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The Direction of Fast Fuel Modeling in the US

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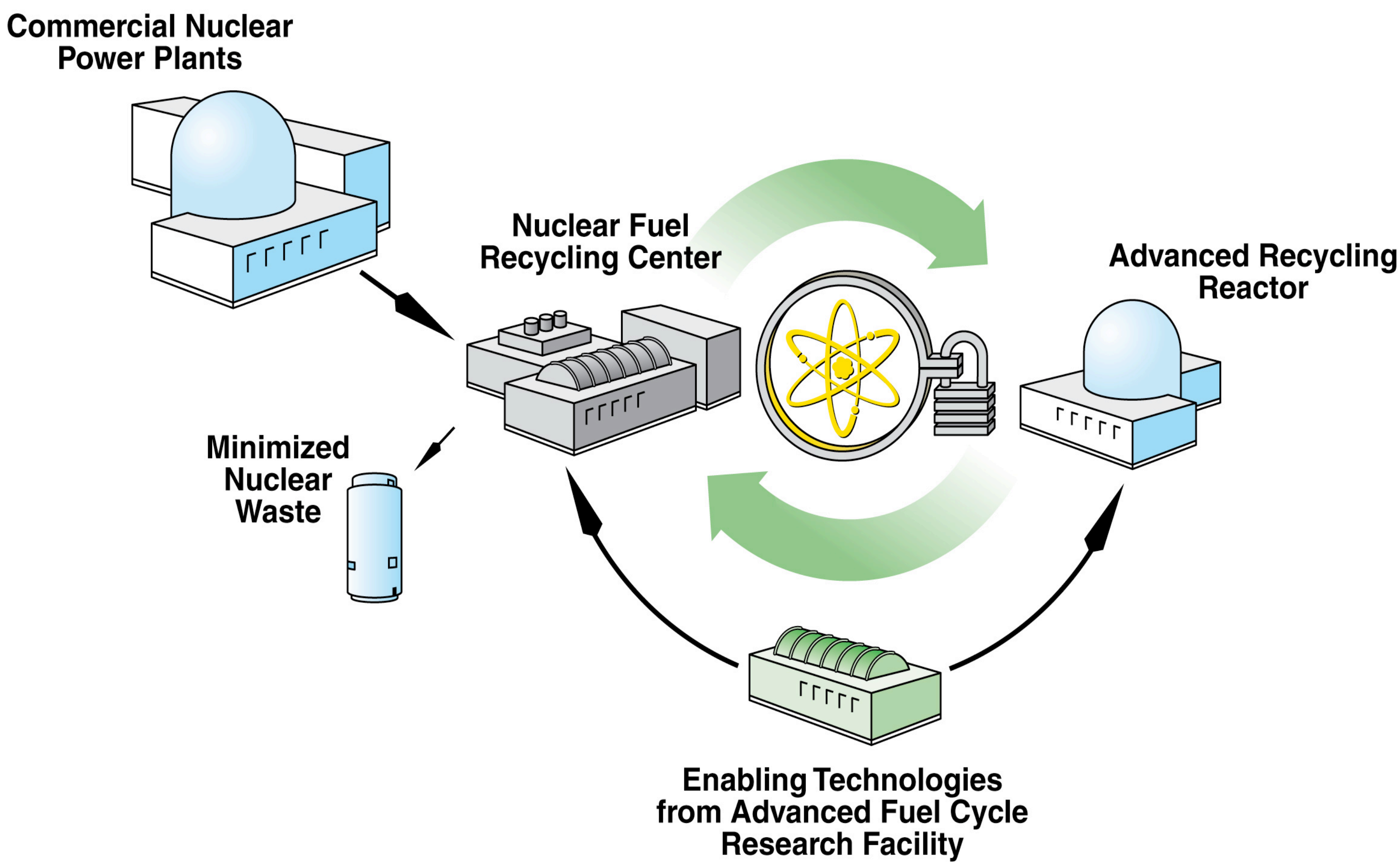
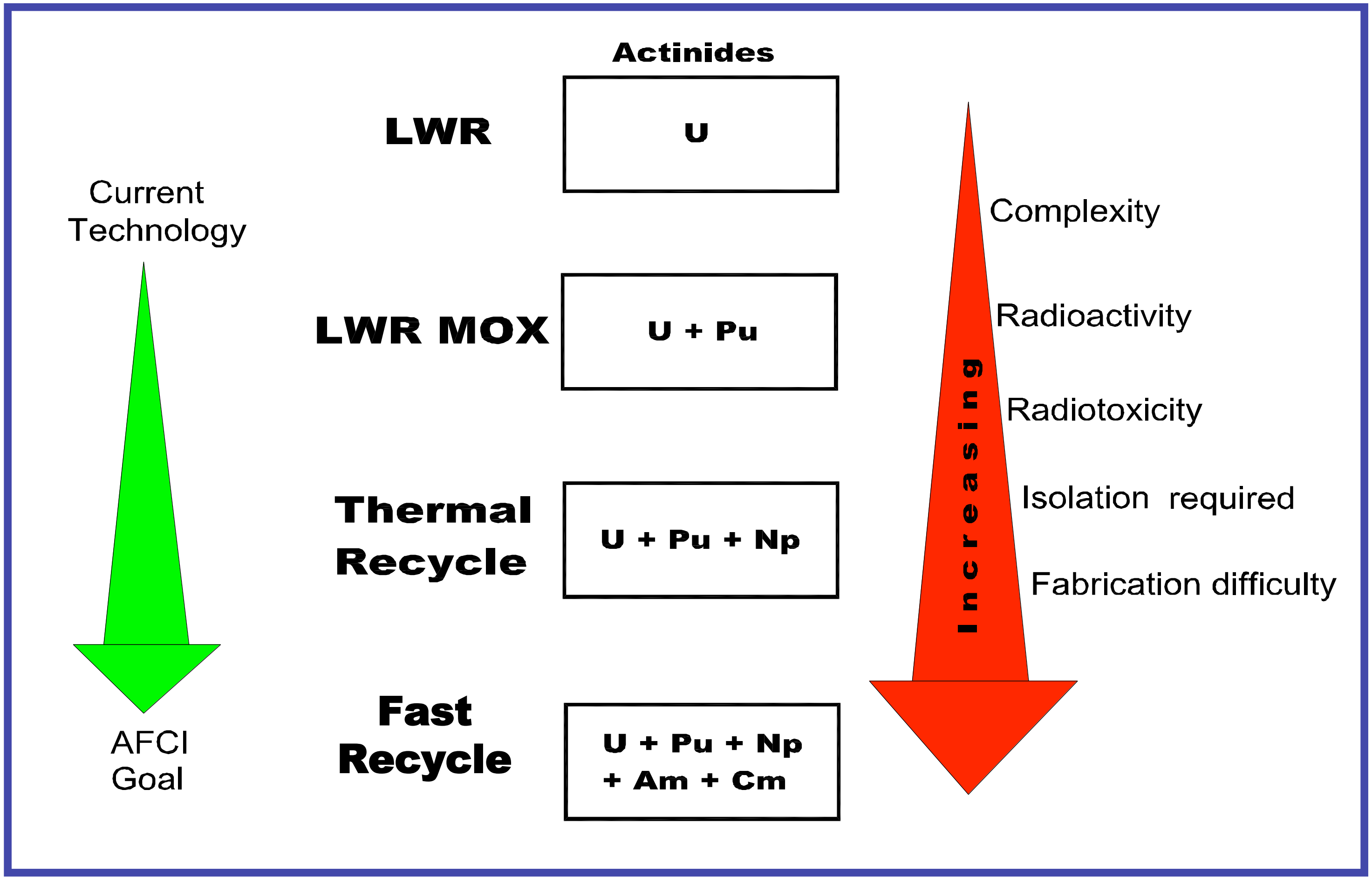
Outline

