Multiscale Techniques Applied to Material Irradiation Damage Analysis

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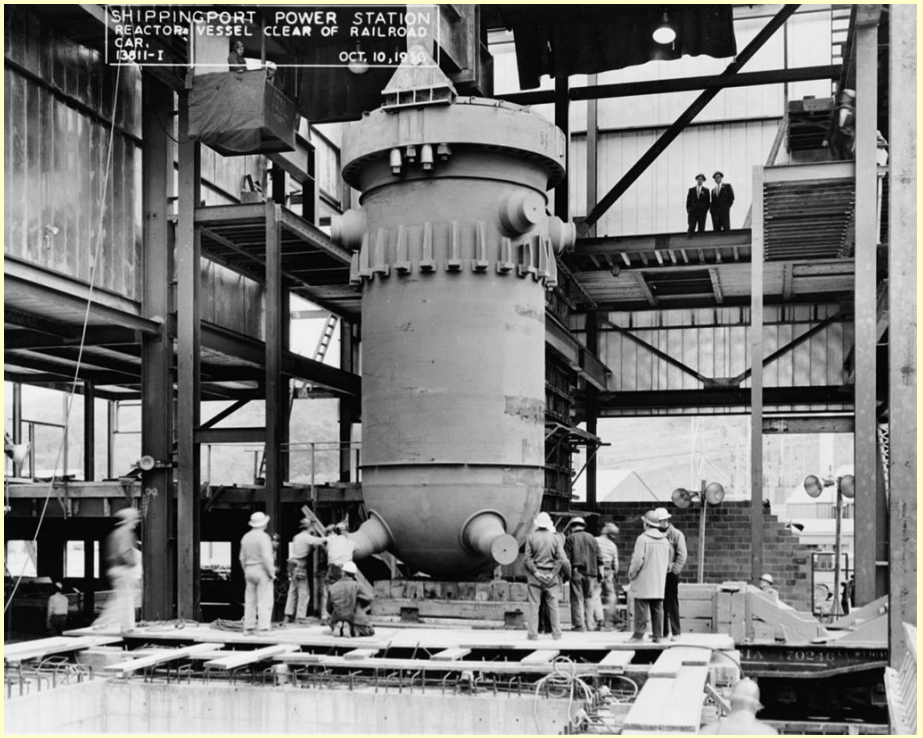
MEEG 591V

