Nuclear Fuel Performance

NE-533

Spring 2024

Last Time

- We derived two analytical solutions for the stress in a pressurized cylinder
  - Thin walled cylinder
  - Thick walled cylinder
- Thermal expansion is a strain that doesn't inherently cause stress
- Thermal expansion can cause stress when there is a temperature gradient
- We have analytical equations for thermal stresses
  - in the cladding
  - in the fuel

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
- 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. 20
- Presentations will take place in-class on Mar. 21 and Mar. 26
- If you have a specific paper that you would like to review and applies to this topic field, present it to me and I will consider it

THERMAL EXPANSION

The gap changes as a function of time

- Both the pellet and the cladding swell

$$\Delta\delta_{gap} = \delta_{gap} - \delta^0_{gap}$$
$$\Delta\delta_{gap} = \Delta\bar{R}_C - \Delta R_f$$
$$\frac{\Delta R_f}{\bar{R}_C} = \alpha_f \left(\bar{T}_f - T_{fab}\right)$$
$$\frac{\Delta R_C}{\bar{R}_C} = \alpha_C \left(\bar{T}_C - T_{fab}\right)$$
$$\Delta\delta_{gap} = \bar{R}_c\alpha_C \left(\bar{T}_C - T_{fab}\right) - \bar{R}_f\alpha_f \left(\bar{T}_f - T_{fab}\right)$$

- But, as the gap decreases, the temperature changes, which again makes the gap change
- The solution using the analytical equations is iterative, due to the dependence of the gap size and temperature

Example

Calculate the steady state temperature profile in the rod, including thermal expansion

- LHR = 200 W/cm, δ^0_{gap} = 30 μm, R_f = 0.6, T_{co} = 600 K, $T_{EXP,0}$ = 373 K, k_{gap} = 0.0026 W/cm-K, t_C= 0.06 cm, α_f = 11.0e-6 1/K, α_C = 7.1e-6 1/K

$$\Delta\delta_{gap} = \bar{R}_c\alpha_C\left(\bar{T}_C - T_{fab}\right) - \bar{R}_f\alpha_f\left(\bar{T}_f - T_{fab}\right) \;=\; \Delta R_c - \Delta R_f$$

$$\Delta T_{gap} = \frac{LHR}{2\pi R_f k_{gap}/\delta_{gap}}$$

- So, T_{IC} = 600 + 18.7 = 618.7 K, T_s = 679.9 K, T_0 = 1210.5 K
- First, we will deal with expansion in the cladding
  - Av(R_c) = 0.6 + 30e-4 + 0.06/2 = 0.633 cm
  - Av(T_C) = (600+618.7)/2 = 609.4 K
  - ΔR_c = 0.633*7.1e-6*(609.4 – 373) = 0.0011 cm

Calculate the steady state temperature profile in the rod, including thermal expansion

- Second, we deal with the fuel
  - Av(Tf) = (1210.5 + 680)/2 = 945.25 K
  - ΔR_f = 0.6*11e-6*(945.3 – 373) = 0.00378 cm

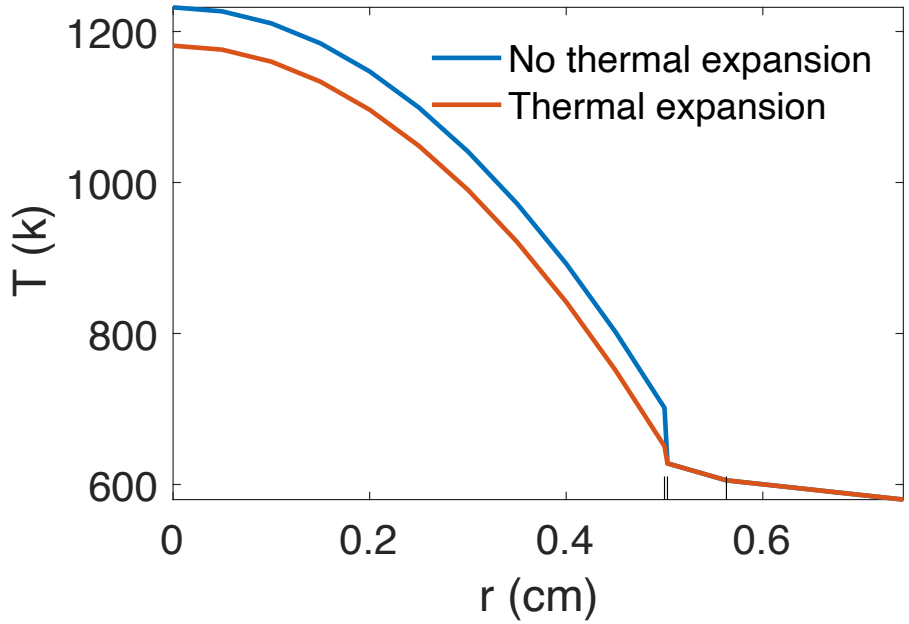
$$\Delta\delta_{gap} = \bar{R}_c\alpha_C\left(\bar{T}_C - T_{fab}\right) - \bar{R}_f\alpha_f\left(\bar{T}_f - T_{fab}\right)$$

- The total change in the gap is 0.0011 – 0.0038 = -0.0027
- However, that means the gap is smaller and so our temperatures were wrong!

This calculation is repeated until the gap width stops changing significantly

- The change in the gap does NOT affect the coolant or outer cladding temperatures, just the gap and fuel temperatures
- Does fuel centerline temp go up or down with correction?

Iteration	δ_{gap} (cm)	T_s (K)	T_0 (K)
0	0.003	701	1232
1	0.00066	644	1174
2	0.00097	652	1182
3	0.00094	651	1181
4	0.00094	651	1181

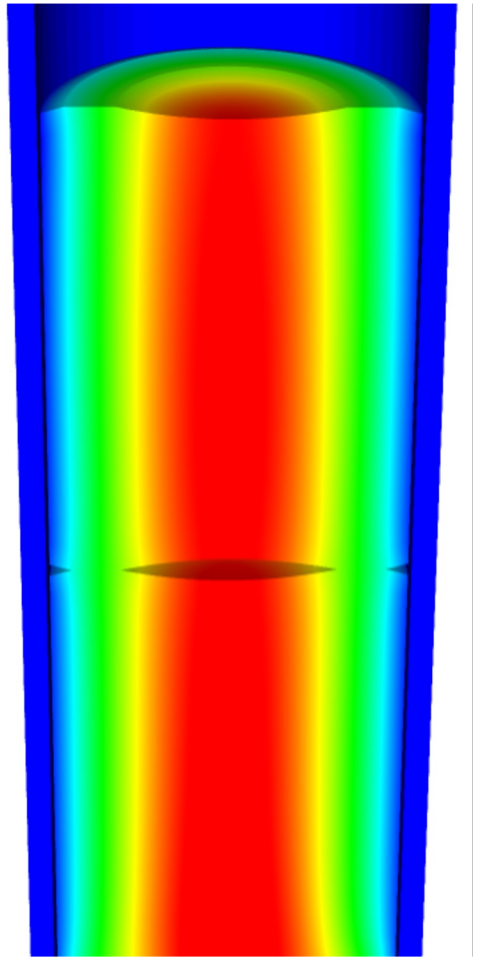


LAST BIT OF MECHANICS

Relating Displacements to Stress

- We have been determining the stress due to some internal pressure (or temperature)
- Often, the information more readily obtainable are the displacements
- Utilizing the previous equations, can use displacement to stress relationships for our geometry

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} + \frac{\partial \sigma_{rz}}{\partial z} = 0 \qquad \frac{1}{r}\frac{\partial (r\sigma_{rz})}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} = 0$$