- Objective of the GNEP Transmutation Fuel Program
- What does a fuel rod do?
- How does it do it?
- How do current fuel performance code simulate fuel behavior?
- How can we apply recent developments in computational sciences to design the next generation of fuel performance codes?

GNEP seeks to close the fuel cycle



GNEP fuels are much more challenging to fabricate and operate



Source: K. Pasamehmetuglo, INL

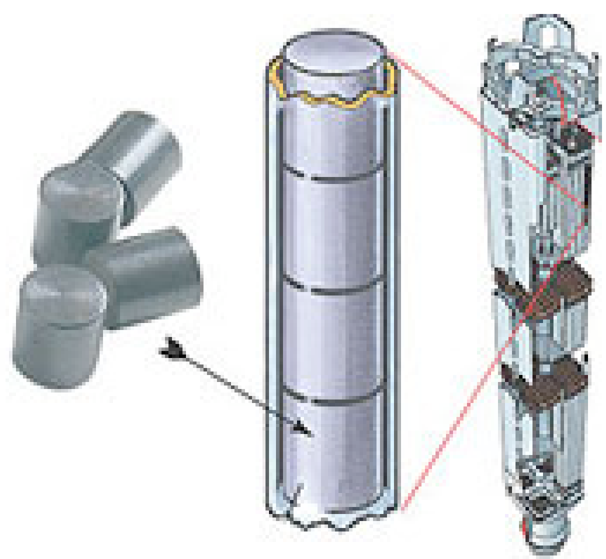
What is a nuclear fuel rod required to do?

- **General fuels requirements**
  1. Generate heat at a ~constant rate
  2. Transfer heat reliably and uniformly to the power generation systems
  3. Not release fission products
  4. Do it safely
  5. Do all four for as long as possible

- **GNEP fuels requirements**
  1. TRU transmutation

Fuel Requirements

From performance perspective, only requirement is nuclei with sufficient density to sustain steady-state chain reaction.

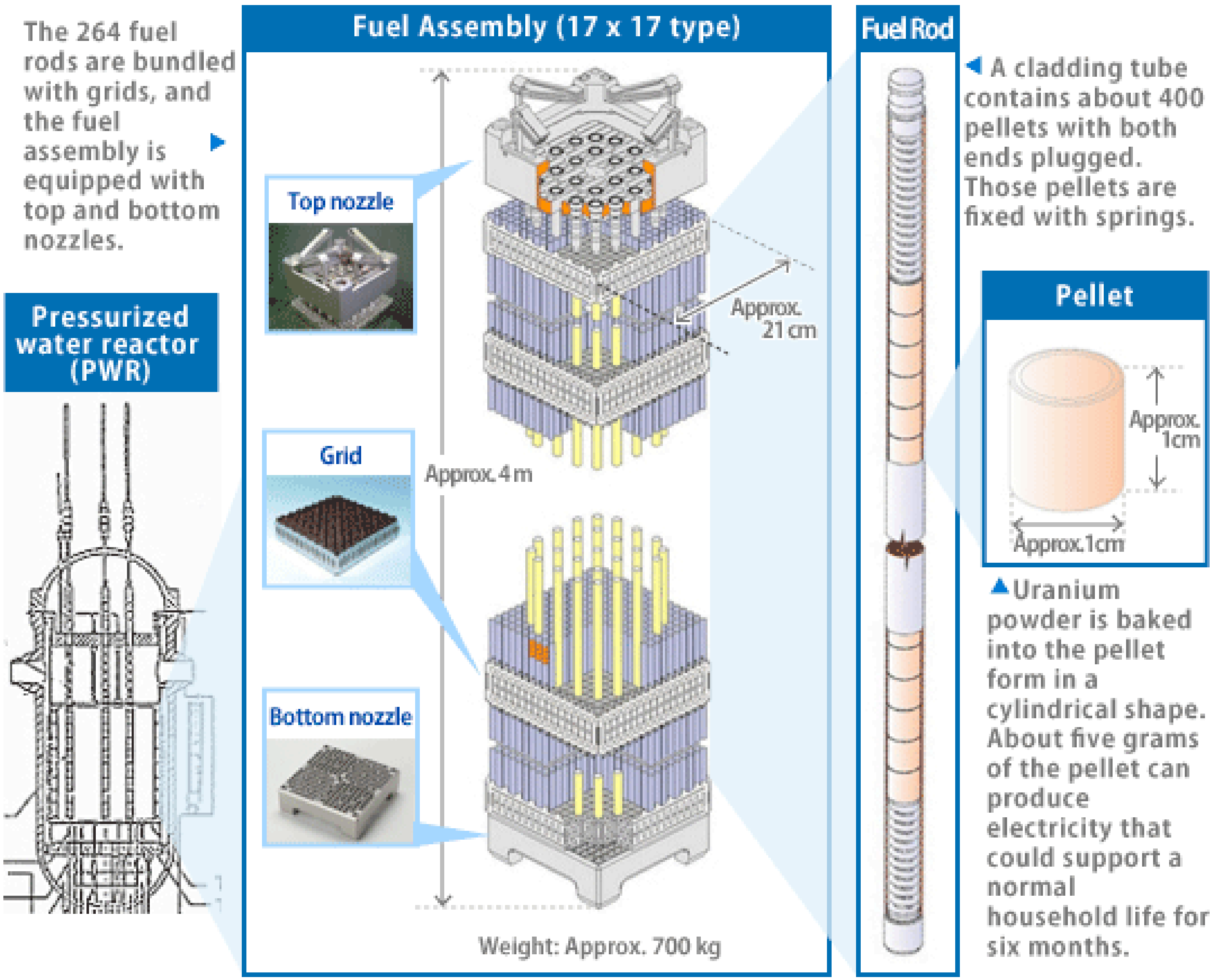


From materials perspective, there are few requirements:

