PennState
College of Engineering

NucE 497: Reactor Fuel Performance

Lecture 18: Property evolution

February 20, 2017
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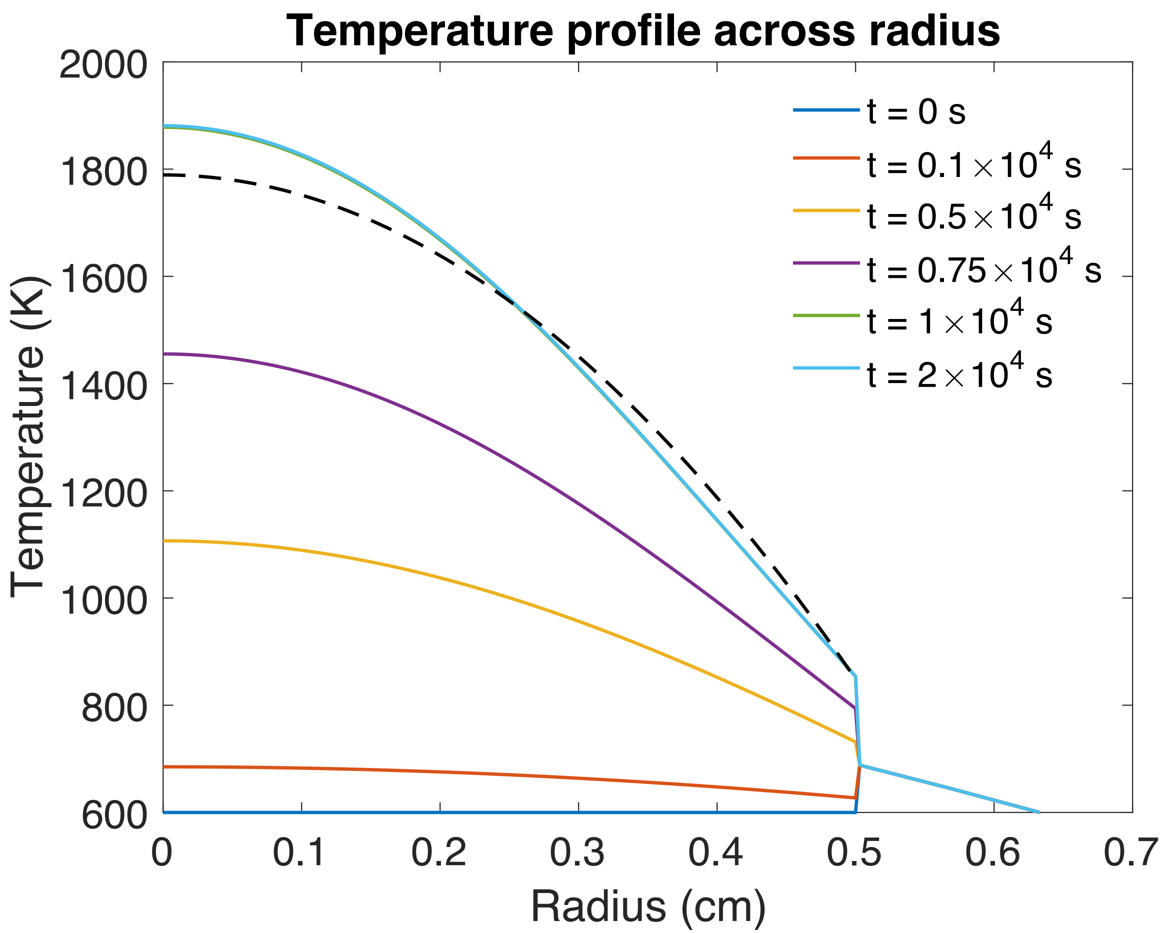
Today we will begin module 4, talking about property evolution and an intro to materials science

- Module 1: Fuel basics
- Module 2: Heat transport
- Module 3: Mechanical behavior
- Module 4: Materials issues in the fuel
  - **Property evolution and Intro to materials science**
  - Chemistry
  - Grain growth
  - Fission products and fission gas
  - Densification, swelling, and creep
  - HBS
  - Fracture
  - Thermal conductivity
- Module 5: Materials issues in the cladding
- Module 6: Accidents, used fuel, and fuel cycle

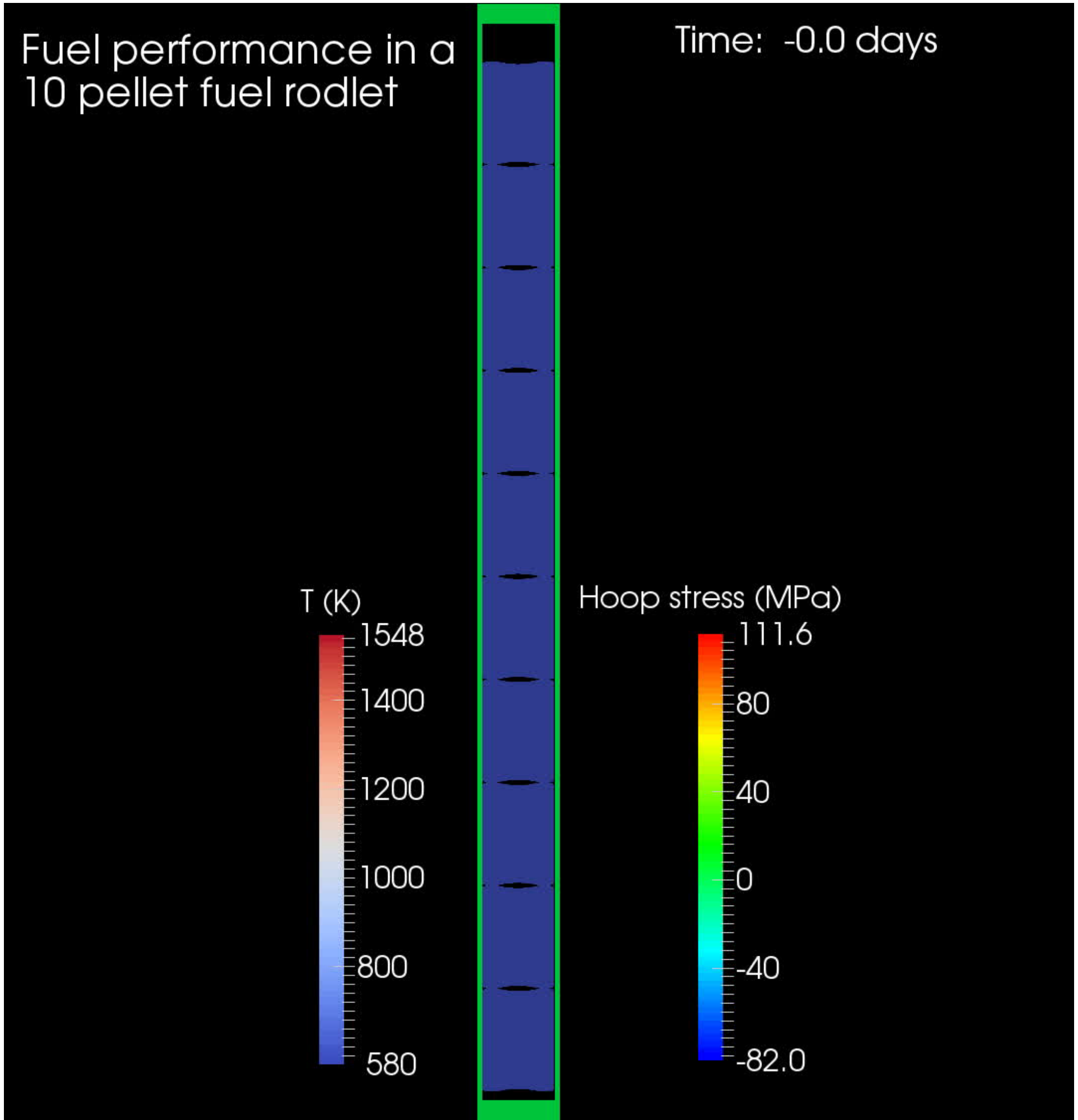
Here is some review from last time

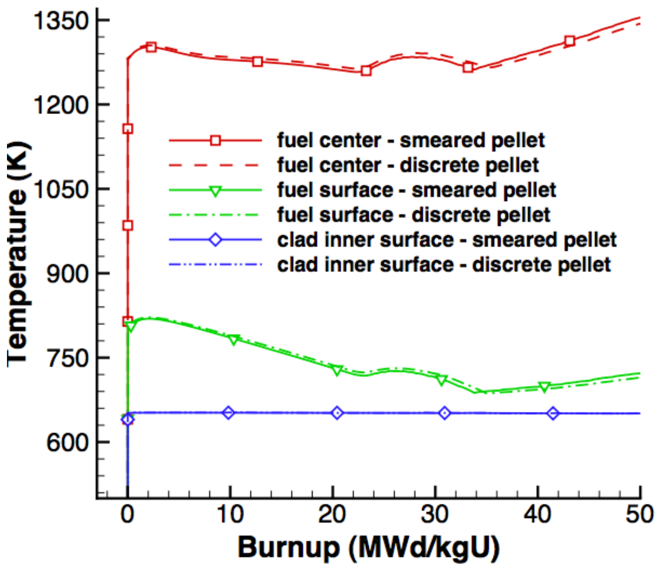
- What two things must a fuel performance code calculate?
  a) The stress and temperature in the fuel
  b) The temperature in the fuel and stress in the cladding
  c) The stress in the fuel and the temperature in the cladding
  d) The stress and temperature in the cladding
- Which is true about FRAPCON?
  a) It is no longer under production
  b) It is a 1.5D transient code
  c) It is certified by the NRC
  d) It can model a missing pellet surface