Assuming problem is axisymmetric

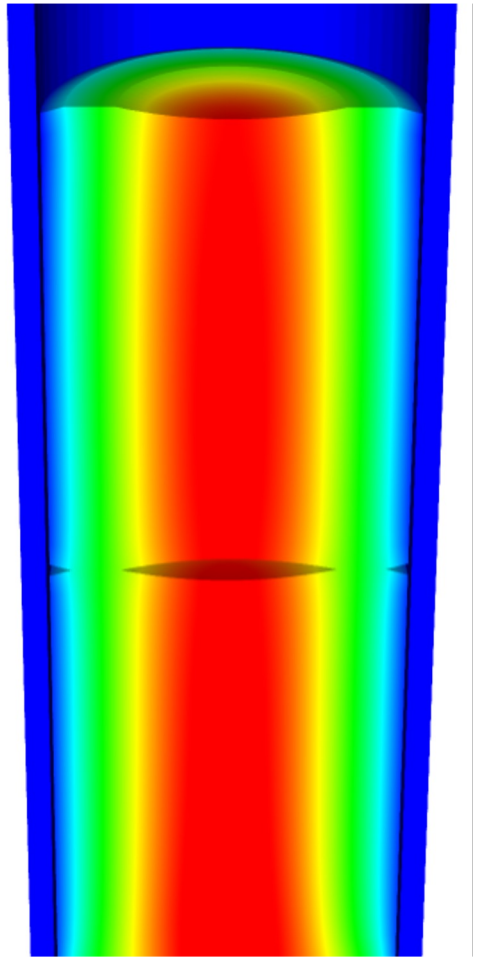
$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rk(T)\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k(T)\frac{\partial T}{\partial z}\right) + Q(r,z)$$

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} + \frac{\partial \sigma_{rz}}{\partial z} = 0 \qquad \frac{1}{r}\frac{\partial (r\sigma_{rz})}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} = 0$$

$$\boldsymbol{\sigma} = \boldsymbol{\mathcal{C}}(\boldsymbol{\epsilon} - \alpha(T - T_{fab})\mathbf{I}) \qquad \epsilon_{rr} = \frac{1}{E}\left(\sigma_{rr} - \nu(\sigma_{\theta\theta} + \sigma_{zz})\right) + \alpha\Delta T$$

$$\epsilon_{rr} = \frac{\partial u_r}{\partial r},\ \epsilon_{\theta\theta} = \frac{u_r}{r}, \epsilon_{zz} = \frac{\partial u_z}{\partial z}, \epsilon_{rz} = \frac{1}{2}\left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\right)$$

$$\boldsymbol{\epsilon} = \begin{bmatrix} u_{r,r} & (u_{r,z} + u_{z,r})/2 & 0 \\ (u_{r,z} + u_{z,r})/2 & u_{z,z} & 0 \\ 0 & 0 & u_r/r \end{bmatrix}$$



Solve for the stress from the strain

- Assume isotropic materials
- Can perform matrix multiplication for the calculation of the stress, given the displacements

$$\begin{bmatrix} \sigma_{rr} \\ \sigma_{zz} \\ \sigma_{\theta\theta} \\ \sigma_{rz} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & \nu & 0 \\ \nu & 1-\nu & \nu & 0 \\ \nu & \nu & 1-\nu & 0 \\ 0 & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix} \begin{bmatrix} u_{r,r} \\ u_{z,z} \\ u_r/r \\ (u_{r,z}+u_{z,r})/2 \end{bmatrix}$$

Further simplify the problem to be 1D

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q \qquad \boldsymbol{\sigma} = \boldsymbol{\mathcal{C}}(\boldsymbol{\epsilon} - \alpha(T - T_{fab})\mathbf{I})$$
$$0 = \nabla \cdot \boldsymbol{\sigma} \qquad \boldsymbol{\epsilon} = \tfrac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)$$

- No change in Z:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r k(T) \frac{\partial T}{\partial r}\right) \qquad \frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0$$

$$\boldsymbol{\epsilon} = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix} \qquad \begin{bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu \\ \nu & 1-\nu \end{bmatrix} \begin{bmatrix} u_{r,r} \\ u_r/r \end{bmatrix}$$

Determine the strain and stress in the pellet for 1D case

- Assume the radial displacement in the fuel pellet is $u_r(r) = 0.05r$ cm.
- What is the strain tensor? $\boldsymbol{\epsilon} = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix}$ At the outer edge: $\boldsymbol{\epsilon} = \begin{bmatrix} 0.05 & 0 \\ 0 & 0.05 \end{bmatrix}$

- We are dealing with UO_2, so E = 200 GPa and v = 0.345

$$\begin{bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu \\ \nu & 1-\nu \end{bmatrix} \begin{bmatrix} u_{r,r} \\ u_r/r \end{bmatrix}$$

  - C_{11} = E (1 – v)/((1+v)(1–2 v)) = 200*(1–0.345)/(1.345*(1–2*.345)) = 314.2 Gpa
  - C_{12} = E v/((1+v)(1–2 v)) = 200*0.345/(1.345*(1–2*.345)) = 165.5 Gpa
- Now we can calculate the stresses
  - σ_{rr} = 0.05*314.2 + 0.05*165.5 = 23.98 GPa
  - $\sigma_{\theta\theta}$ = 0.05*165.5 + 0.05*314.2 = 23.98 GPa

$$\sigma = \begin{bmatrix} 23.98 \\ 23.98 \end{bmatrix}$$

Example problem

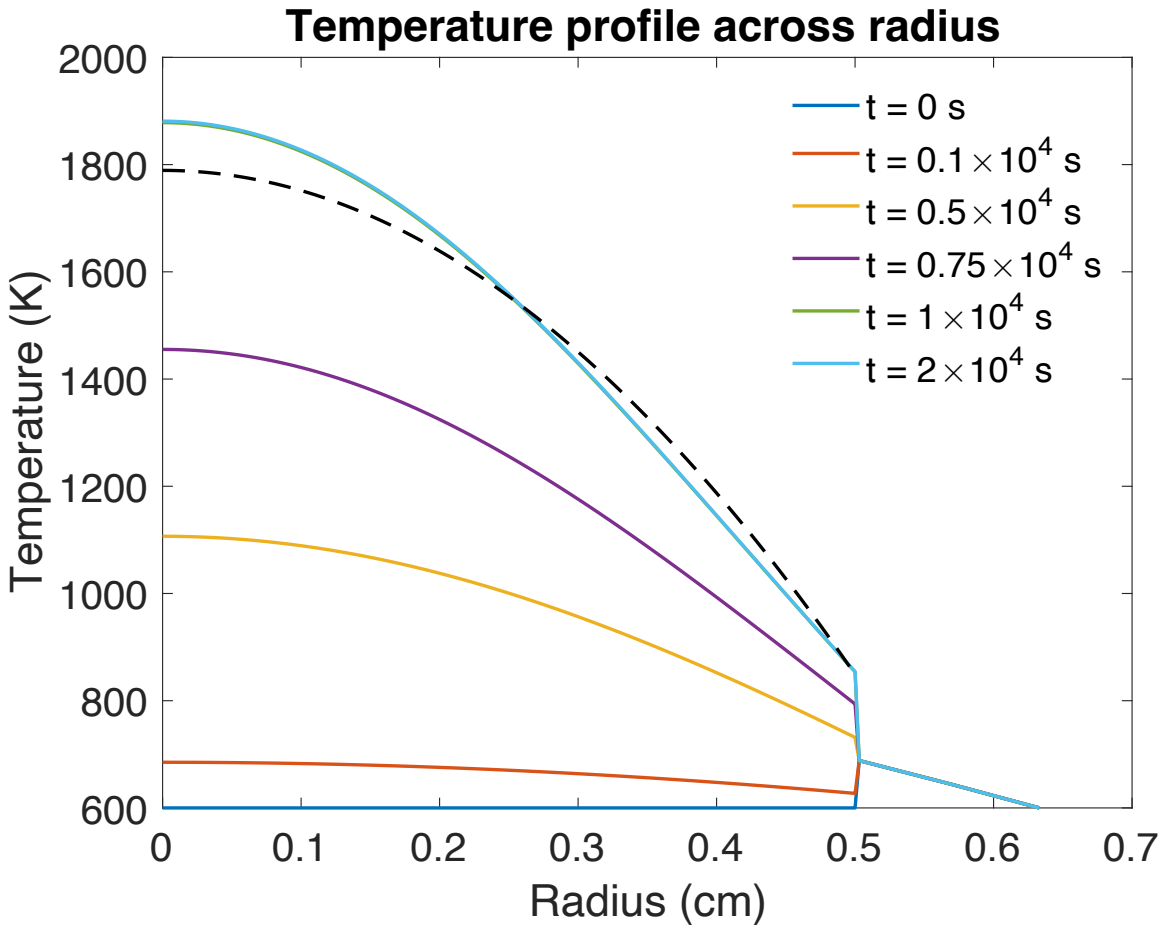
- Compute the stress and strain tensors in the center and at the outer edge (r = 0.5 cm) in 1D axisymmetric coordinates in a fuel pellet with $u_r(r) = r^2/5$. C_{11} = 314.2 Gpa, C_{12} = 165.5 Gpa. $\boldsymbol{\epsilon} = \begin{bmatrix} u_{r,r} & 0 \\ 0 & u_r/r \end{bmatrix}$