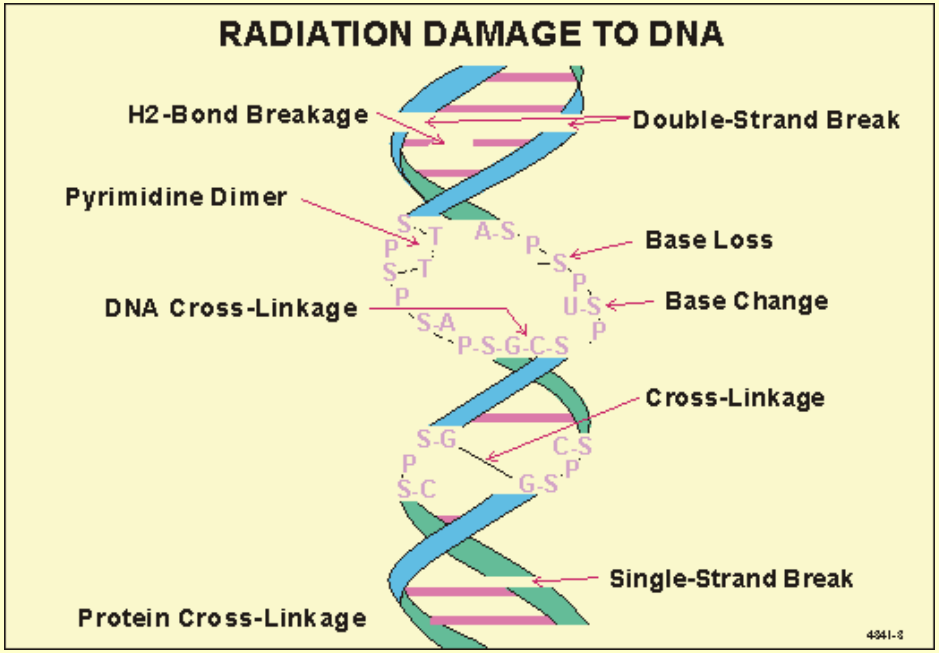
Outline

- Motivations
- Mechanisms
- Review of methods
- Application

Motivations

- Understand mechanicsms by which radiation interacts with materials





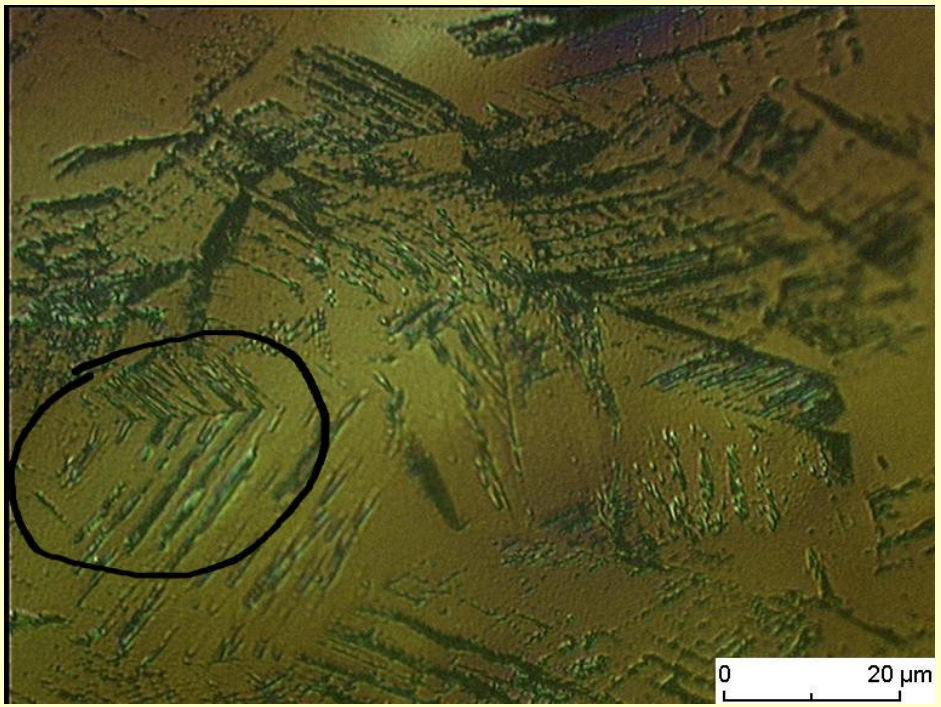
- Produce materials and procedures that better take account of this behavior
- Multiple length and time scales important!

- *Radiation Sources and effects.* <*http://www.radiation-scott.org/radsource/3-0.htm*>. Retrieved 12/2/15.

- <https://en.wikipedia.org/wiki/Reactor_pressure_vessel#/media/File:Shippingport_LOC_135430pu.jpg>

Mechanisms of Interactions in Metals

- Primary Knock-On Atoms (PKA's)
- E_k dependent on radiation type/energy
  - Neutrons high E_k
  - electrons low E_k