- •Density of fission nuclei
- •Pellet maintains structural integrity
- •Good thermal conductivity
- •Retains fission products
- •Not rupture clad

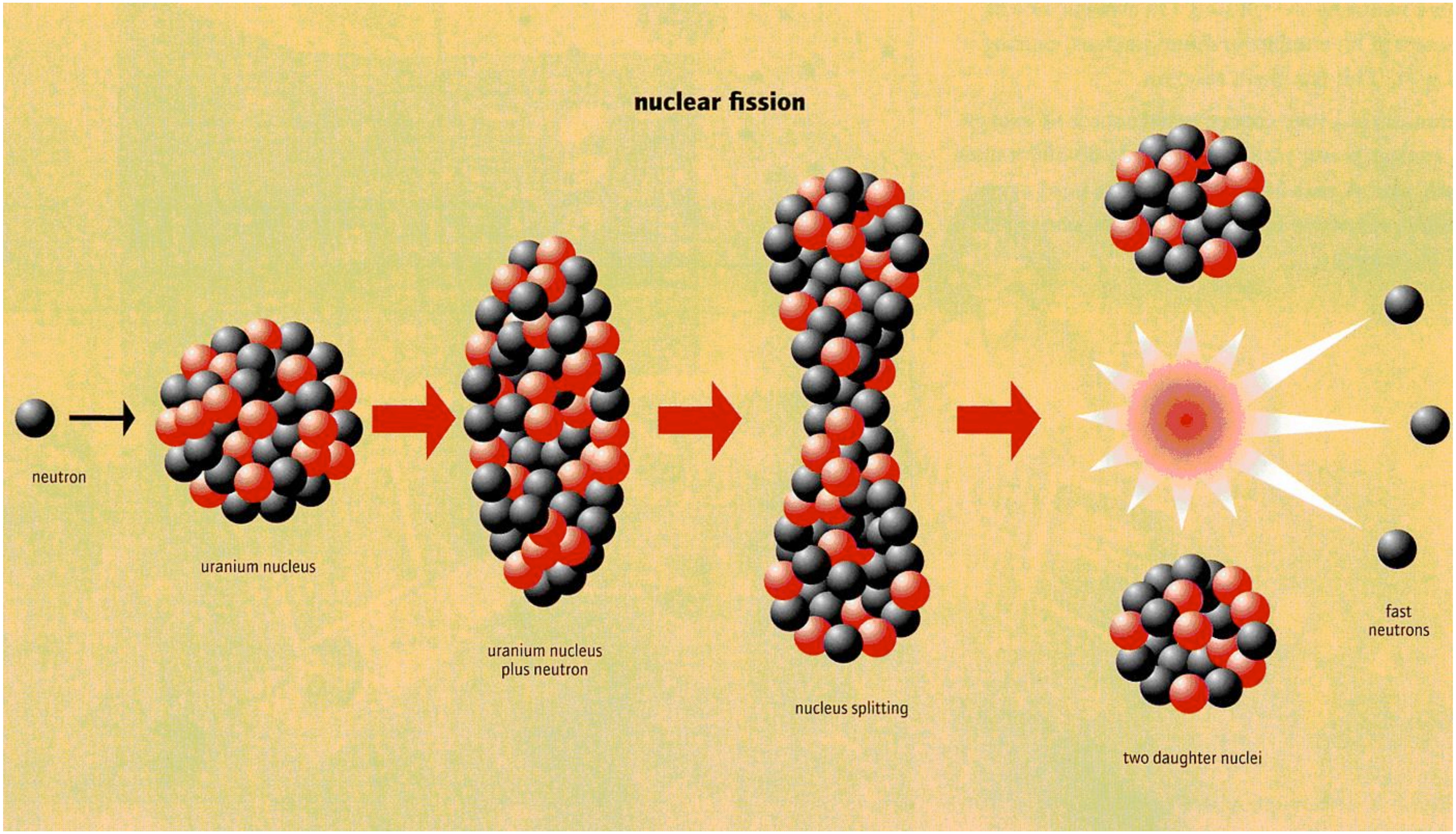
*Source: http://www.skb.se/default2____14877.aspx

Light Water Reactors



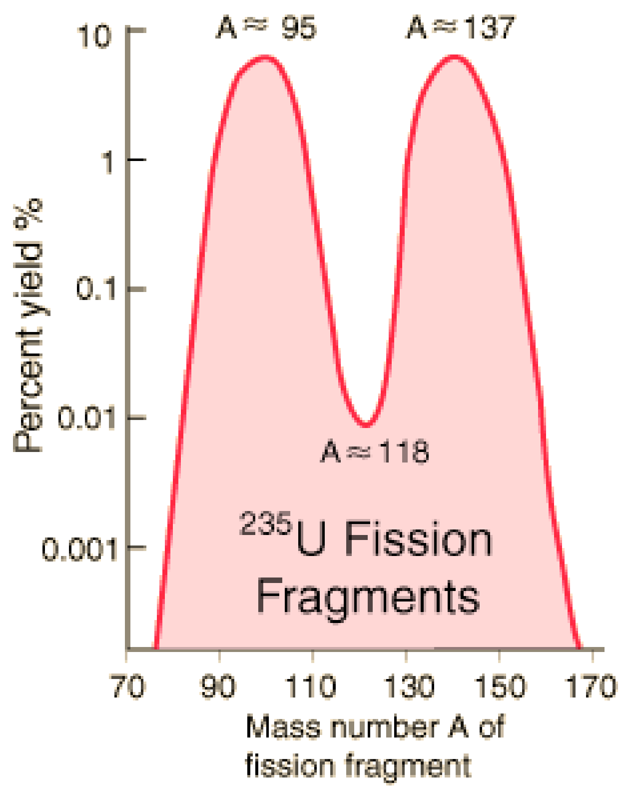
Source: www.nfi.co.jp/e/product/prod02.html