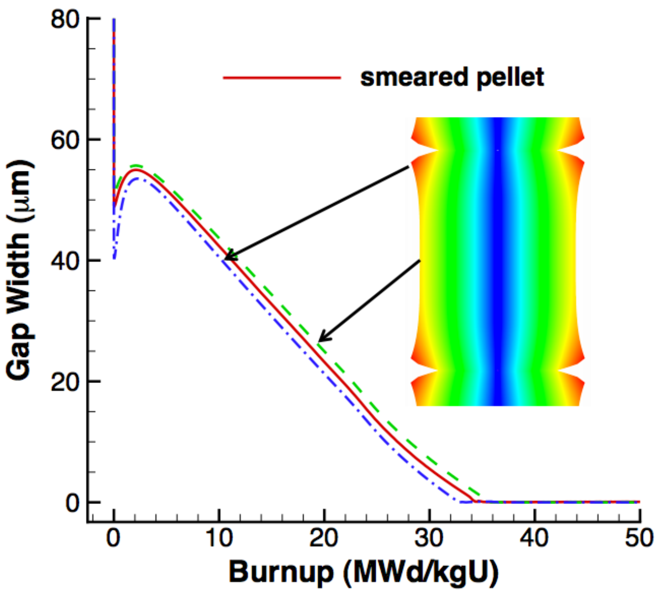
Using everything we have learned so far, nothing changes once the fuel and cladding reach steady state



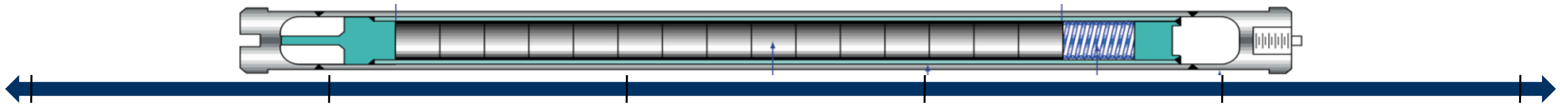
That is not the case in actual fuel







We have to change the properties with time, due to changes that take place in the microstructure



Insertion in reactor **Removal from reactor**

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

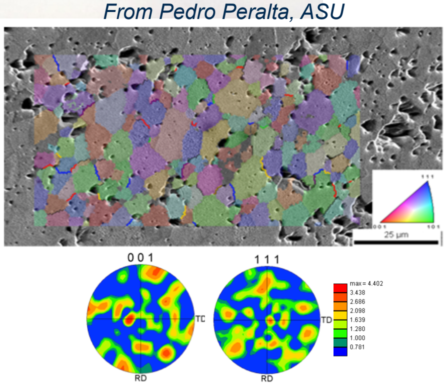
Early life
- Thermal expansion
- Fracture
- Point defect and fission gas generation
- Fuel Densification

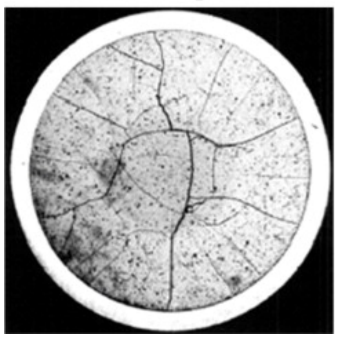
Mid Life
- Point defect diffusion
- Point defect clustering
- Fission gas segregation to GB and voids
- Bubble nucleation

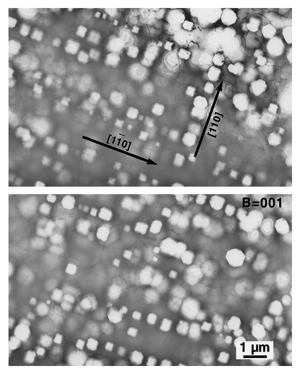
Late life
- Fission product swelling
- Bubble percolation and fission gas release
- Cladding creep
- Fuel creep

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

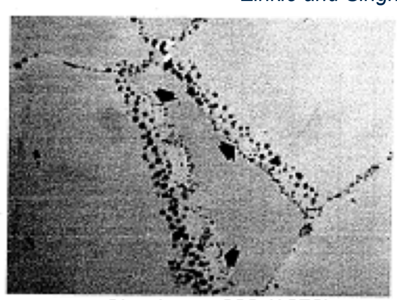
From Pedro Peralta, ASU





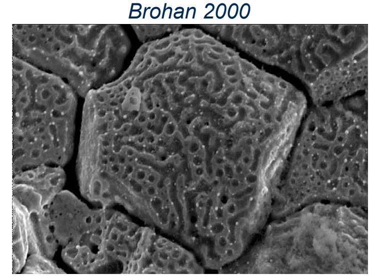


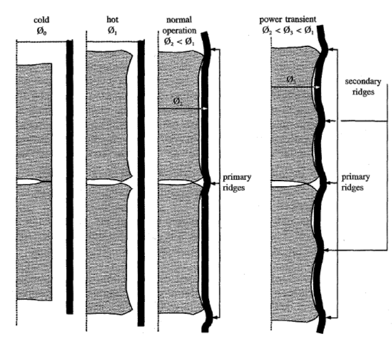
Zinkle and Singh 2000

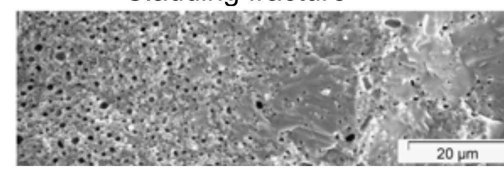


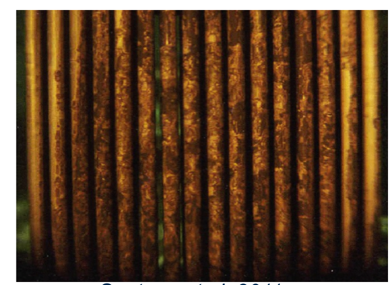
Olander, p. 323 (1978)

Brohan 2000

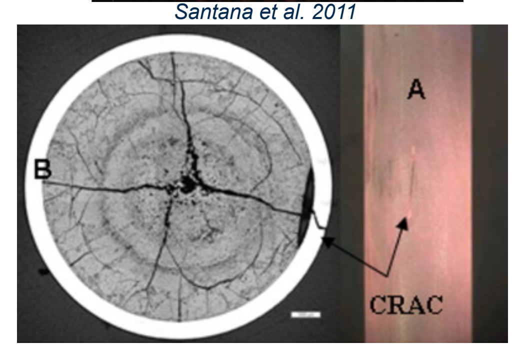








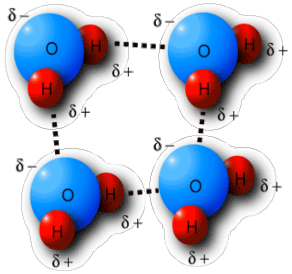
Santana et al. 2011



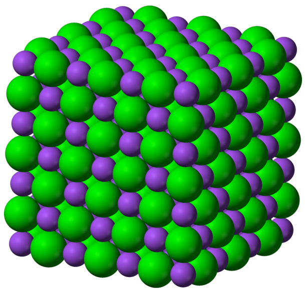
Before we can go into the microstructure changes, we need to summarize some materials science concepts