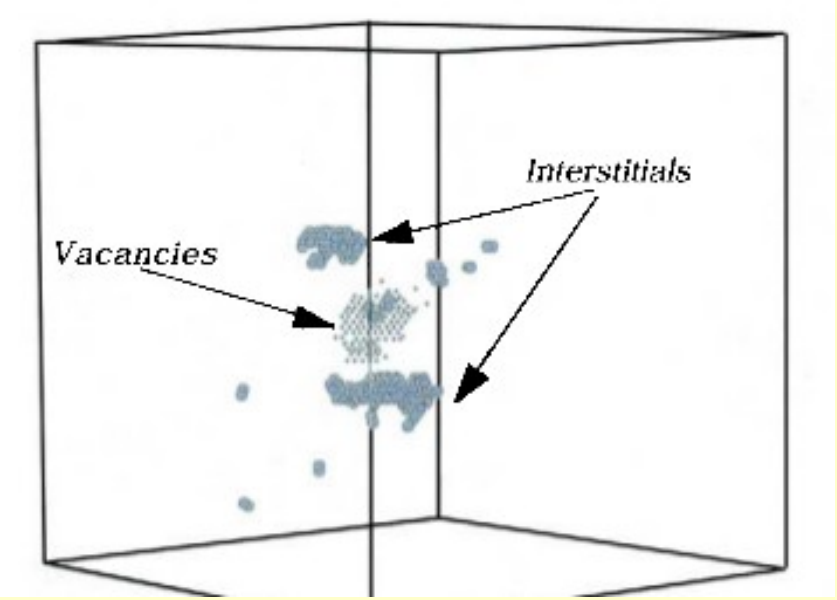


[1]

Austentite (FCC) → Martensite (BCT)

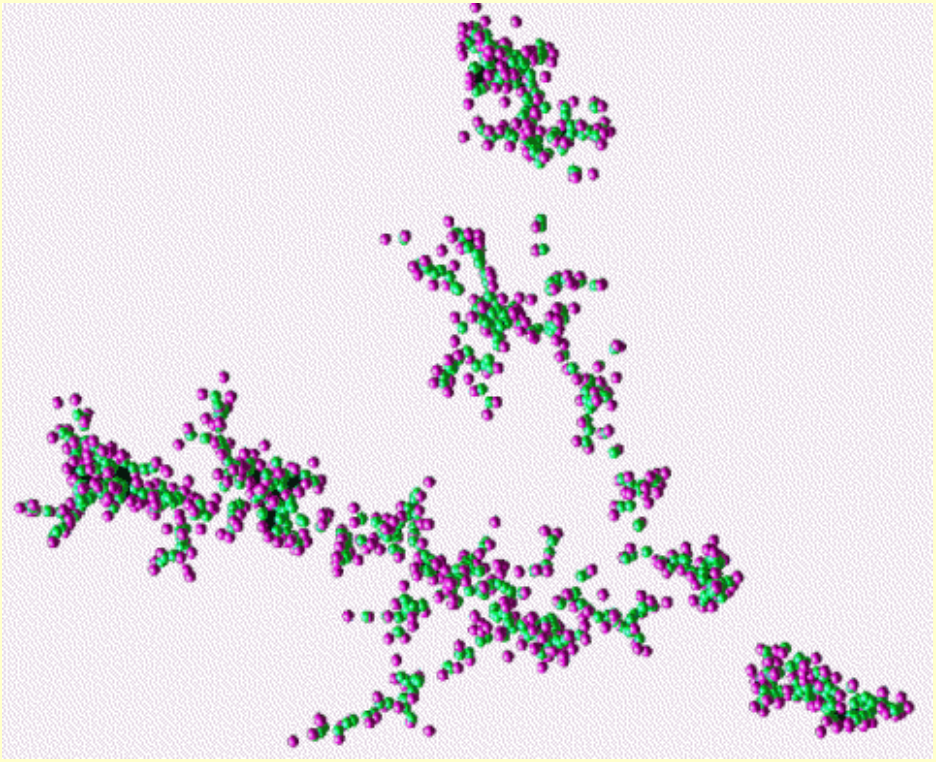
Defects and Interstitials

- PKA's result in displacement of secondary atoms
- "Cascade" of displacements



[2]

Property changes



- Defects (Dislocations) build up and result in property changes
  - Work hardening
  - Embrittlement
  - Loss of ductility

- Atomistic Simulations of Radiation Damage in Metals. <http://cmcsn.phys.washington.edu/book/export/html/507>. Retrieved 12/2/15.