- First, calculate the strain tensor
- $\varepsilon_{rr} = u_{r,r} = 2r/5$
- $\varepsilon_{\theta\theta} = u_r/r = r/5$
- At the center there is no strain; at the outer edge $\boldsymbol{\epsilon} = \begin{bmatrix} 0.2 & 0 \\ 0 & 0.1 \end{bmatrix}$

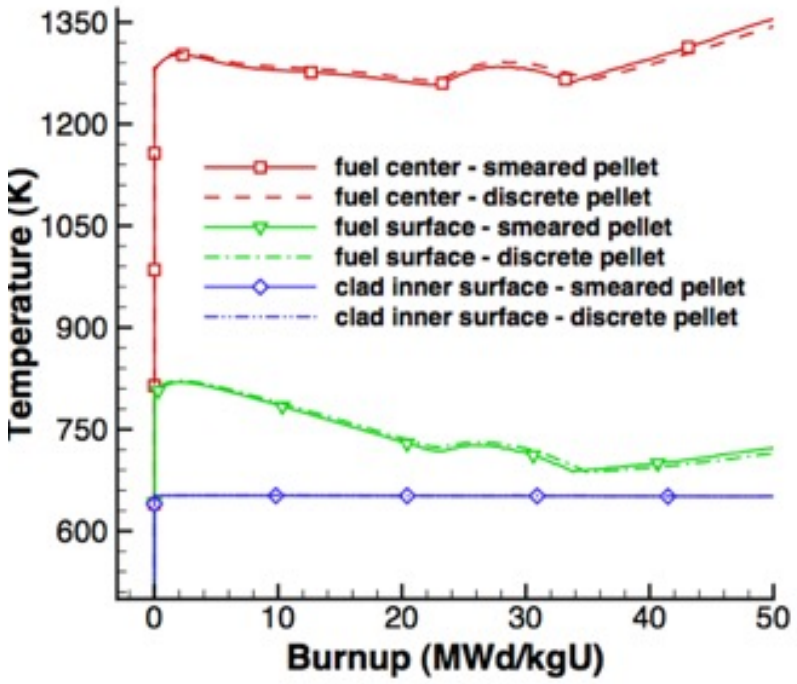
- To calculate the stress, convert to a strain vector and multiply by elastic constant matrix
- The stress in the center is zero
- On the outer edge
  - σ_{rr} = 0.2*314.2 + 0.1*165.5 = 79.4 GPa
  - $\sigma_{\theta\theta}$ = 0.1*314.2 + 0.2*165.5 = 64.52 GPa

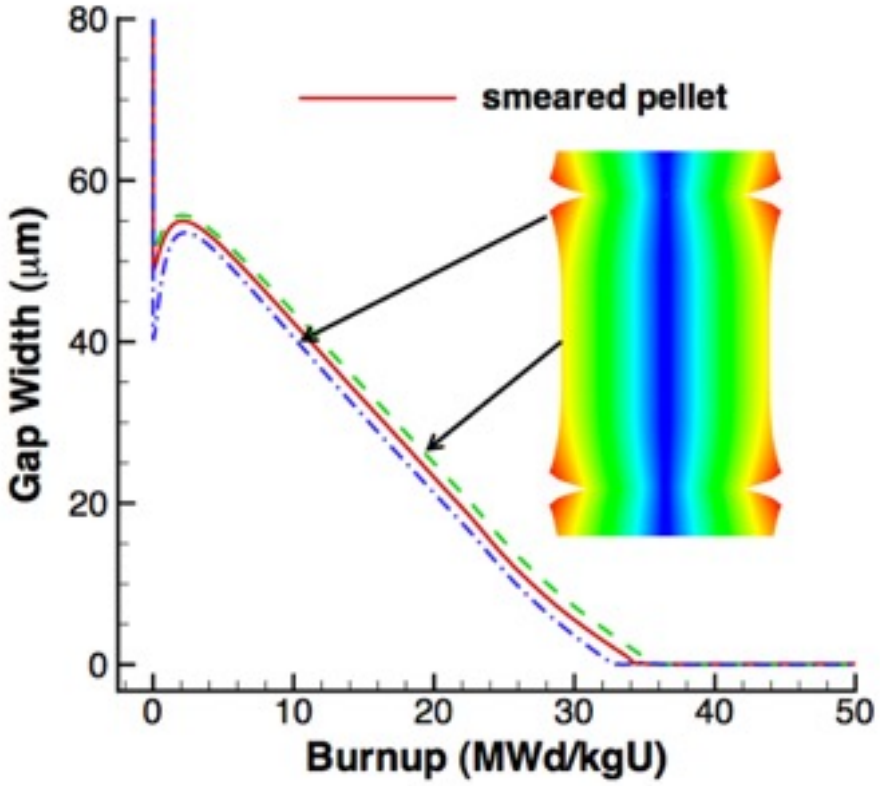
MATERIAL PROPERTY EVOLUTION

Pretty much everything we have learned so far, nothing changes once the fuel and cladding reach steady state



Fuel is dynamic!





Property changes due to microstructure evolution during reactor operation must be considered

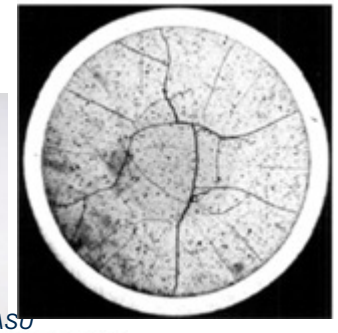
Insertion in reactor

Removal from reactor

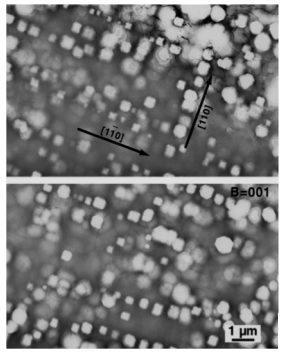
Fuel Fabrication
- Sintered UO^2
- Height 2 cm
- Diameter 1 cm
- ~10 μm grain size
- Density > 95%

From Pedro Peralta, ASU

Early life
- Thermal expansion
- Fracture
- Point defect and fission gas generation
- Fuel Densification



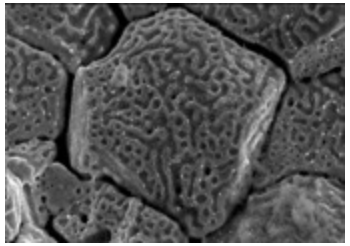
Mid Life
- Point defect diffusion
- Point defect clustering
- Fission gas segregation to GB and voids
- Bubble nucleation