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

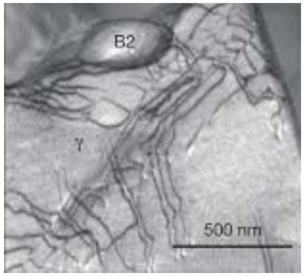
Chemical bonds



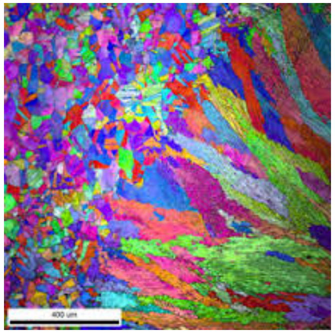
Crystal structure



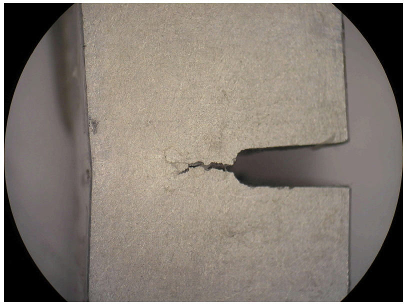
Defect interactions



Microstructure

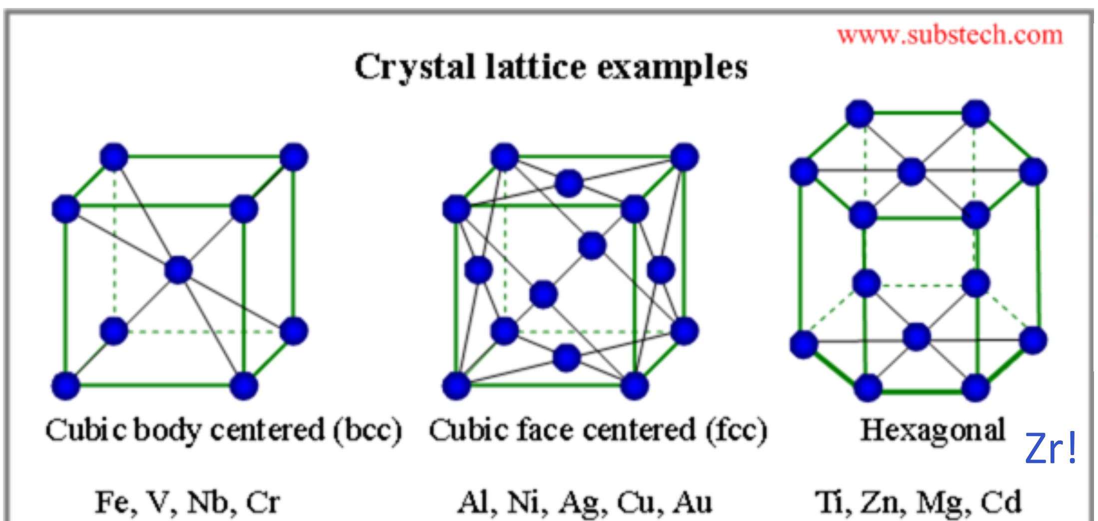


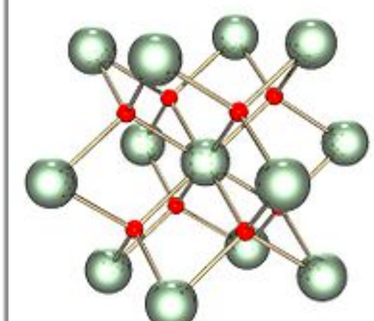
Material properties and performance



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

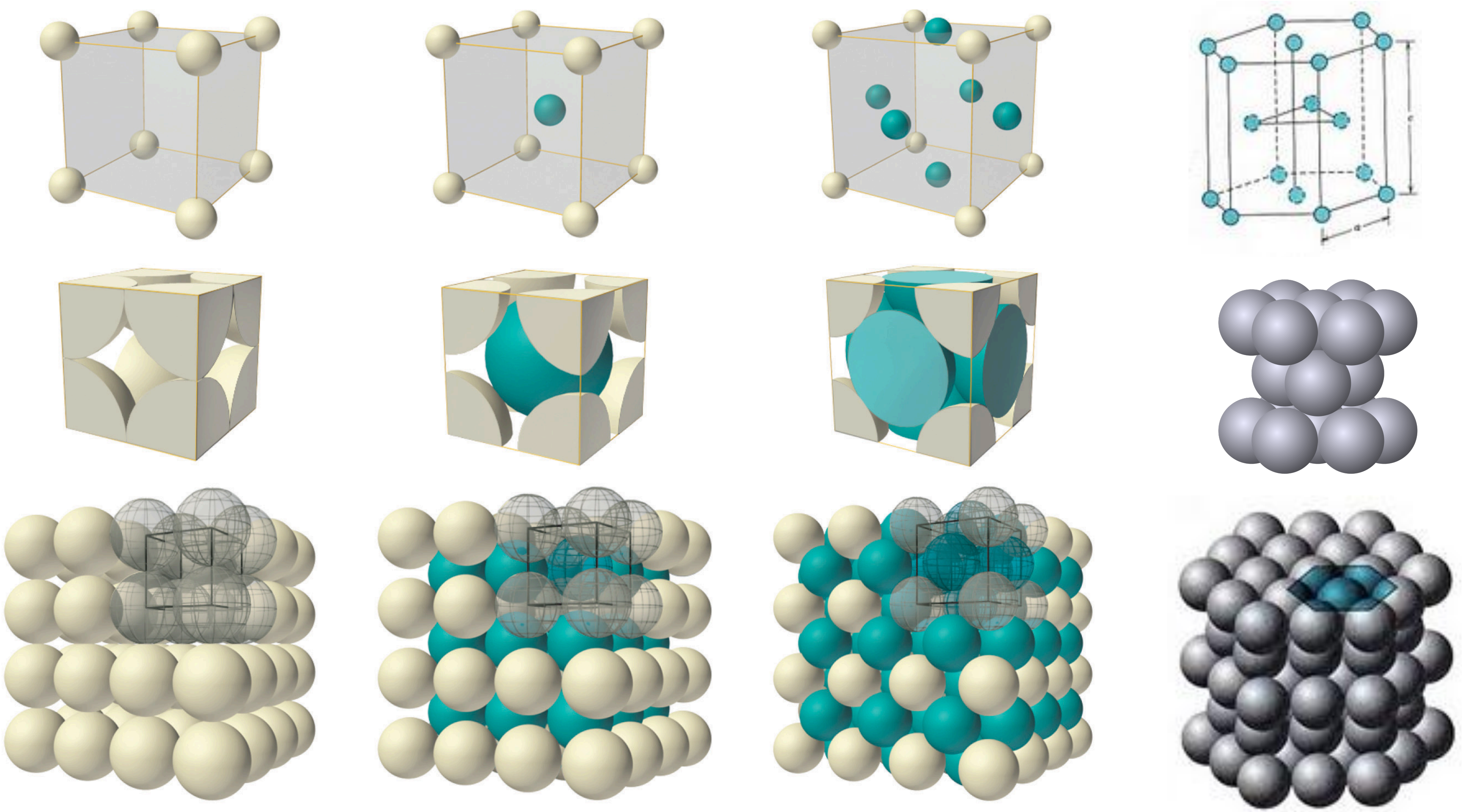
- The atoms of many materials form an organized lattice, these are called **crystalline materials.** All reactor materials are crystalline.
- Materials with atoms without an organized lattice are called **amorphous.** A common amorphous material is glass.
- The configuration of the atoms in the lattice impacts the properties of the material (density, thermal expansion coefficient, elastic modulus, etc.)
- The study of material crystal structure is called **crystallography.**





Fluorite structure of UO^2

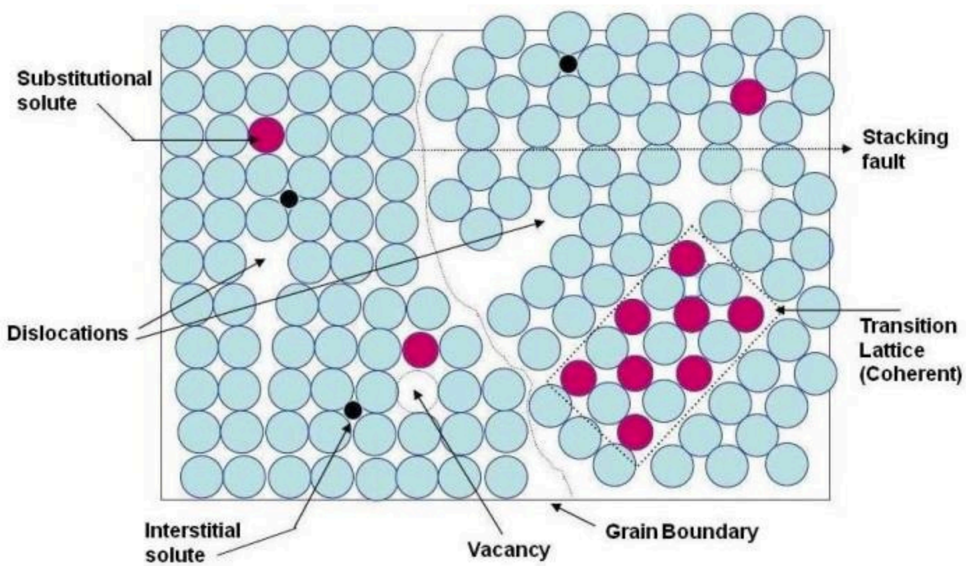
All major nuclear materials are either cubic or hexagonal



(a) Simple cubic (b) Body-centered cubic (c) Face-centered cubic (d) Hexagonal close packed

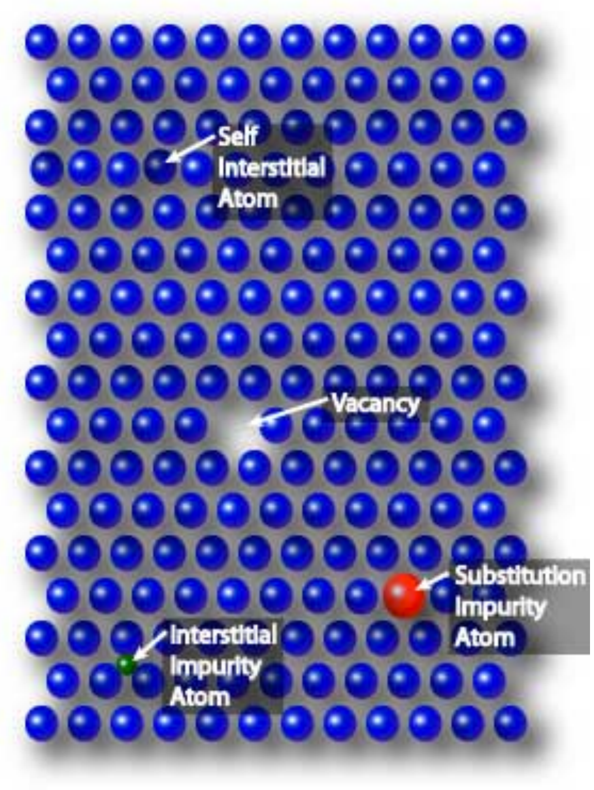
Even in crystalline materials, the lattices are not perfect, they have defects

- “Materials are like people; it is the defects that make them interesting”
- Defects can be 0D, 1D, 2D, 3D
- The interactions between defects seriously impact material properties and how they perform.



