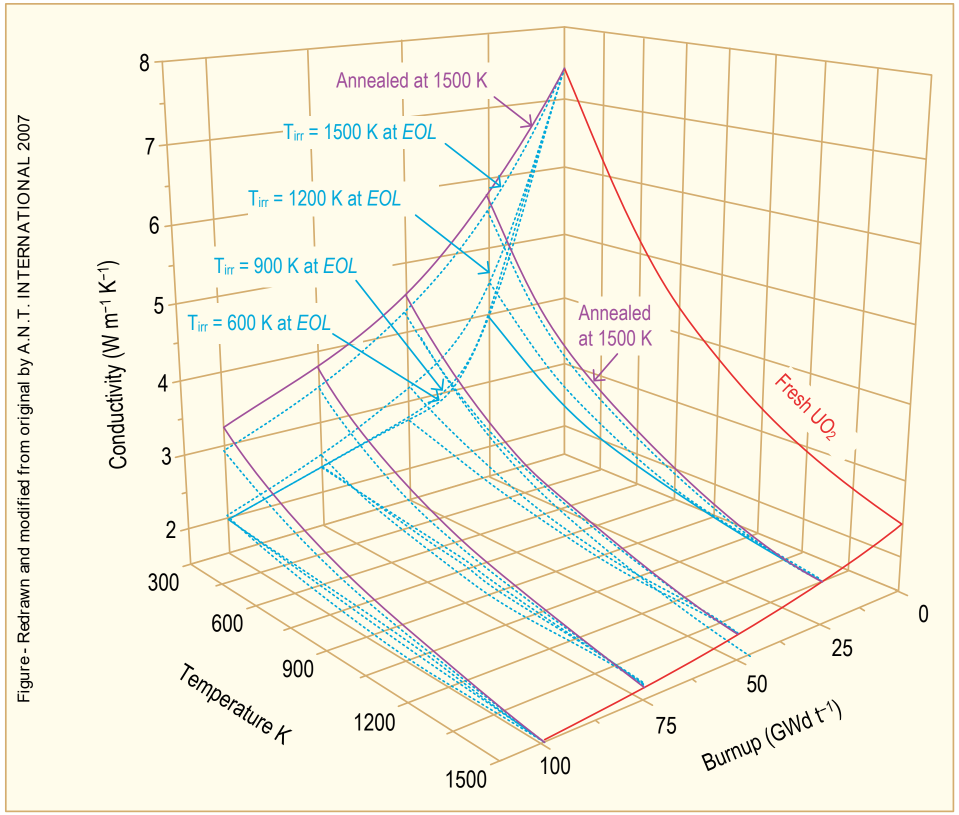
  - Where t = T/1000
  - The first part of the equation describes the phonon interactions
  - The second part describes electronic transport which becomes significant at high temperature



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

- One 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

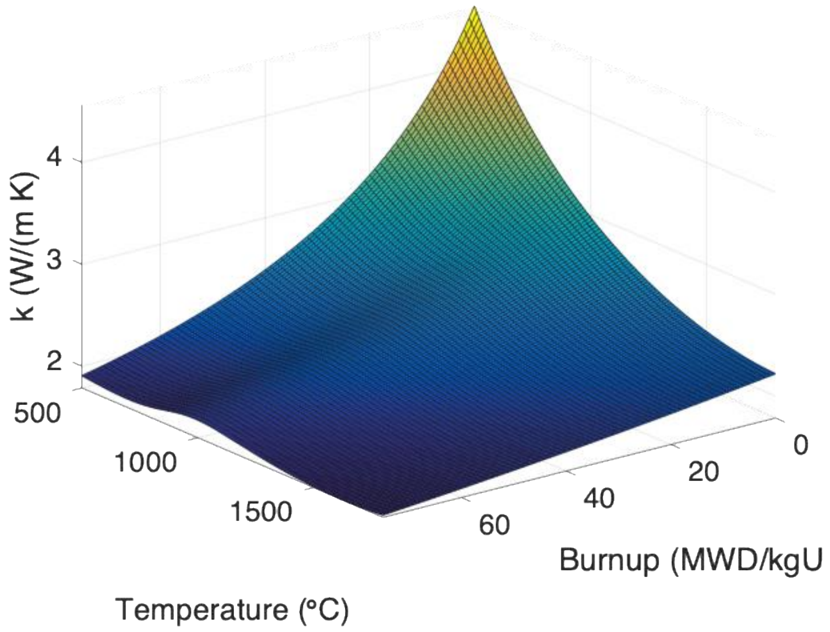
$$k = (1 - R_f(T))k_{ph1}(T,\beta) + R_f(T)k_{ph2}(T,\beta) + k_{el}(T)$$