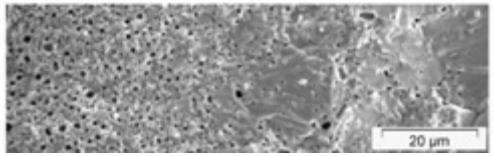
Zinkle and Singh 2000

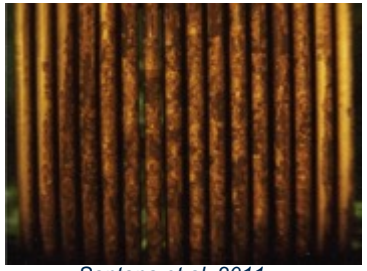
Late life
- Fission product swelling
- Bubble percolation and fission gas release
- Cladding creep
- Fuel creep

Brohan 2000

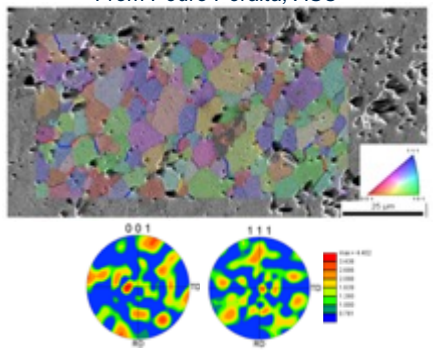


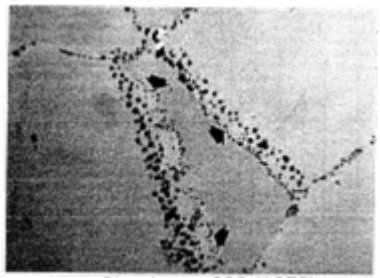
Fuel failure
- Pellet/cladding interaction
- Cladding corrosion
- Cladding fracture



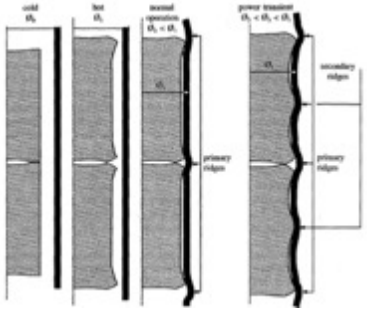


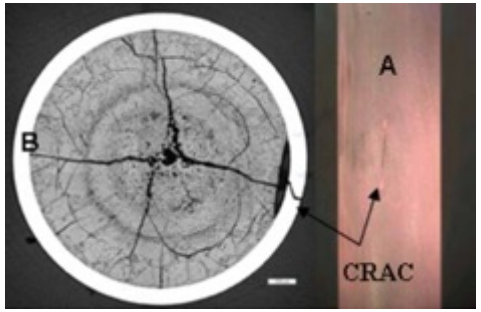
Santana et al. 2011





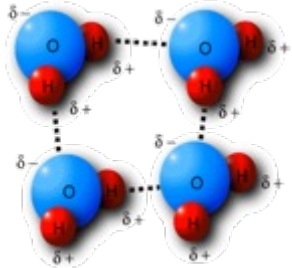
Olander, p. 323 (1978)



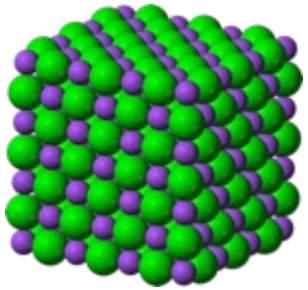


The properties and performance of a material are a result of factors across various length scales