Various Crystal Defects

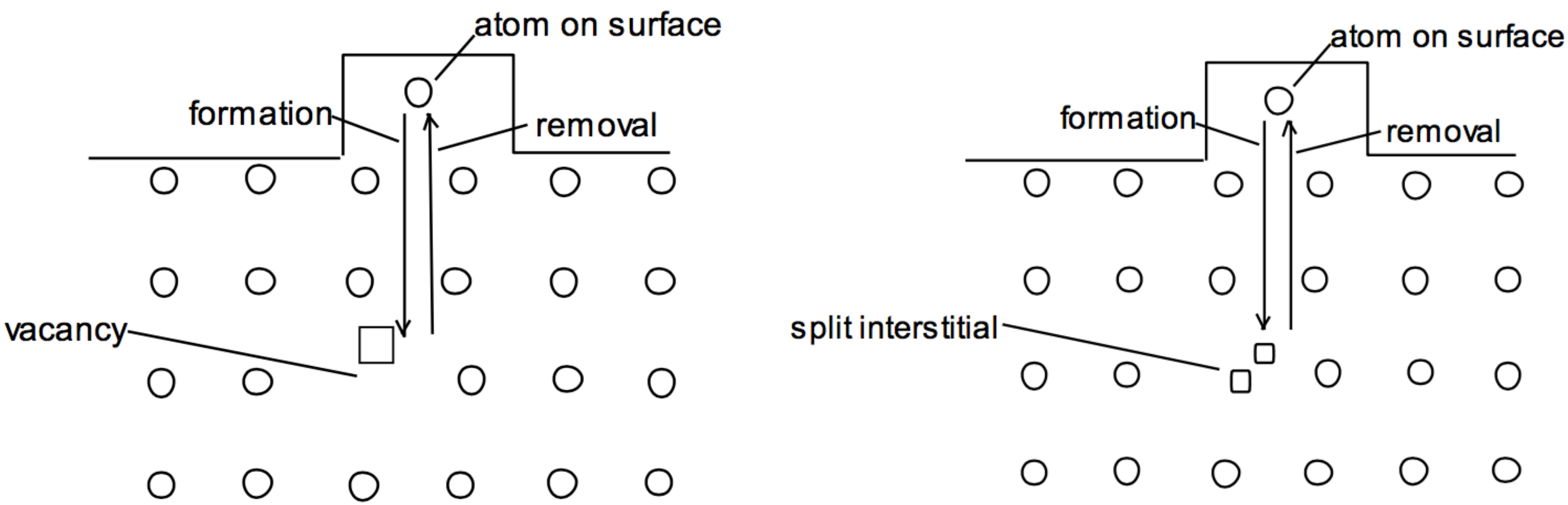
Point defects (zero-dimensional defects) are lattice imperfections related to one or two lattice sites



- There are several types of point defects
  - **Vacancies**
  - **Self interstitial atoms (SIA)**
  - **Interstitial impurity atoms**
  - **Substitution impurity atoms**
- Point defects control the mobility of atoms and, therefore influence all processes that depend on diffusion

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)

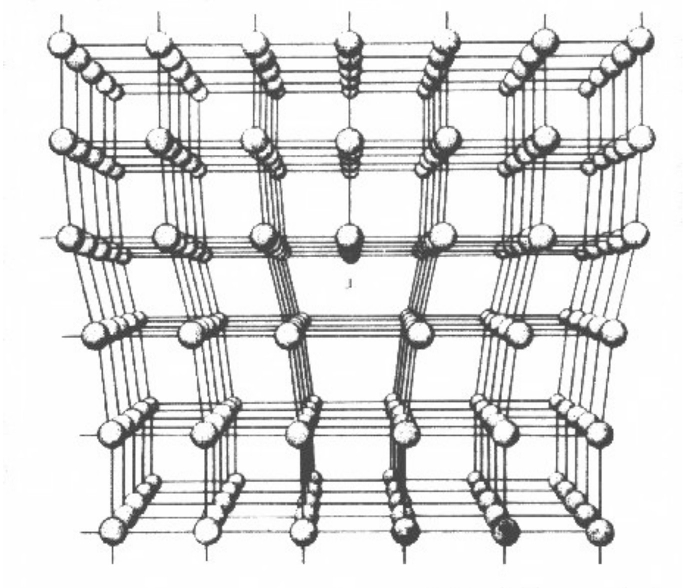


- We define the number of vacancies or interstitials in terms of a concentration. Total number of atoms is *N*

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

Dislocations are imperfections associated with a line of lattice sites (one dimensional defect)

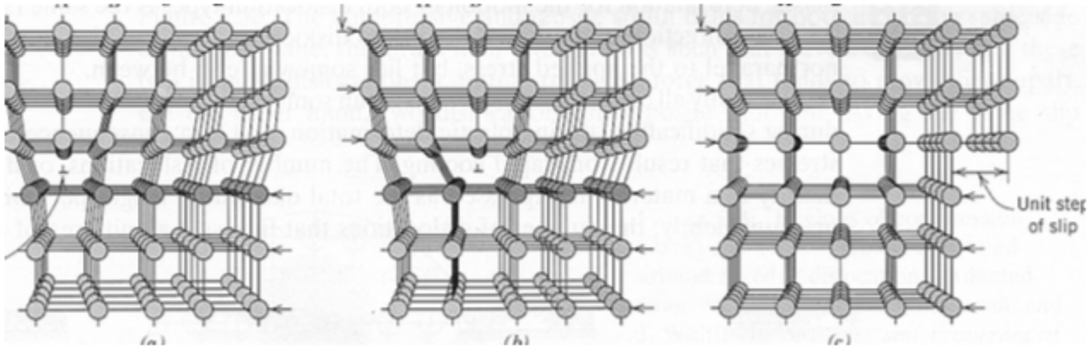
- In a dislocation, an extra half plane of atoms is inserted into the lattice.



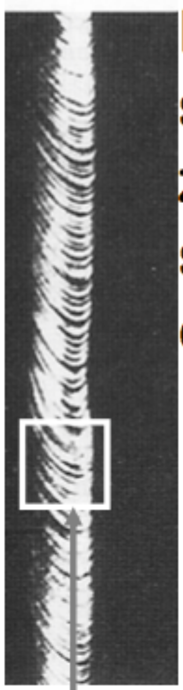
- Dislocation motion controls the plastic (permanent) deformation of crystalline materials

Plastic deformation occurs due to dislocation motion

- A dislocation is a line defect.
- When it moves, only a small number of bonds are broken at a time



Adapted from Fig. 7.1, *Callister 6e.* (Fig. 7.1 is adapted from A.G. Guy, *Essentials of Materials Science*, McGraw-Hill Book Company, New York, 1976. p. 153.)

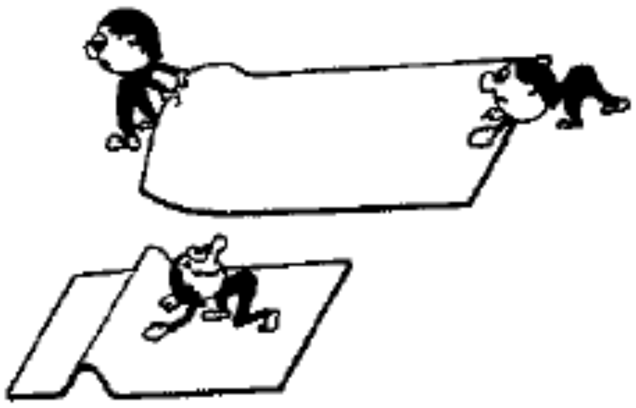


Plastically stretched zinc single crystal.