Basic Nuclear Physics
Fission Event

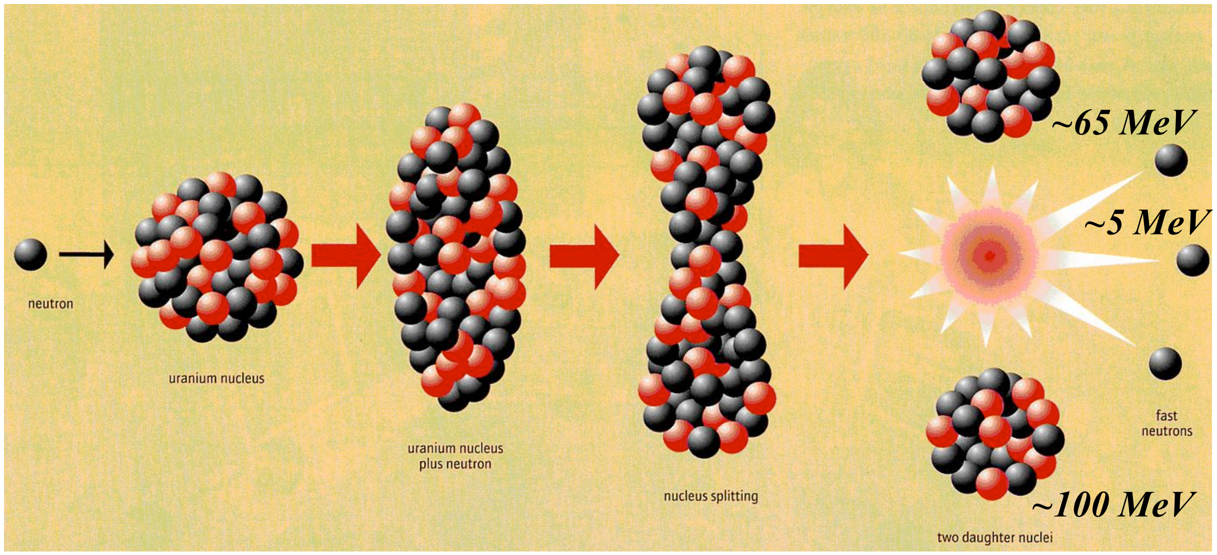


Basic Nuclear Physics
Fission energy and fragments

Kinetic Energy, heavy fragment	~65 MeV
Kinetic Energy, light fragment	~100 MeV
Kinetic Energy, fission neutron	5 MeV
Prompt γ-ray energy	5 MeV
β-decay energy	5 MeV
γ-decay energy	5 MeV
Neutrino energy	11 MeV
Total energy	196 MeV



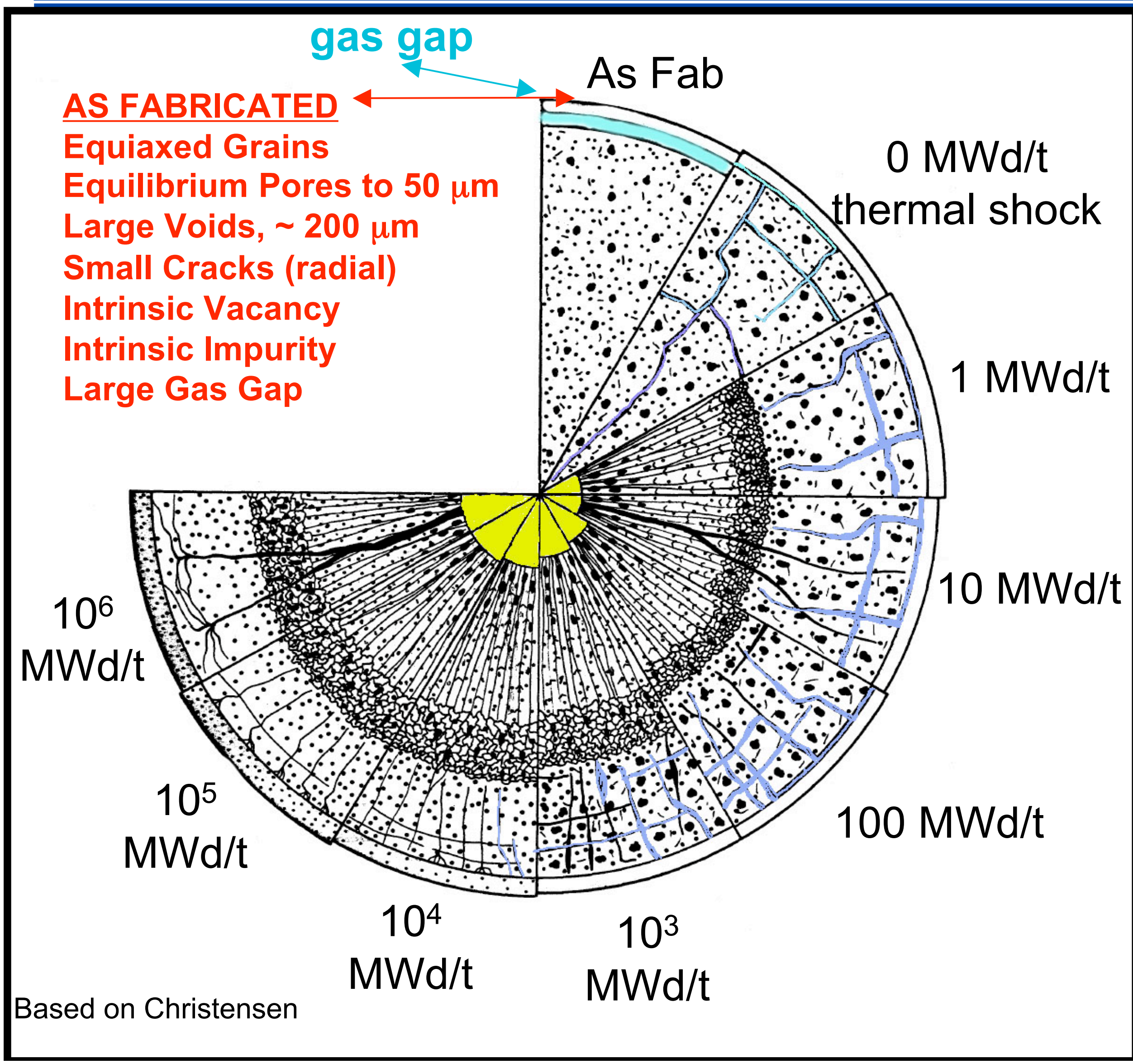
Basic Nuclear Physics
Some Consequences of Fission



- **Neutron irradiation damage**
- **Fission Fragment irradiation damage**
  - **heat generation**
  - **local melting**
- **Changing chemistry**
  - **O/M ratio**
  - **phase changes ?**
- **Swelling**
  - **additional atoms**
  - **fission gas production**

Complexity of the problem

Courtesy L. Snead



As Irradiated

Crack Evolution

Radiation Defects
- Vacancy/Interstitial
- Dislocations
- Small Clusters
- Voids (central void)