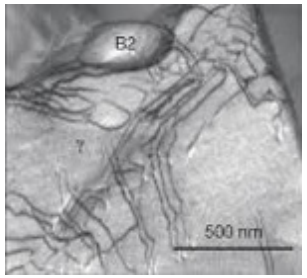
Chemical bonds



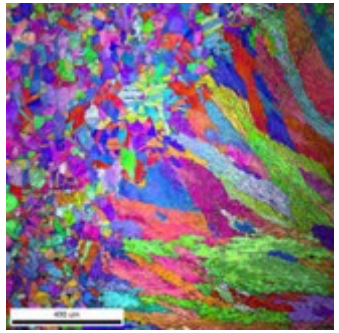
Crystal structure



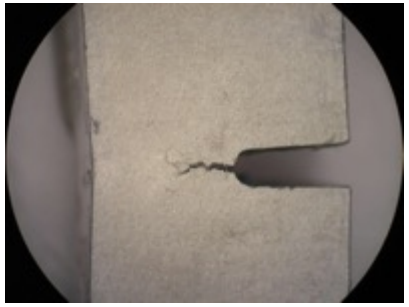
Defect interactions



Microstructure

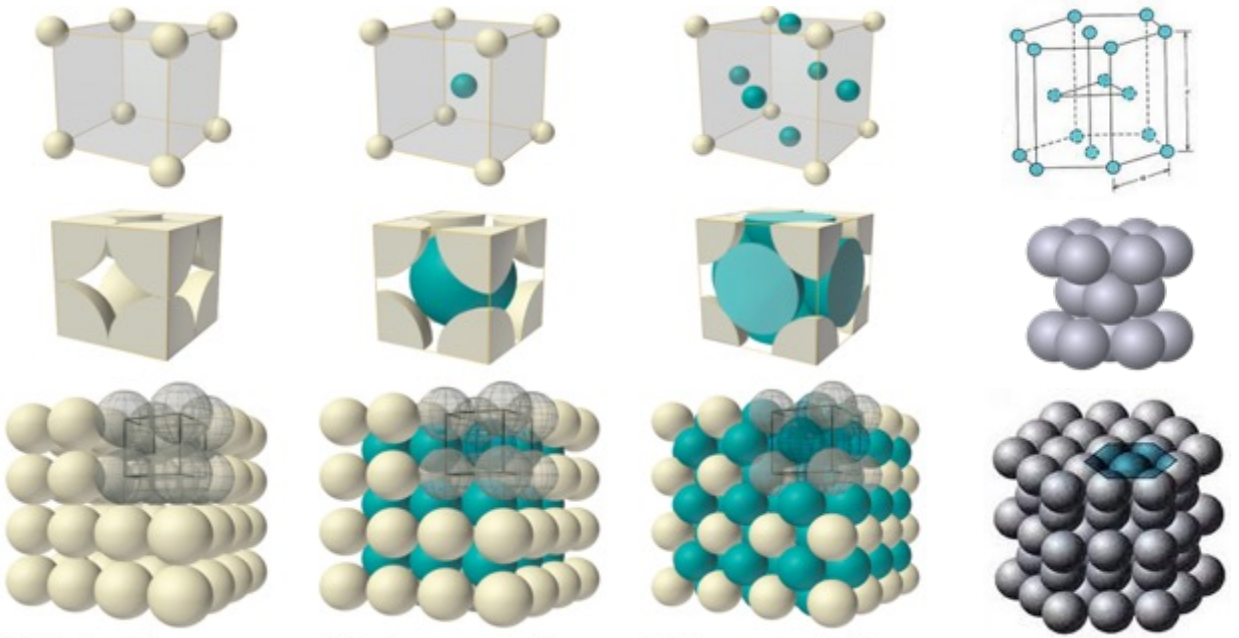


Material properties and performance



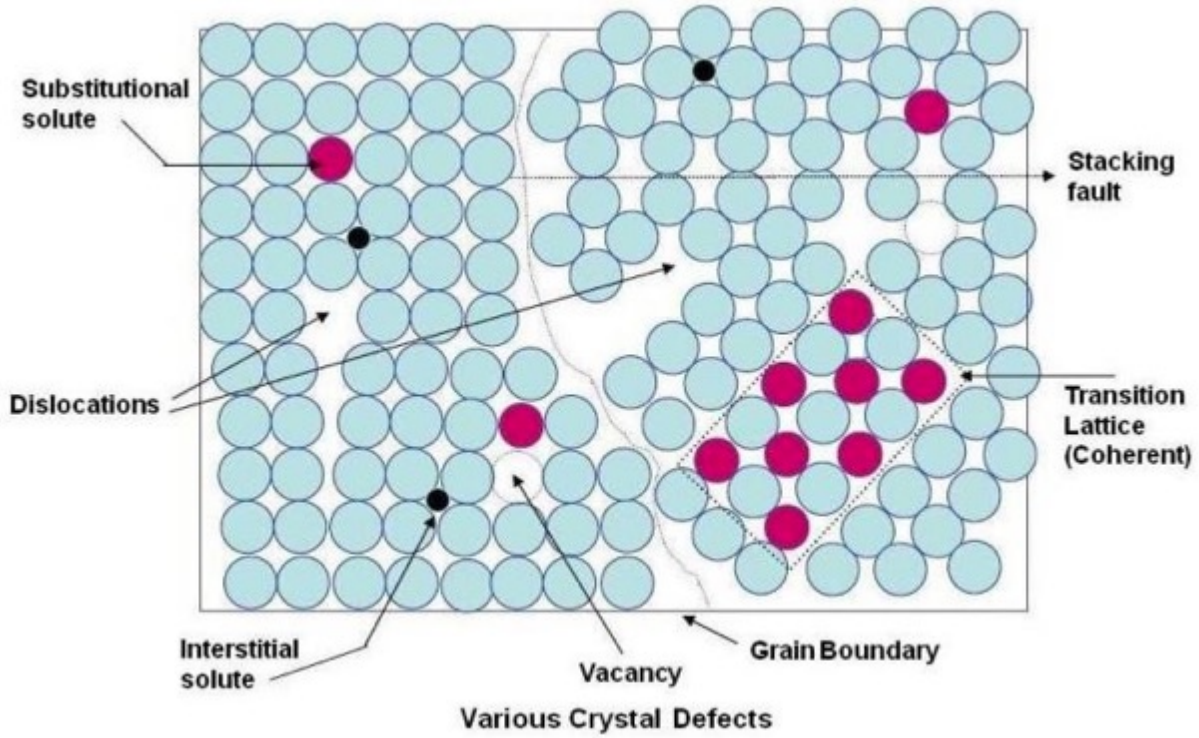
The crystal structure of a material is the shape of the ordered structure of the atoms

- The atoms of many materials form an organized lattice, these are called **crystalline materials.** All reactor materials are crystalline.
- The configuration of the atoms in the lattice impacts the properties of the material (density, thermal expansion coefficient, elastic modulus, etc.)
- All major light water nuclear materials are either cubic or hexagonal



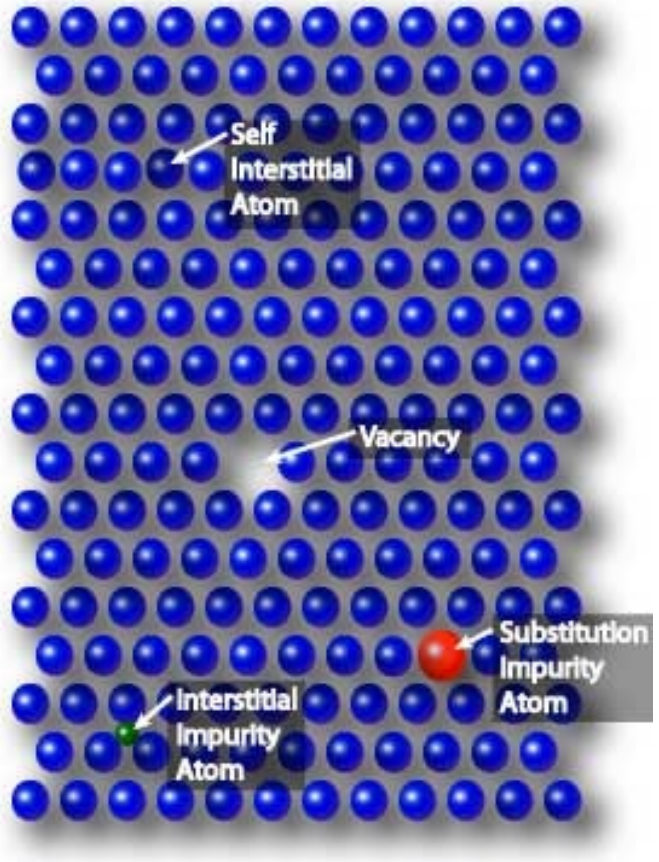
Crystalline materials

- In crystalline materials, the lattices are not perfect, they have defects
- Defects can be 0D, 1D, 2D, 3D
- The interactions between defects seriously impact material properties and how they perform



Point defects

- Point defects (zero-dimensional defects) are lattice imperfections related to one or two lattice sites
- There are several types of point defects
  - **Vacancies**
  - **Self interstitial atoms (SIA)**
  - **Interstitial impurity atoms**
  - **Substitutional impurity atoms**
- Point defects control the mobility of atoms and, therefore influence all processes that depend on diffusion



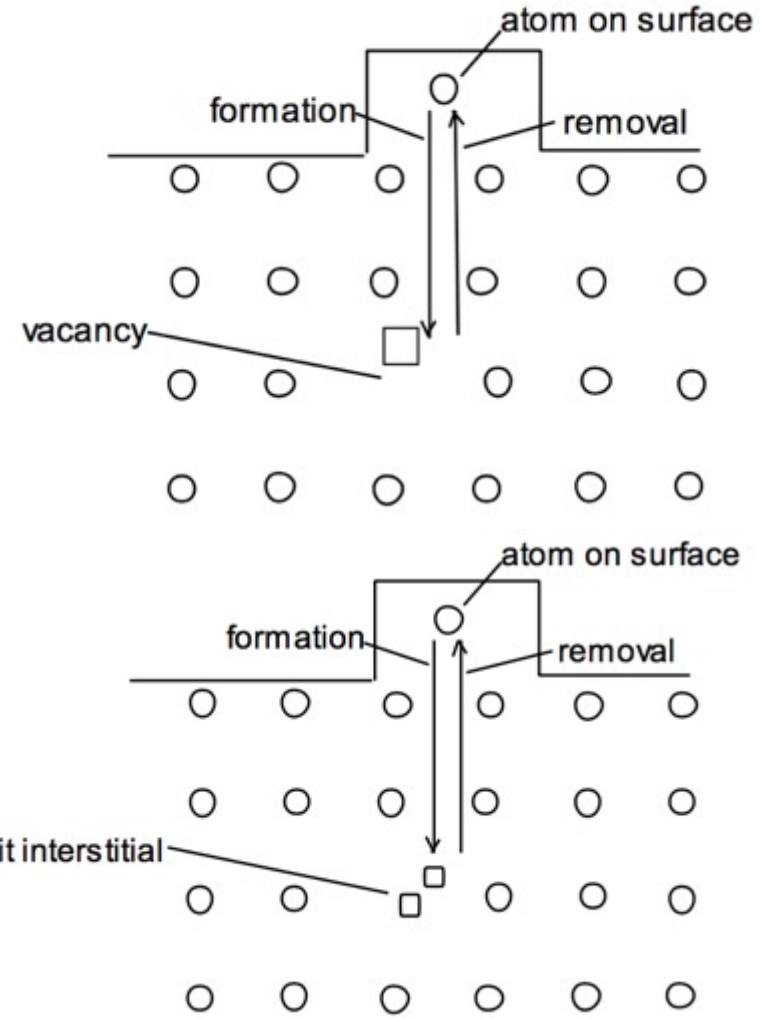
Point defects

- Vacancies and interstitials form naturally in materials
- Extra atoms can sit on a surface, creating a vacancy, or a surface can have a missing atom, creating a self interstitial atom (SIA)
- We define the number of vacancies or interstitials in terms of a concentration

$$C_V = \frac{N_V}{N_S} = \frac{number\ of\ \ empty\ sites}{total\ number\ of\ \ sites}$$