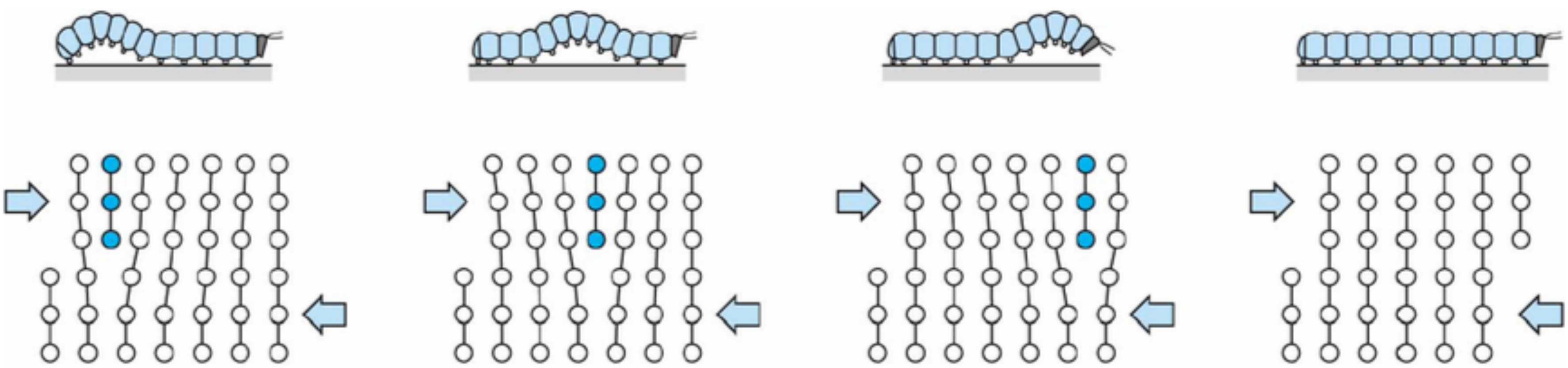
Adapted from Fig. 7.9, *Callister 6e.* (Fig. 7.9 is from C.F. Elam, *The Distortion of Metal Crystals*, Oxford University Press, London, 1935.)

Adapted from Fig. 7.8, *Callister 6e.*

Analogies for this behavior include moving a carpet, or the motion of a caterpillar

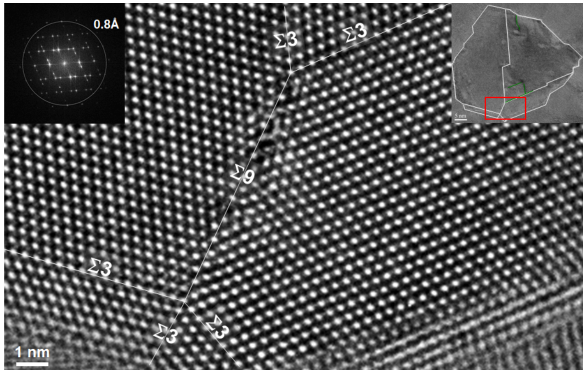


[E. Weber]

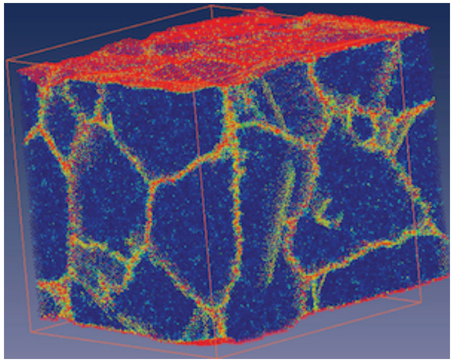


Grain boundaries are planes where misoriented crystal lattices meet (two dimensional)

- 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**.



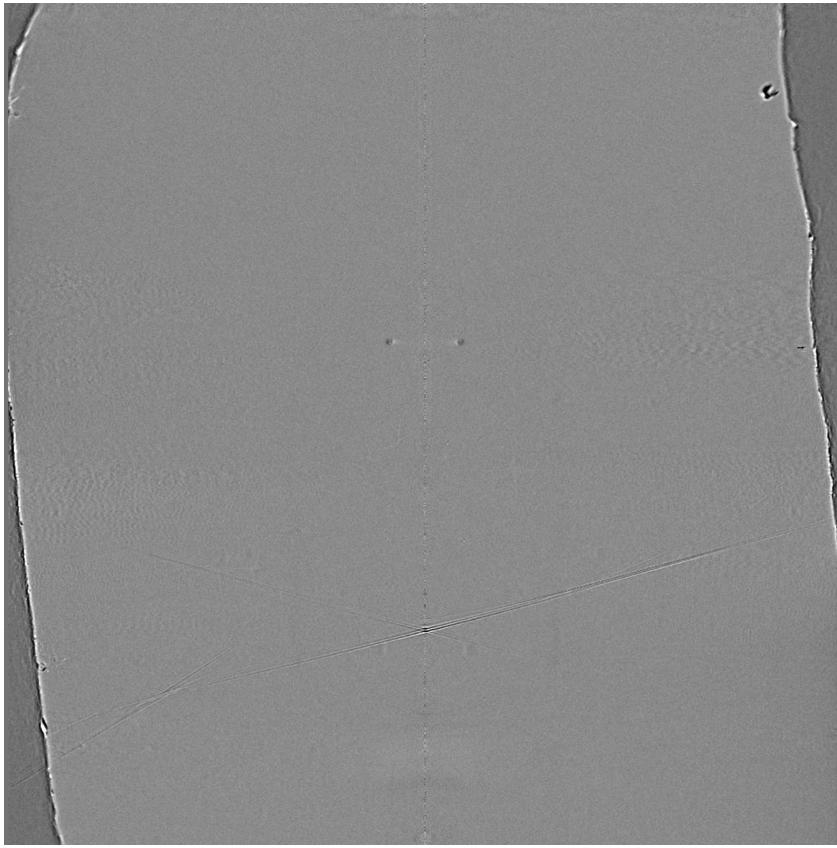
High-res transmission eleectron microscopy can also show individual atoms (palladium) *www.knmf.kit.edu/TEM.php*



Atomistic simulation of grain boundaries in 3D

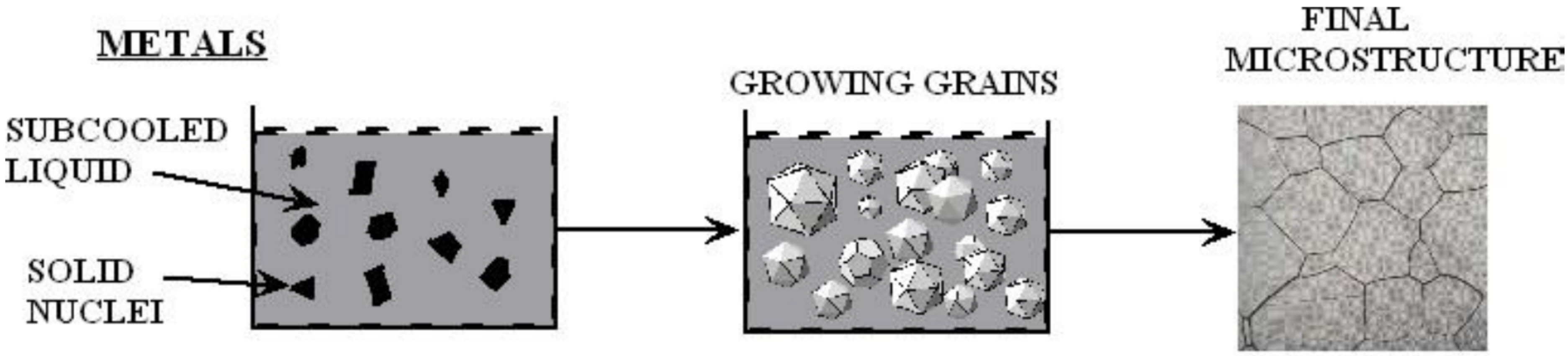
- Most crystalline materials are polycrystalline, not single crystal

Metals are often cast, and polycrystals naturally form during casting



Metals are often cast, and polycrystals natural form during casting

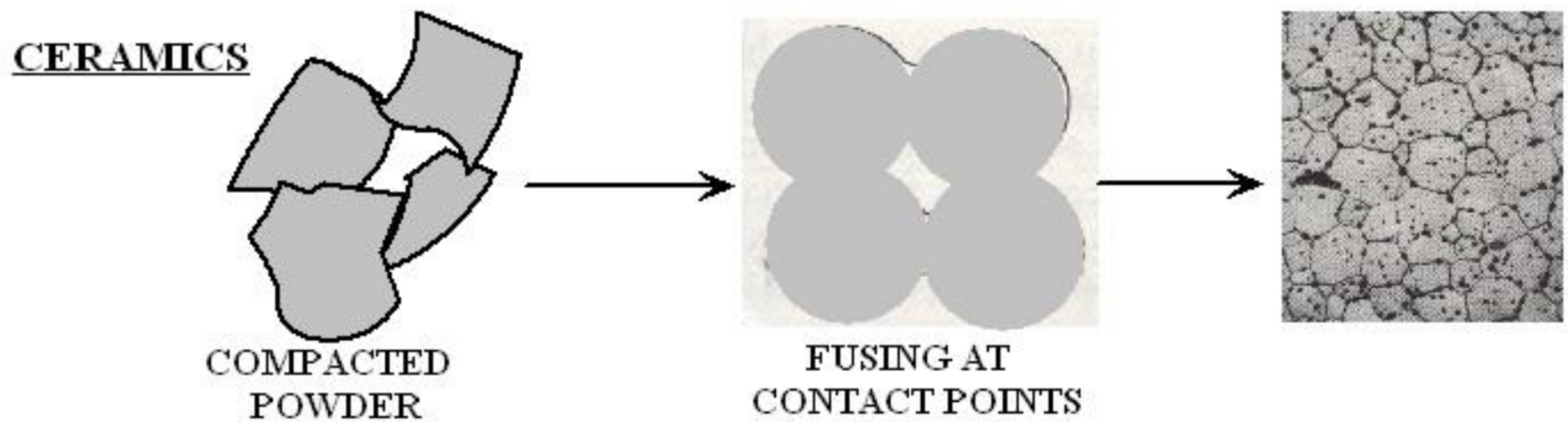
- Solidification begins in different regions of the melt, each with a different orientation.