Columnar Grain Growth

Grain boundary
- Carbide formation

Equiaxed Grain Growth

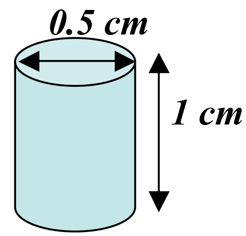
Metallic Inclusion

Solid Solution Impurity

Second Phase Formation

Evolving gas conduction

Fast Reactor Fuel Options

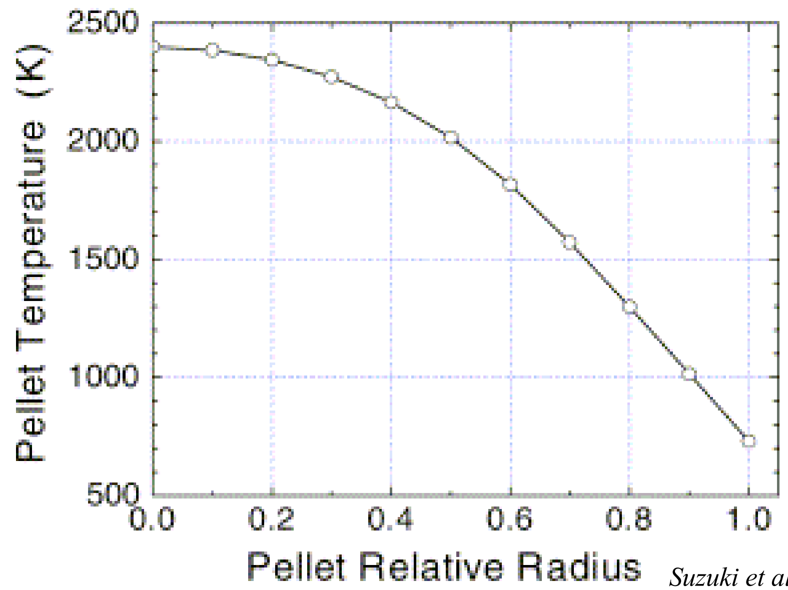


Fast Reactor Fuel Type Fresh Fuel Properties	Metal U-20Pu-10Zr	Oxide UO_2-20PuO_2	Nitride UN-20PuN	Carbide UC-20PuC
Heavy Metal Density, g/cm^3	14.1	9.3	13.1	12.4
Melting Temperature, ºK	1350	3000	3035*	2575
Thermal Conductivity, W/cm-ºK	0.16	0.023	0.26	0.20
Operating Centerline Temperature at 40 kW/m, ºK, and (T/T_{melt})	1060 (0.8)	2360 (0.8)	1000 (0.3)	1030 (0.4)
Fuel-Cladding Solidus, ºK	1000	1675	1400	1390
Thermal Expansion, 1/ºK	17E-6	12E-6	10E-6	12E-6
Heat Capacity, J/gºK	0.17	0.34	0.26	0.26
Reactor Experience, Country	US, UK	RUS, FR, JAP US, UK		IND
Research & Testing, Country	US, JAP, ROK, CHI	RUS, FR, JAP, US, CHI	US, RUS, JAP	IND

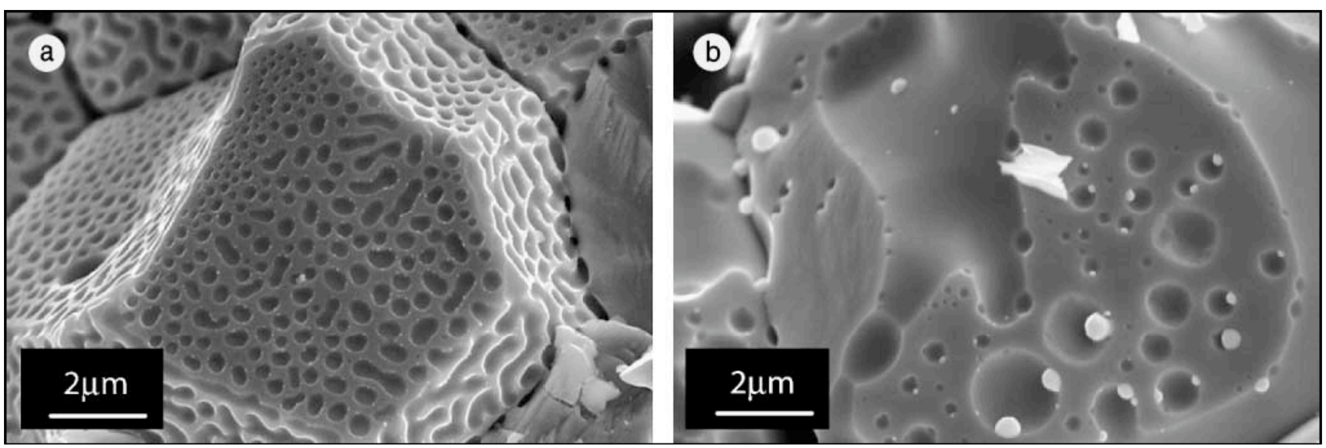
Source: Robert N. Hill and R. A. Wigeland, ANL

LWR Fuel: very little grain growth or other microstructural changes.

LWR fuels
•12 to 15 um grains,10 vol% porosity
•Optimized for FP retention
•Most properties are well behaved
•Very rarely fail