Methods

- In reactor steels, engineering decisions are often made using empirical relations.
  - Extrapolation is dangerous!
  - Performing experiments to model a new system can be difficult
- Experiments do not show events at the atomic scale

- MD simulations provides a window to atomic interaction events
- Dislocation Dynamics Simulations predict changes in material properties

Some Results

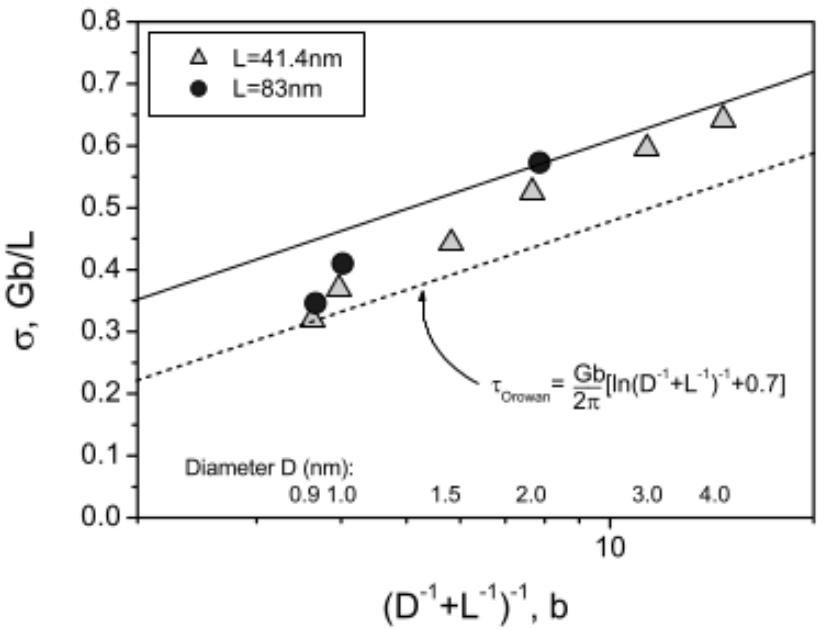


Fig. 11. Stress (units Gb/L) vs. $\tilde{D}/b$ for an edge dislocation to pass a row of voids in an atomic model of Fe at $T = 0$ K. The D and L values are indicated. The dashed and full lines are those for the Orowan stress and for voids with $\gamma_s = 3$, respectively, taken from Fig. 9 for the continuum simulation of [68] with r_0 set equal to b.

- Matches theoretical models in some cases, not in others

[3]

An application

- Understand the mechanisms that drive microstructure change due to irradiation in metallic Uranium fuels

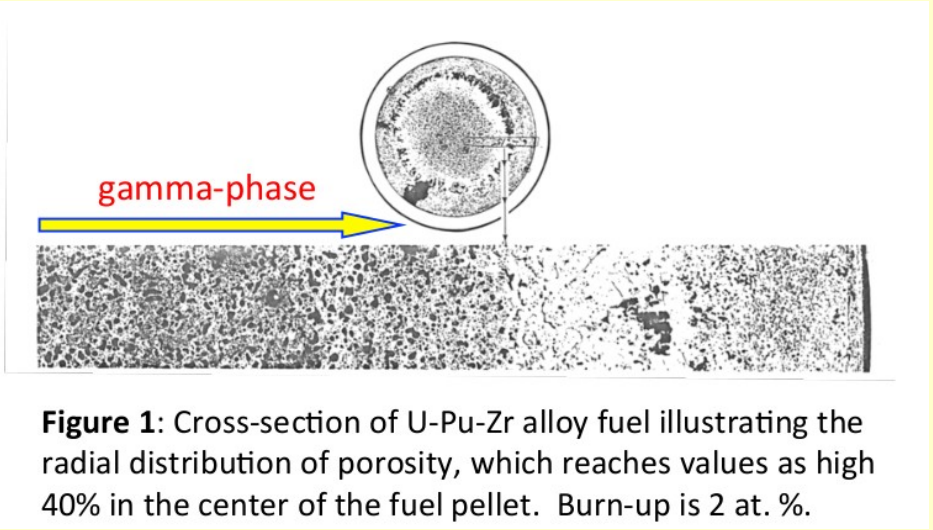


Figure 1: Cross-section of U-Pu-Zr alloy fuel illustrating the radial distribution of porosity, which reaches values as high 40% in the center of the fuel pellet. Burn-up is 2 at. %.

Computational and Experimental Studies of Microstructure-Scale Porosity in Metallic Fuels for Improved Gas Swelling Behavior. Millet Research Group.

Literature References

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