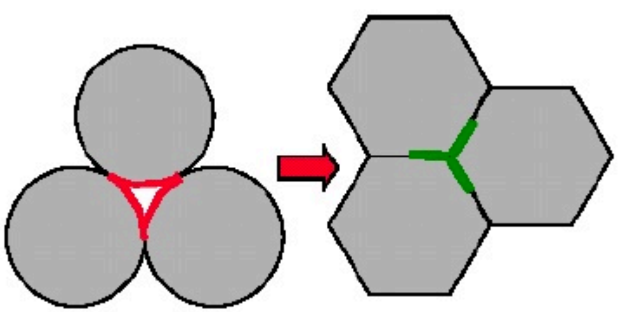
- Once the different regions meet, grain boundaries form between them

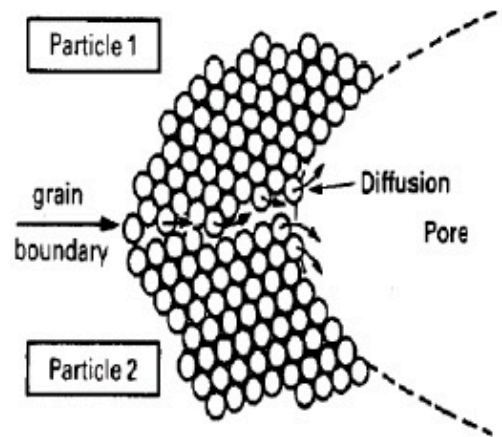
Ceramics are typically sintered, and polycrystals also naturally form from sintering

- In sintering, powders are compacted at high temperature

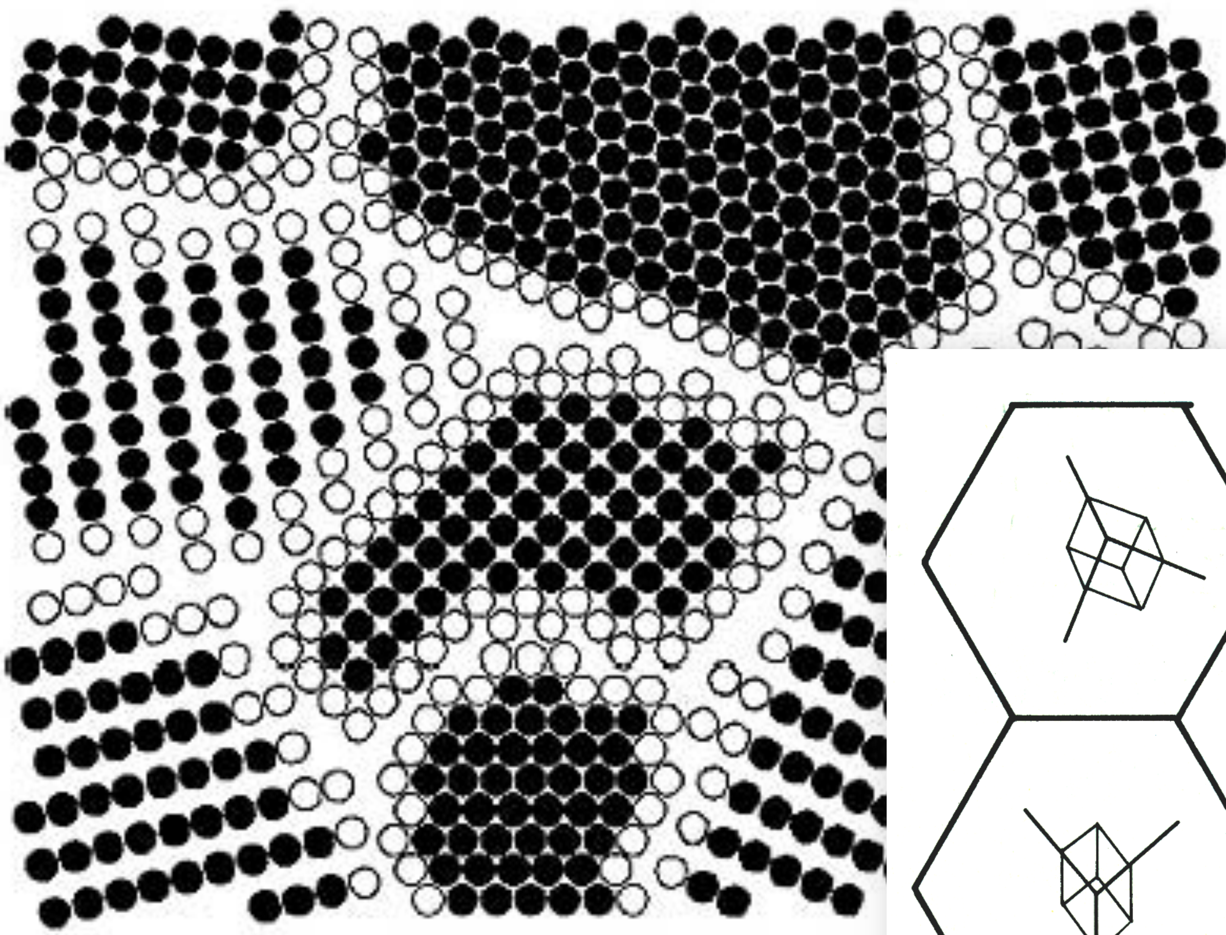


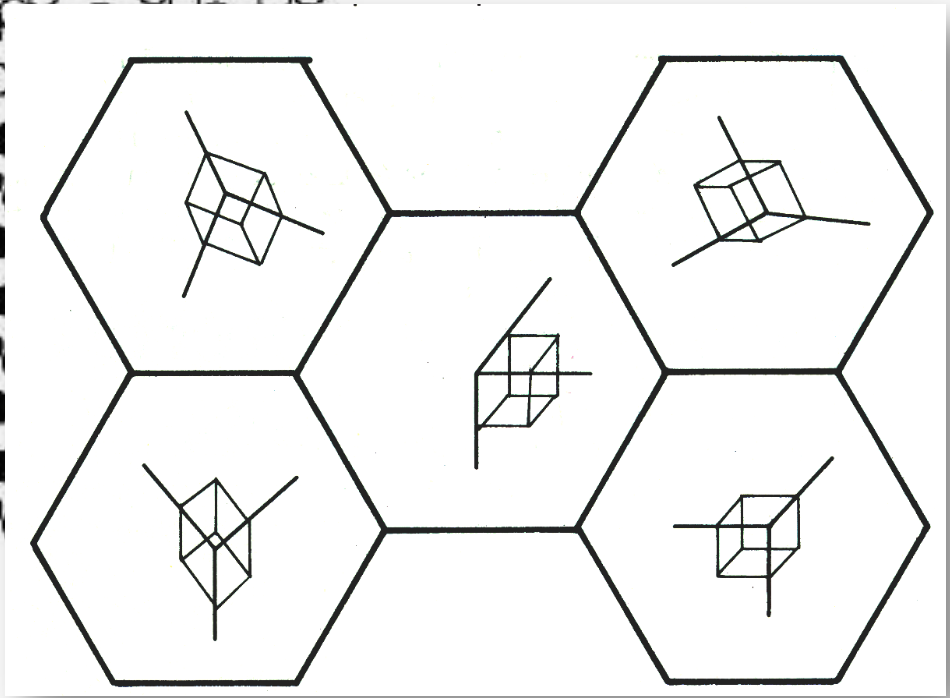
- The particles are each oriented differently, and as the fuse, grain boundaries form