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

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

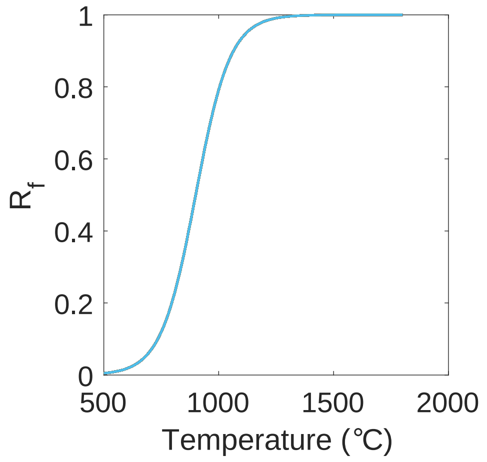
$$k_{ph2} = \frac{1}{(9.592\times10^{-2} + 2.6\times10^{-3}\cdot\beta + (2.5\times10^{-4} - 2.7\times10^{-7}\beta)T}$$

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

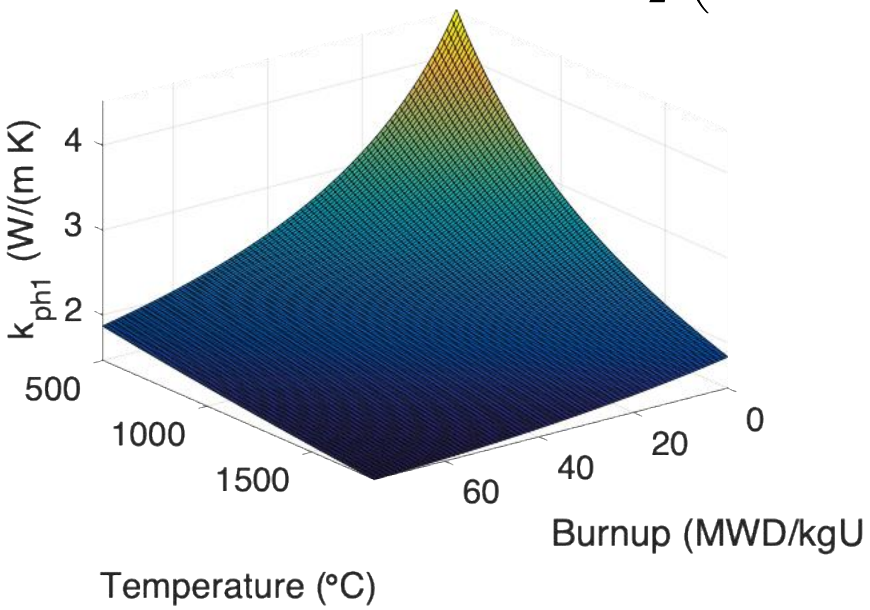


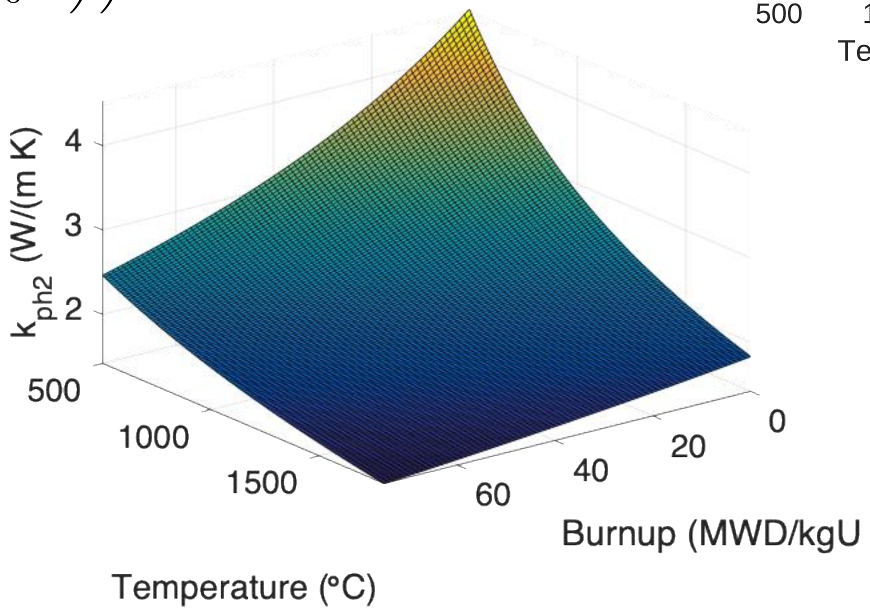
UO2 Thermal Conductivity

- The R_f function switches between two k_{ph} functions, accounting for thermal recovery



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





MOOSE/BISON Models

- https://mooseframework.inl.gov/bison/source/materials/UO2Thermal.html
- Fink-Lucuta
- Halden
- NFIR
- NFI
- Ronchi-Staicu
- Toptan (NCSU alum)