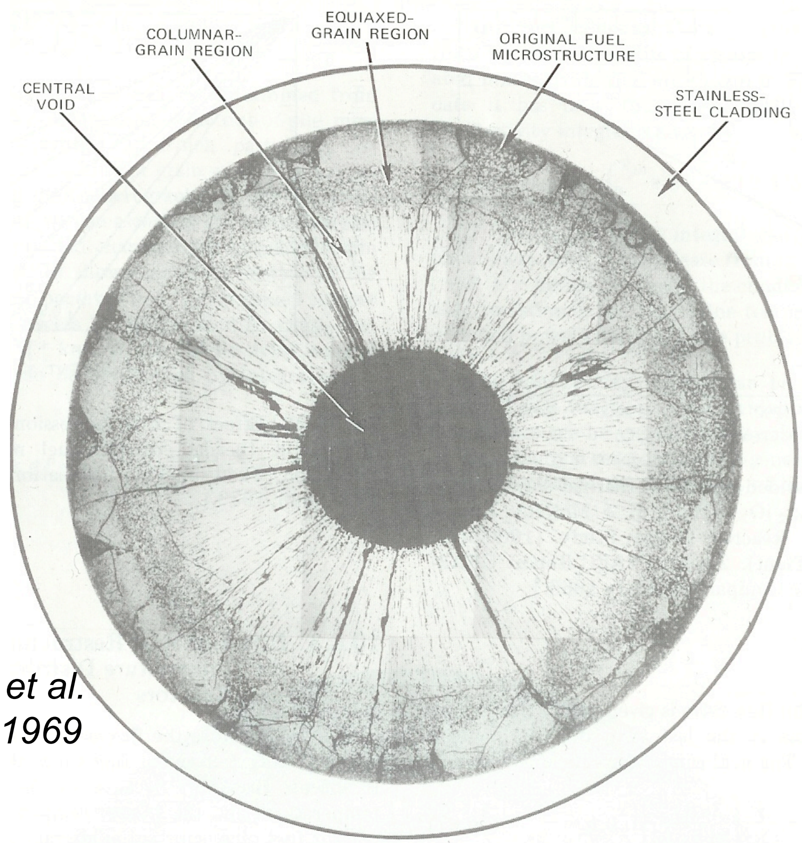


Suzuki et al, NED, 2004

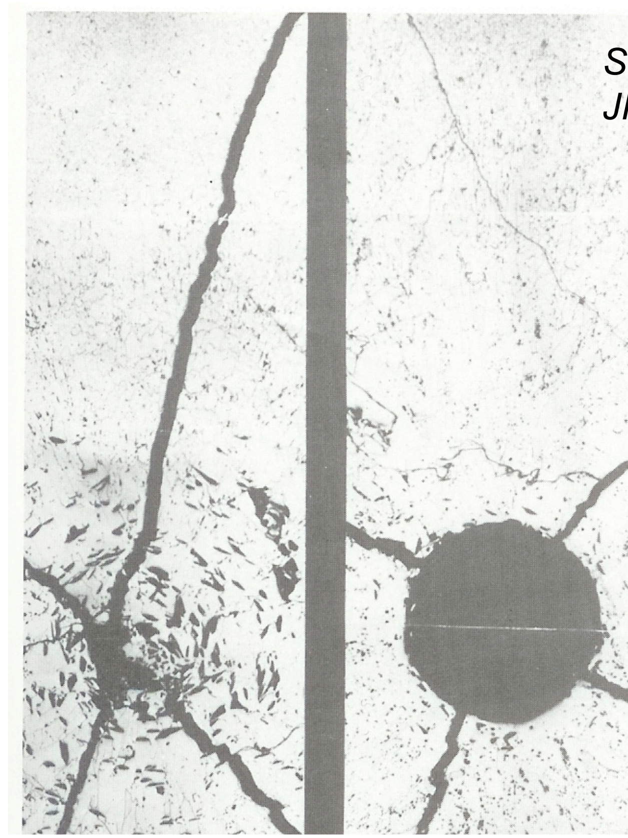


Fisher et al, JNM, 2002

Fast Reactors Oxide Fuels Undergo Microstructural Restructuring during Service

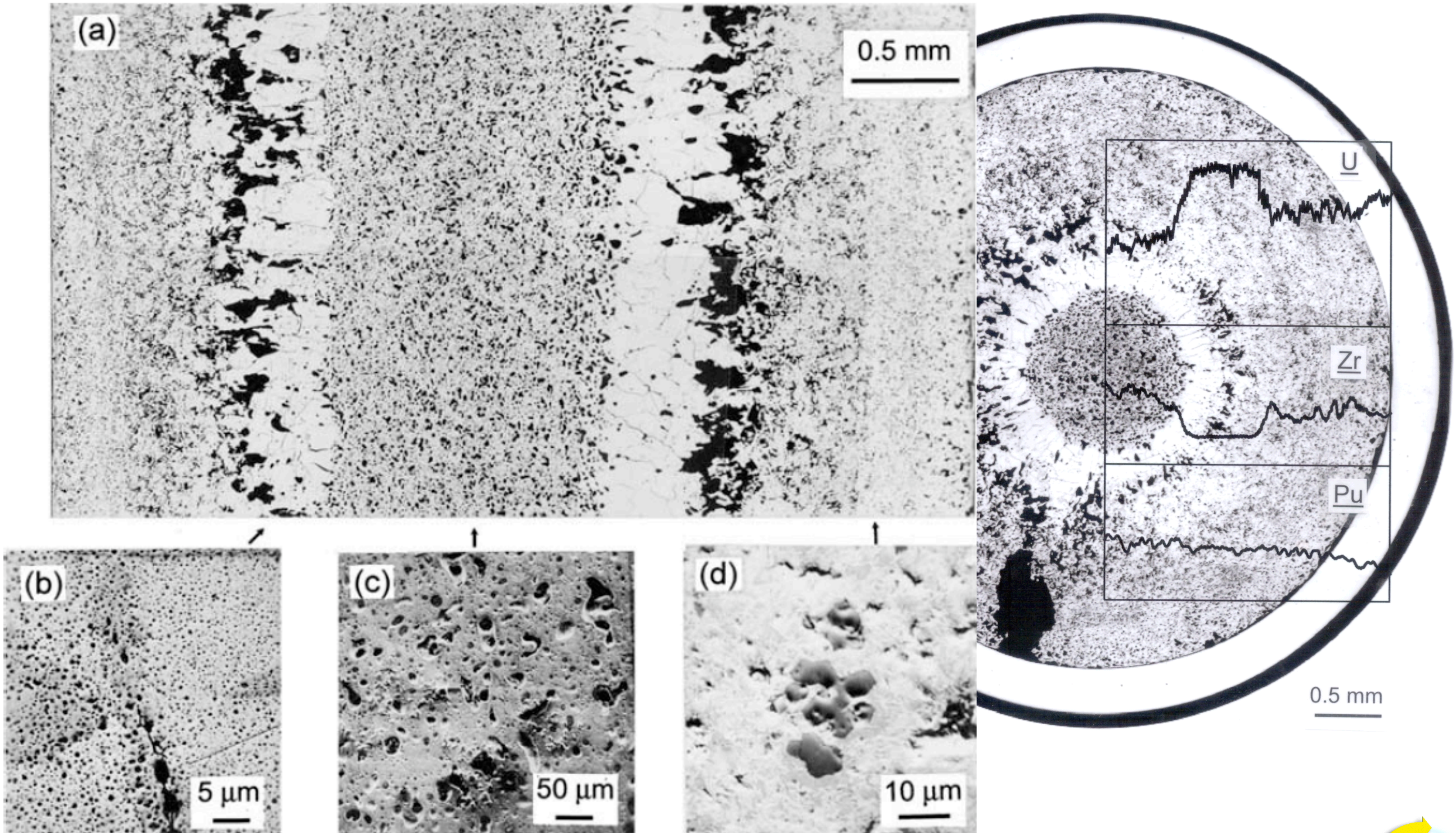


Boyle et al. JNM, 1969



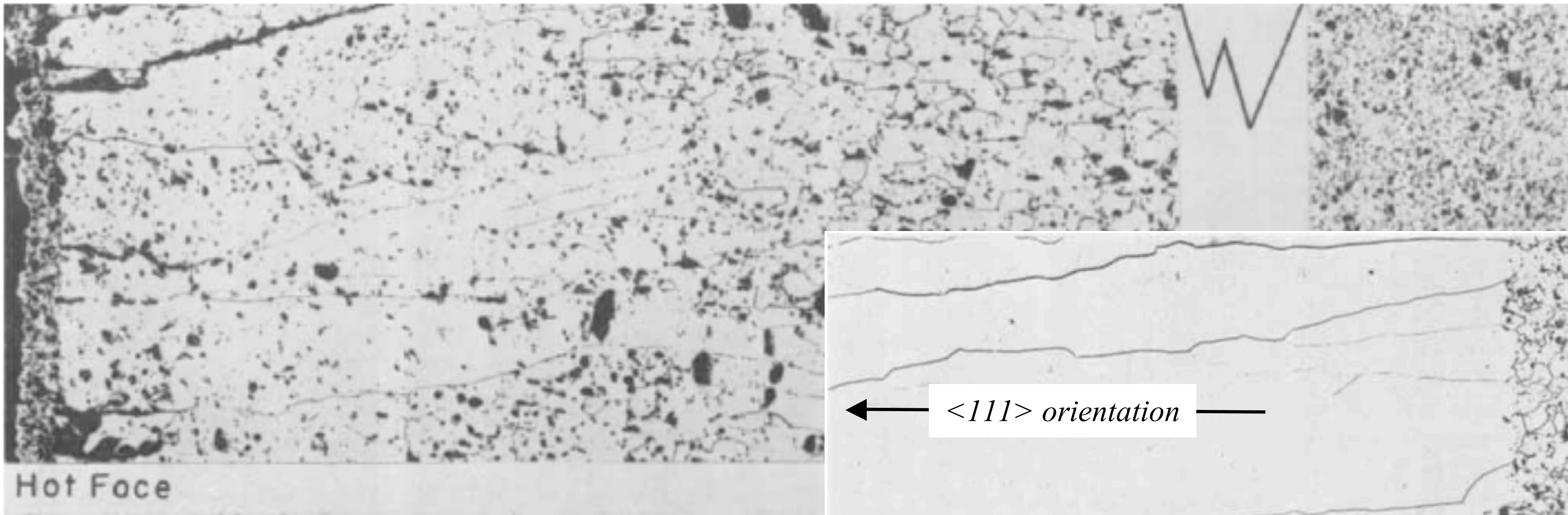
Sens et al. JNM, 1972

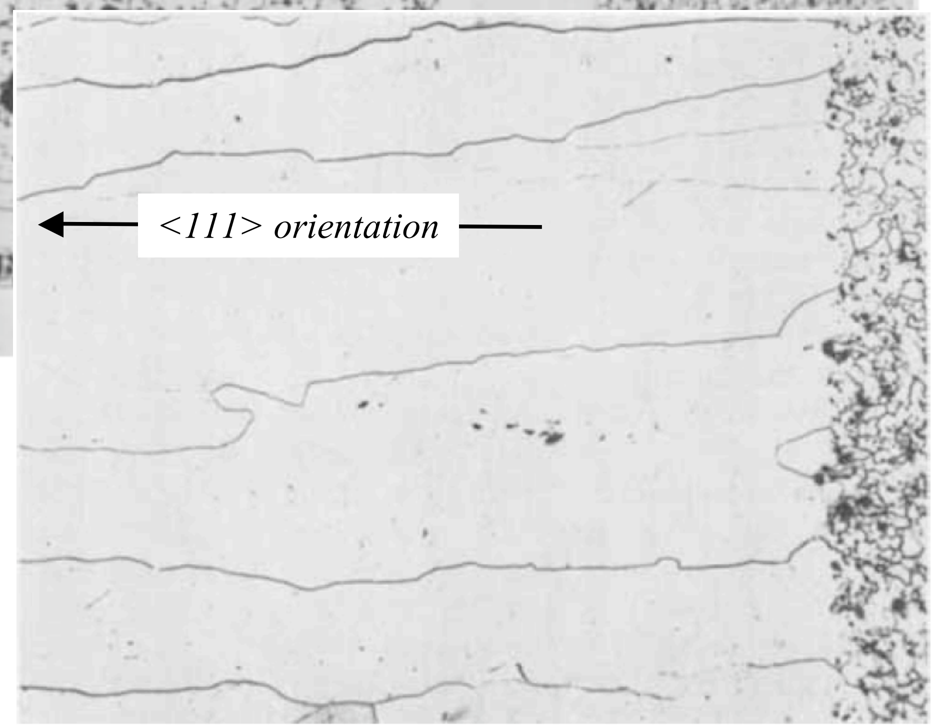