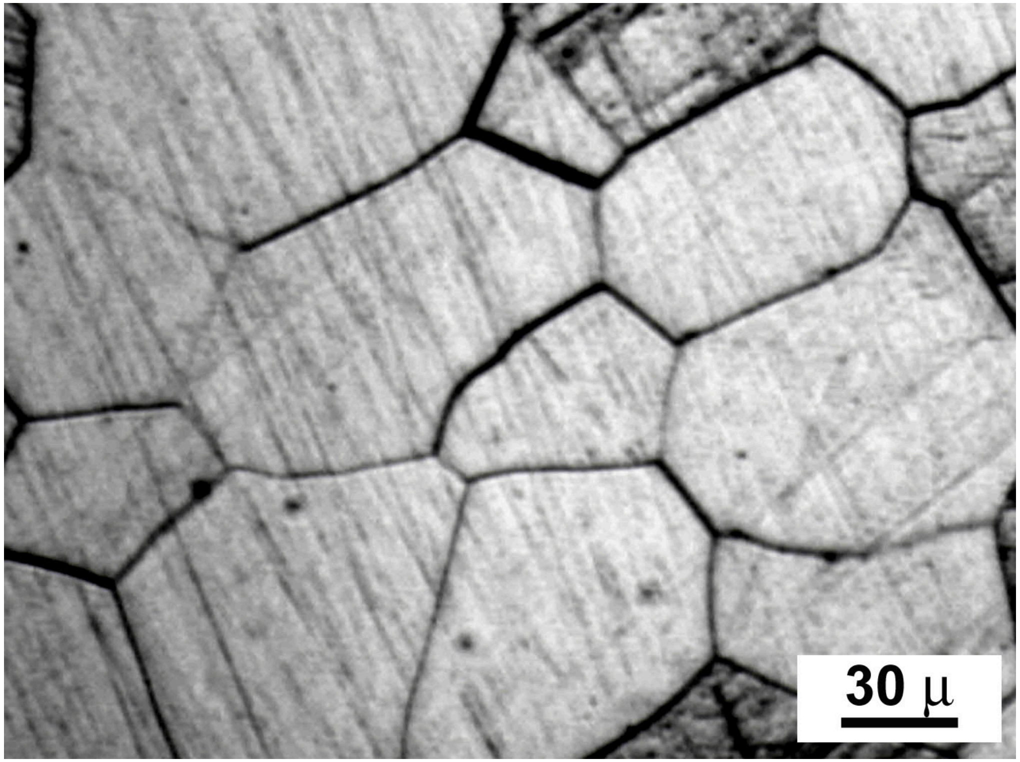
The differences between the grain orientations result in the grain boundary

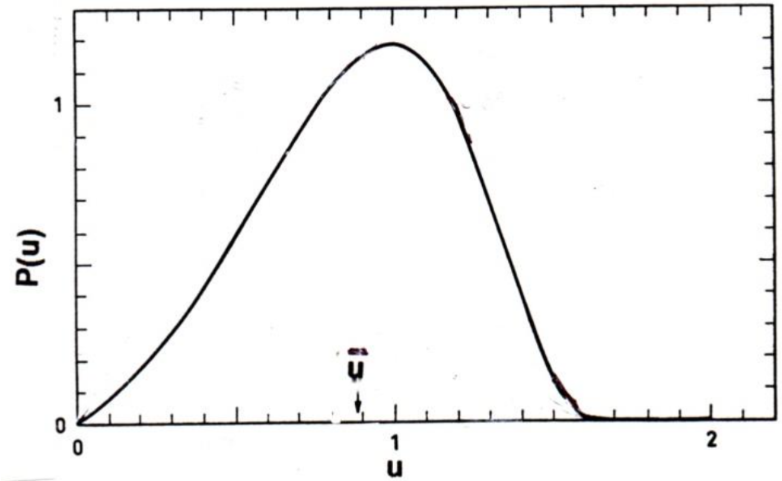




In a polycrystal, there is also a distribution of grain sizes

- Not every grain is the same size
- Therefore, we commonly refer to the **grain size distribution** and the **average grain size**

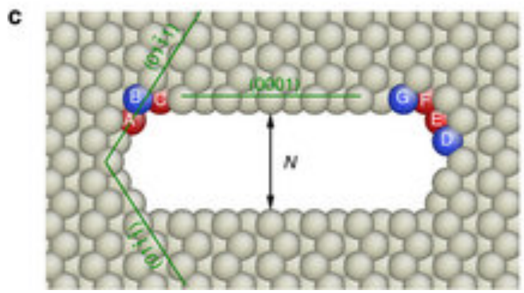


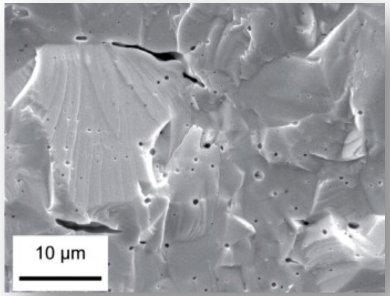


The Hillert distribution is an analytical distribution for grain size. Real materials often vary from this behavior

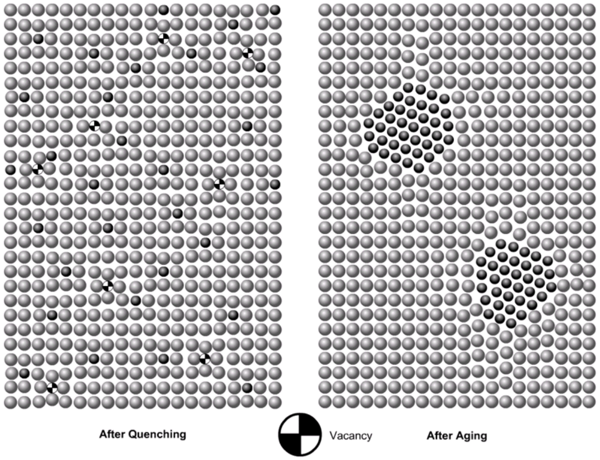
When point defects cluster, they form three dimensional defects

- The energy of a point defects is reduced when several point defects cluster together
- Larger clusters of vacancies are called **voids**



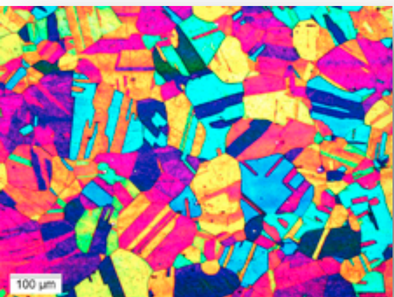


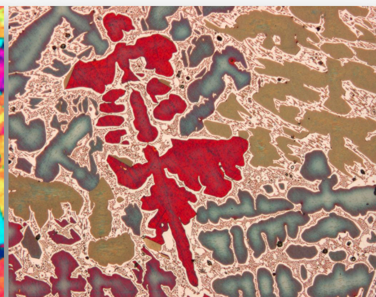
- Clusters of impurity atoms are called **precipitates**

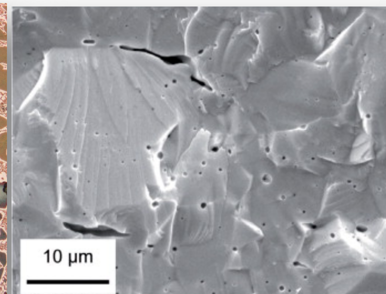


Material microstructure is the structure observable with 25x magnification

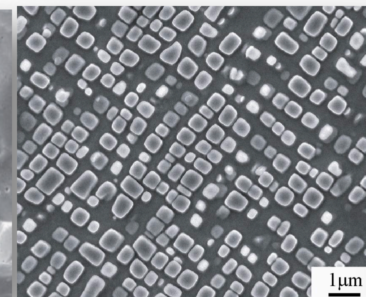
- The microstructure includes grain structure, secondary phases, porosity, and more