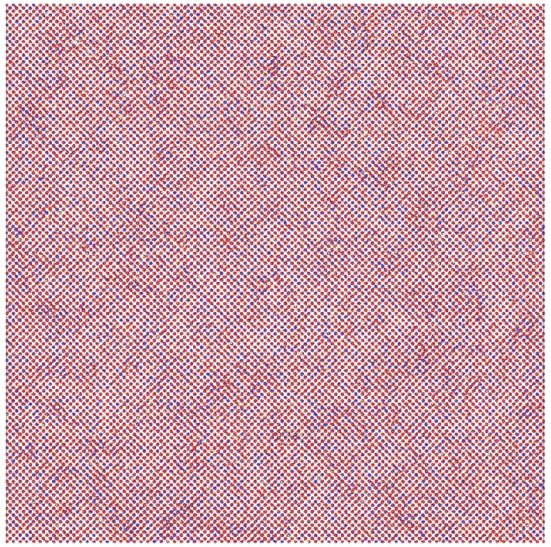
- There exists an equilibrium concentration of point defects

$$C_v = \exp\left(\frac{S_f^v}{k}\right)\exp\left(\frac{-E_f^v}{kT}\right)$$



Radiation damage

- Ionizing radiation can introduce defects into the crystal lattice, called radiation damage
- PKA collisions create a collision cascade, which results in the generation of defects (point and clusters)



Duration (ps)	Event	Result	Parameters
10^{-6}	Transfer of energy from energetic particle	Creation of PKA	$\Sigma_n(E_n, E)$

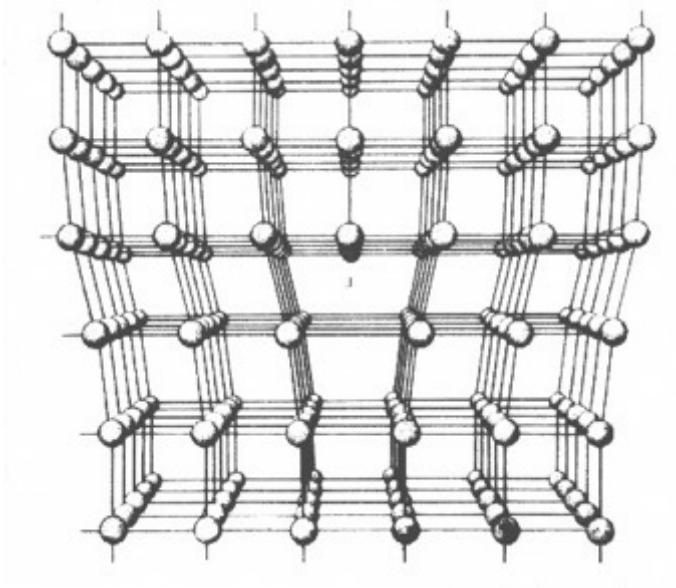
10^{-6} to 0.2	Slowing down of PKA, generation of displacement cascade	Recoil atoms
		Vacancies
		Subcascades
			E_d = energy
			ν_{NRT} = # atoms
			T = energy transferred

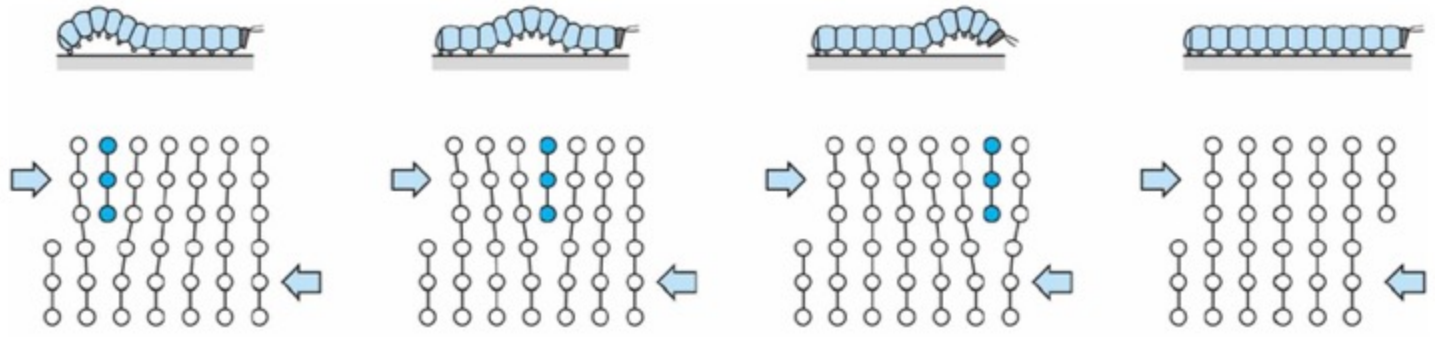
0.2 – 0.3	Thermal spike cool down	Stable interstitials, clusters, atomic mixing	V(T) = # stable defects
			F = clustering fraction

3 – 10	Cascade cooling to bulk solid temperature	SIA depleted zone in cascade core	Loop collapse probability
> 10	Diffusion of defects and interaction with sinks	Microstructure evolution	Many

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

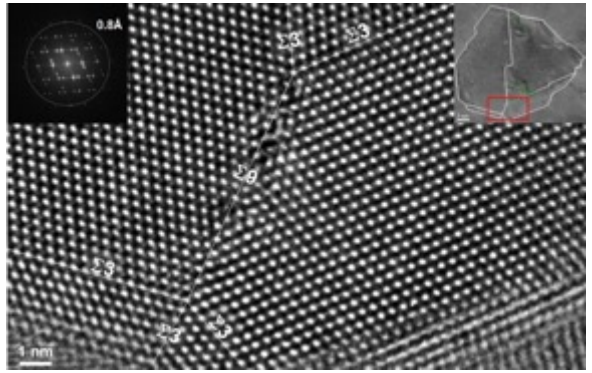
- In a dislocation, an extra half plane of atoms is inserted into the lattice
- When it moves, only a small number of bonds are broken at a time
- Dislocation motion controls the plastic (permanent) deformation of crystalline materials



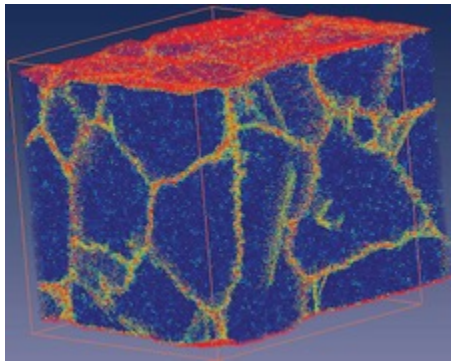


Grain boundaries

- 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**
- Most crystalline materials are polycrystalline, not single crystal