Segragation, grain restructuring and pore migration in U-Pu-Zr fuel.



Ref: Kim, Hofmann, Hayes & Sohn, JNM, 2004

Out-of-pile experiments showing columnar grain growth and axial pore formation in UO_2





Ref: MacEwan and Lawon, JACerS, 1962

Pu redistribution in FBR MOX is a function of O/M ratio.

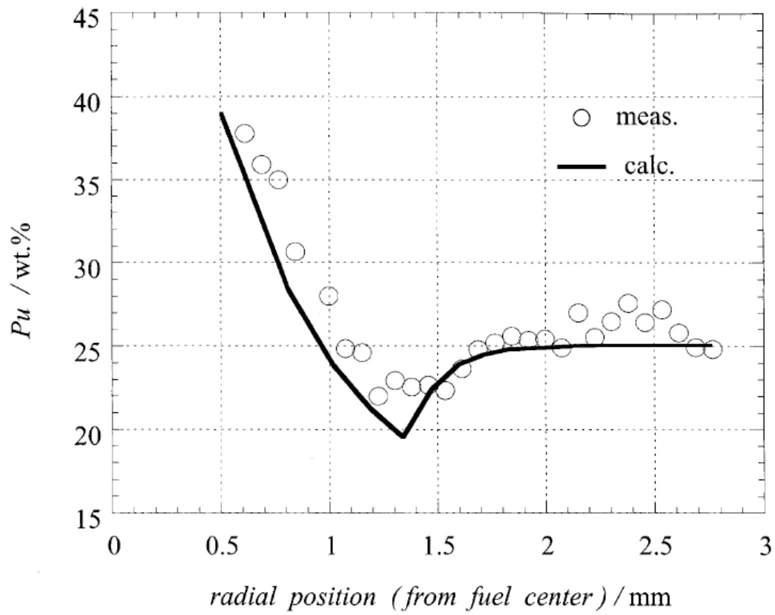


Fig. 3. Radial Pu distribution of XD0992 obtained from PIE (initial O/M = 1.99, initial Pu = 27 wt%).