Annealed Stainless Steel

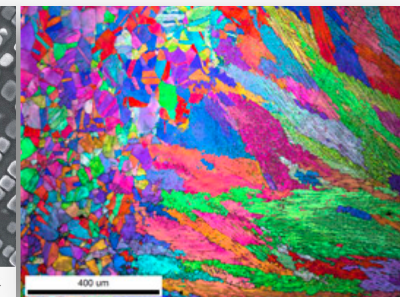

Cast Bronze



Sintered UO2



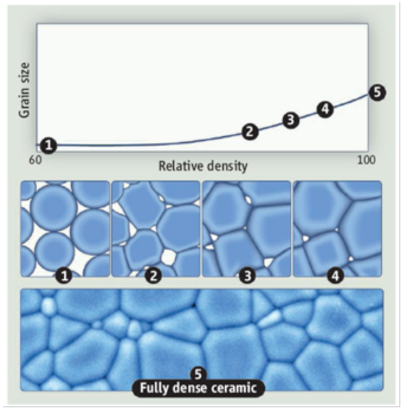
Co-Al-W Superalloy


Friction stir welded stainless steel

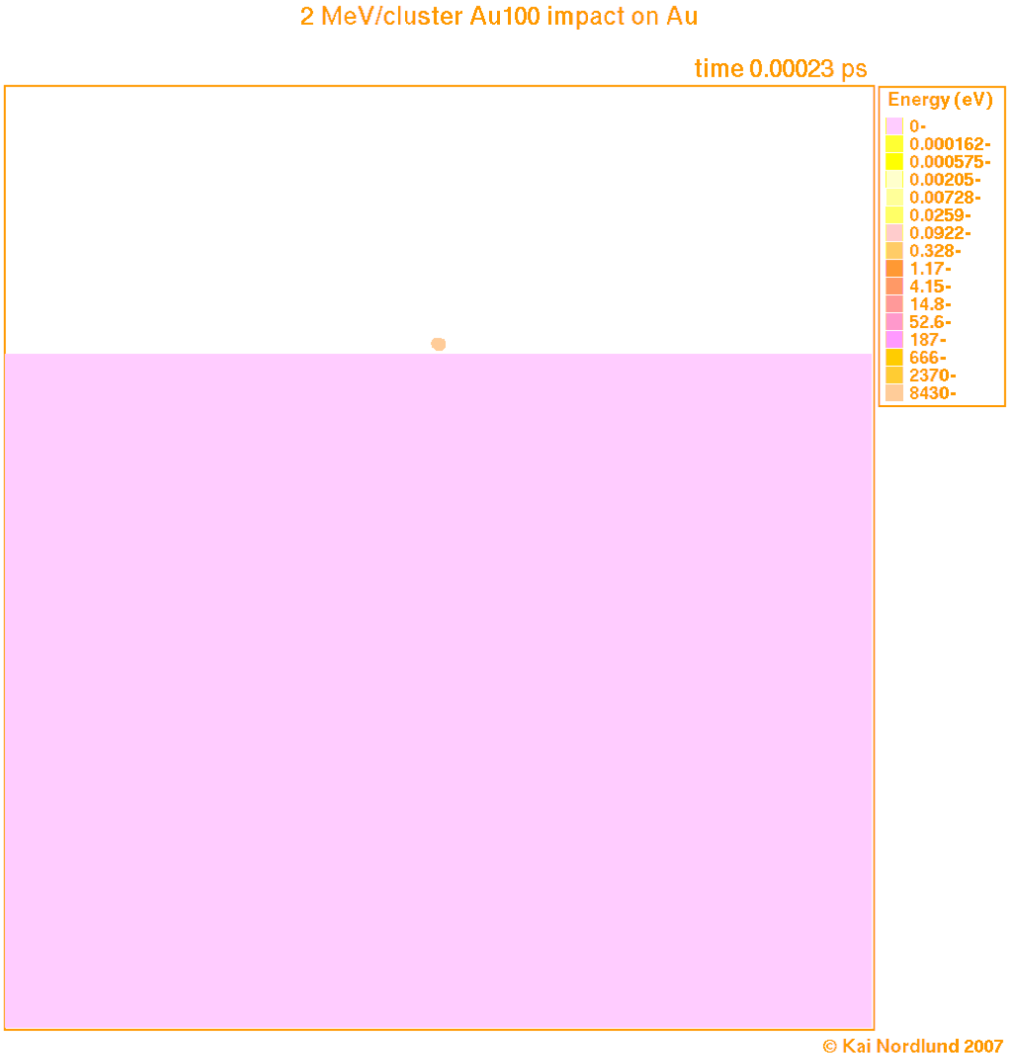
- The microstructure can strongly influence physical properties such as strength, toughness, ductility, hardness, corrosion resistance, high/low temperature behavior or wear resistance.
- These properties in turn govern the application of these materials in industrial practice

The process we use to make a material has 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
- **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
  - Use on many types of materials (metals, ceramics, glasses)
- **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



Ionizing radiation can introduce defects into the crystal lattice, called radiation damage



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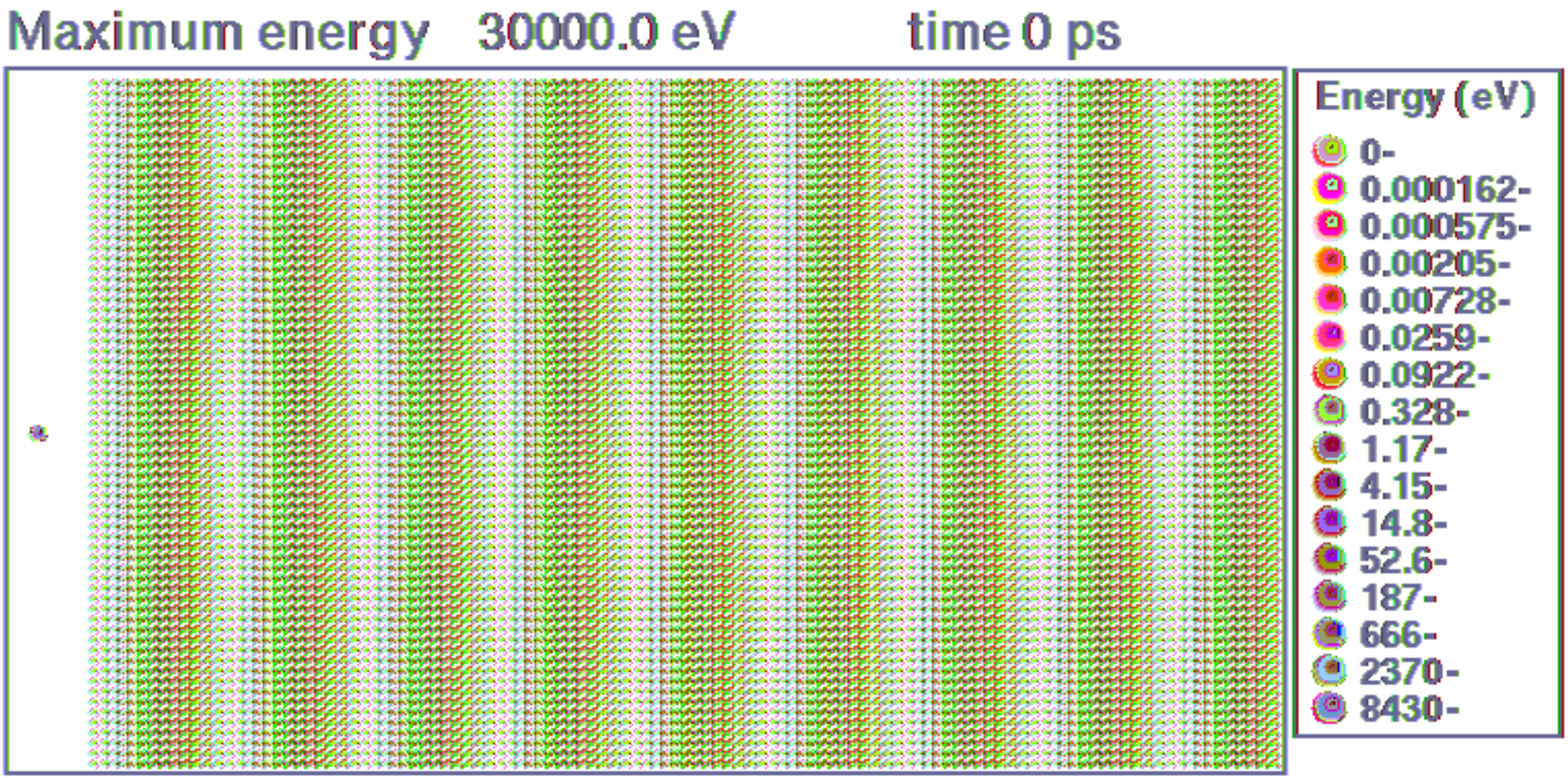
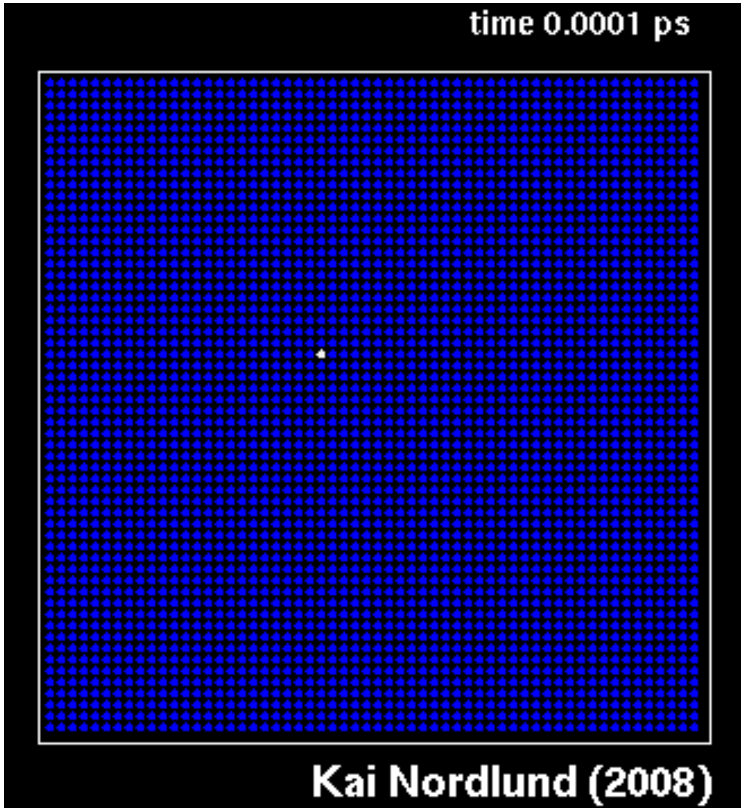


PKA collisions create a collision cascade, which results in the generation of defects (point and clusters)



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 v_{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

Summary

- Even during steady state operation, 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 include vacancies, interstitials, and impurity atoms
  - Dislocations are line defects
  - Grain boundaries are planar defects
  - Voids and precipitates are volume defects
- All materials have defects
- Radiation damage causes many more defects