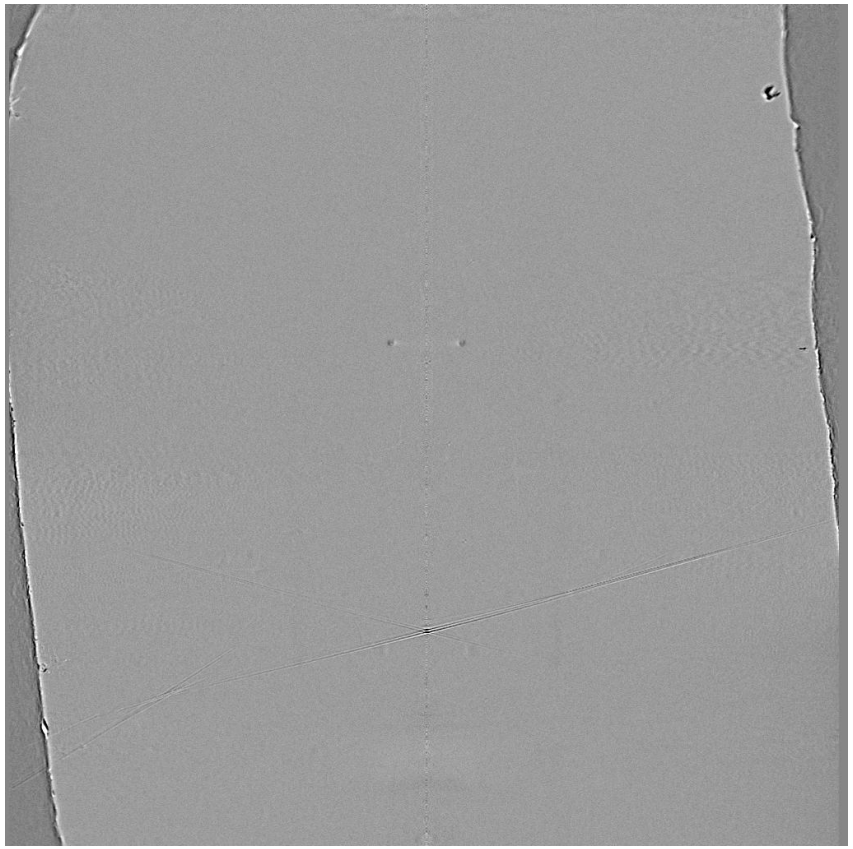


High-res transmission eleectron microscopy can also show individual atoms (palladium) *www.knmf.kit.edu/TEM.php*



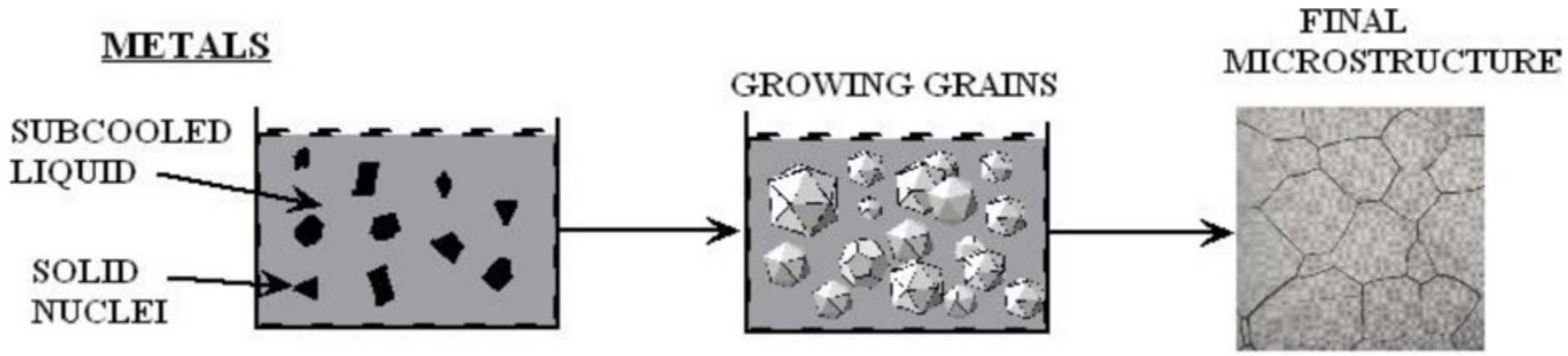
Atomistic simulation of grain boundaries in 3D

Metals are often cast, and polycrystals naturally form during casting



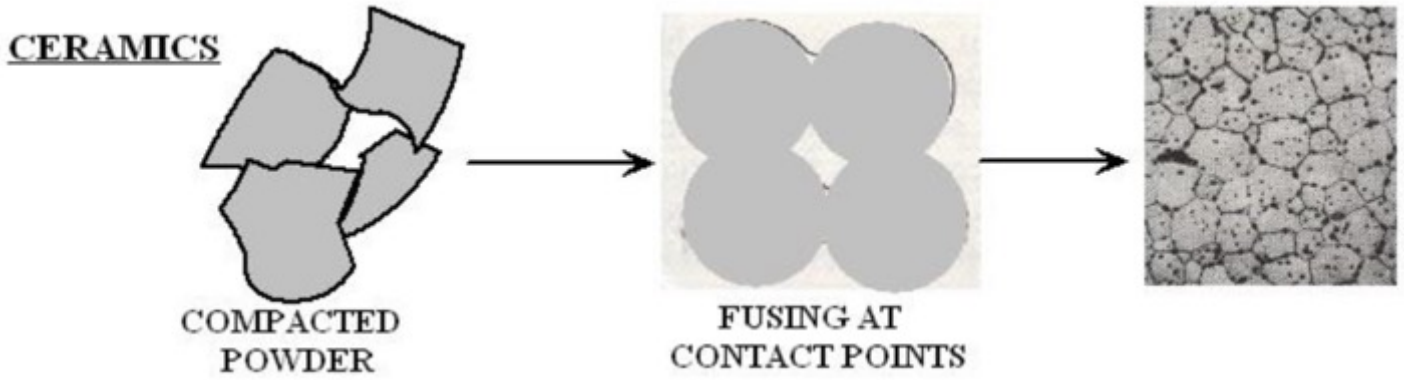
Polycrystals naturally form during casting

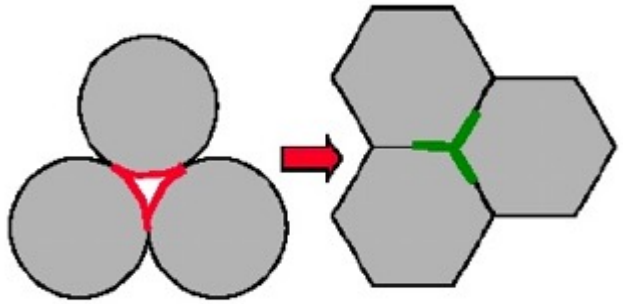
- Solidification begins in different regions of the melt, each with a different orientation
- Once the different regions meet, grain boundaries form between them

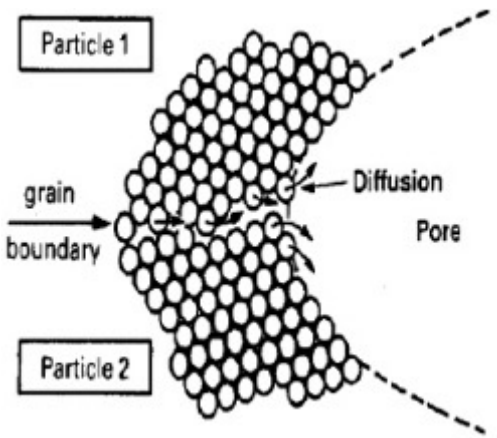


Ceramic sintering

- 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



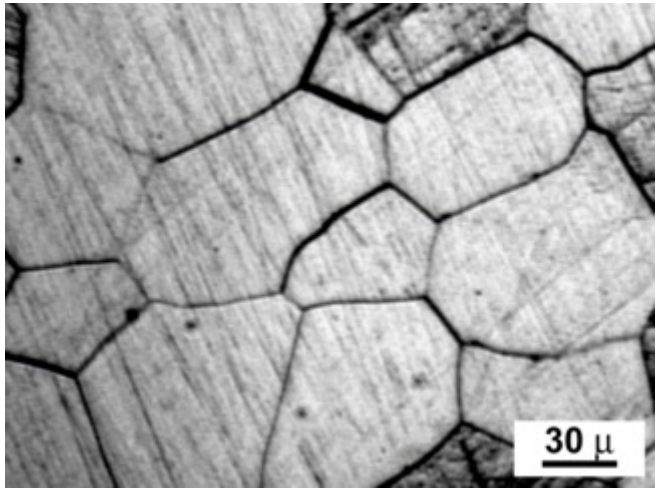


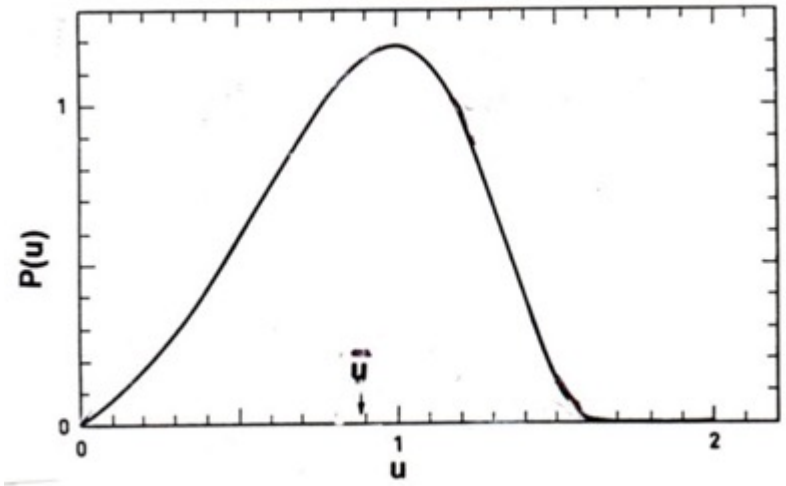


Distribution of grain sizes

- 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

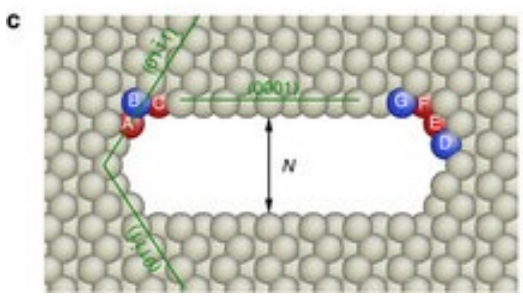
$$P(u) = (2e)^{\beta} \cdot \frac{\beta u}{(2-u)^{2+\beta}} \cdot \exp \frac{-2\beta}{2-u}$$

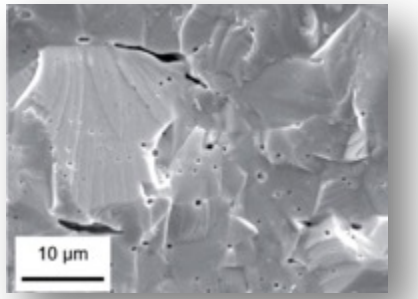


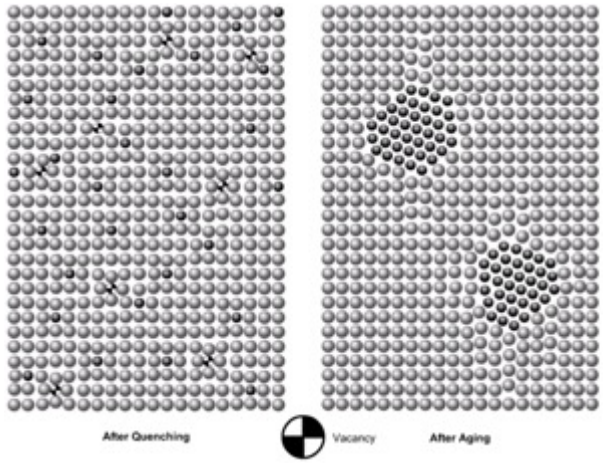


3D Defects

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

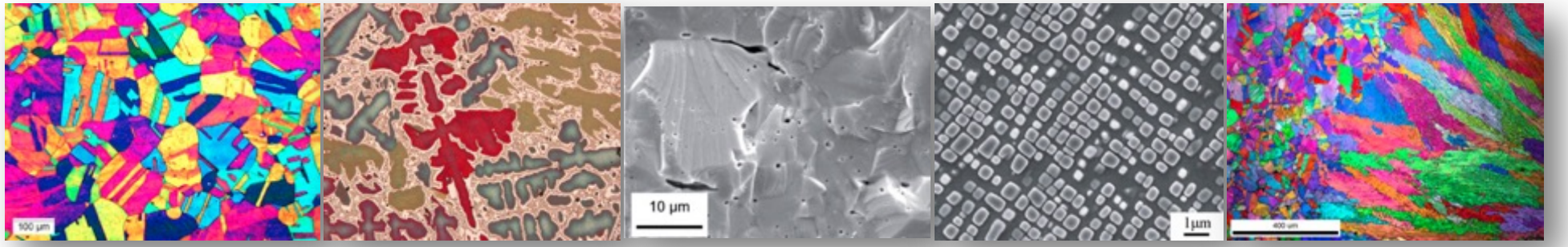






Microstructure

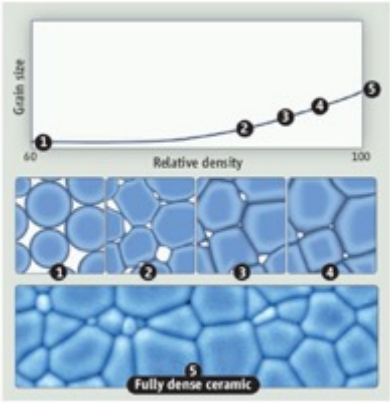
- Material microstructure is the structure observable with 25x magnification
- The microstructure includes grain structure, secondary phases, porosity, and more
- The microstructure can strongly influence physical properties such as strength, toughness, ductility, hardness, corrosion resistance, high/low 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**

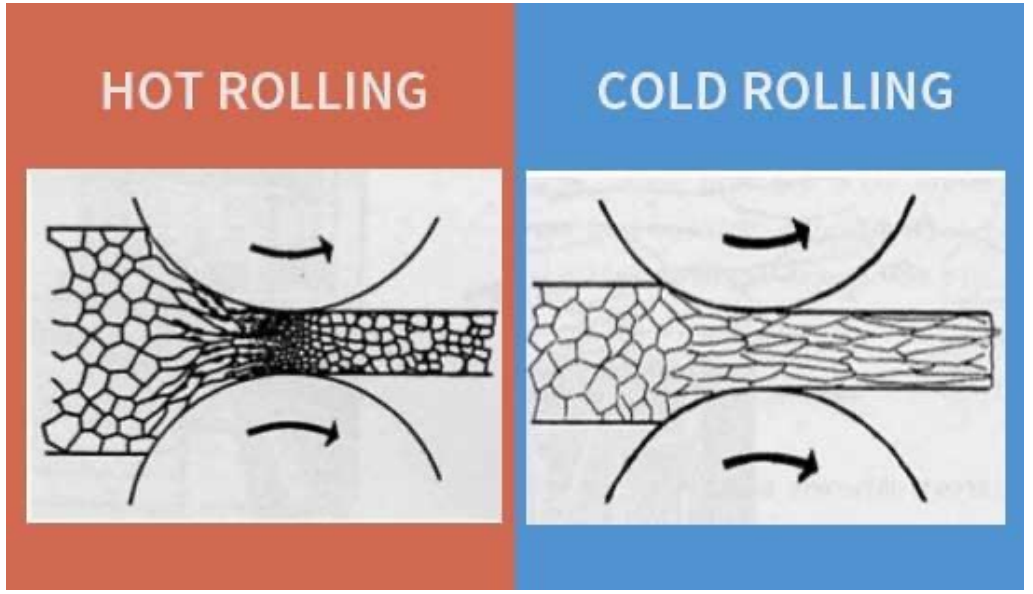


Material processing

- 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