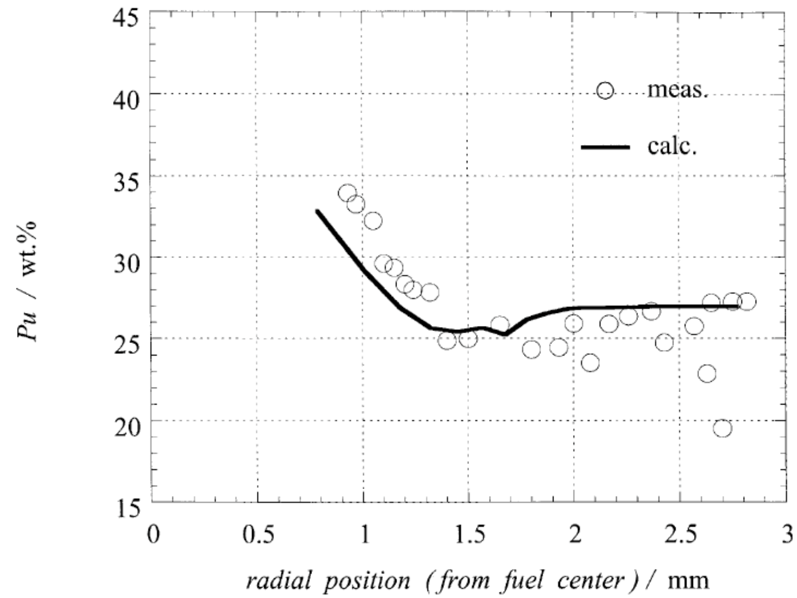
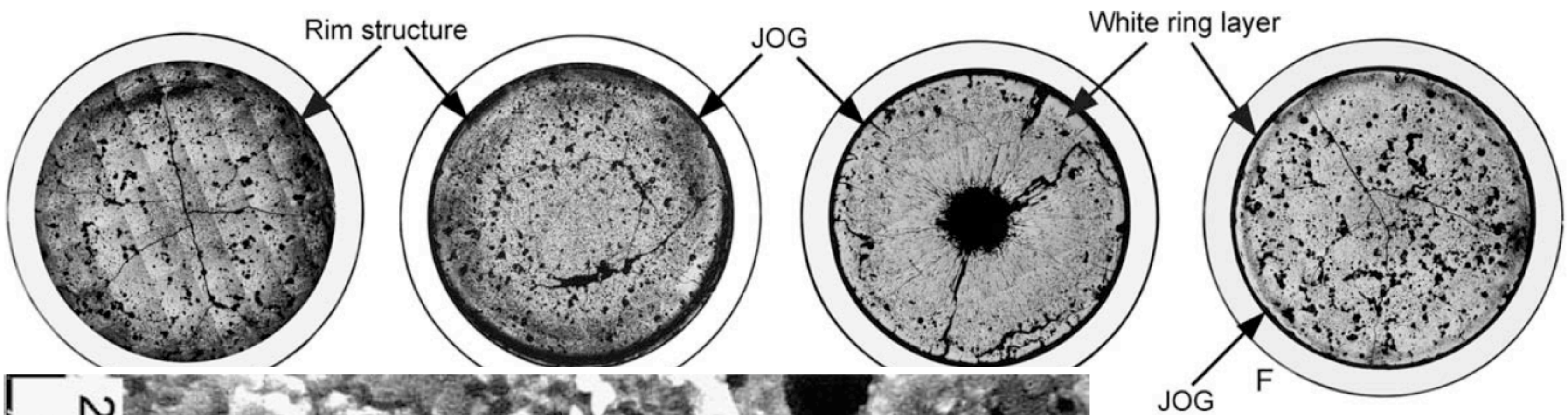
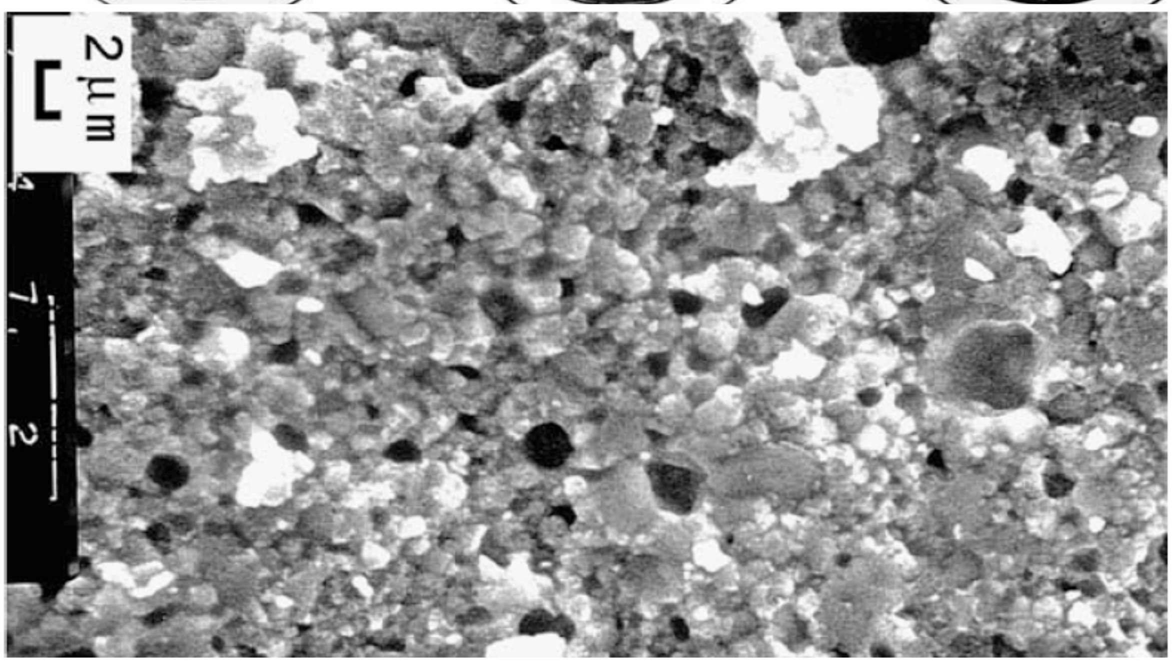


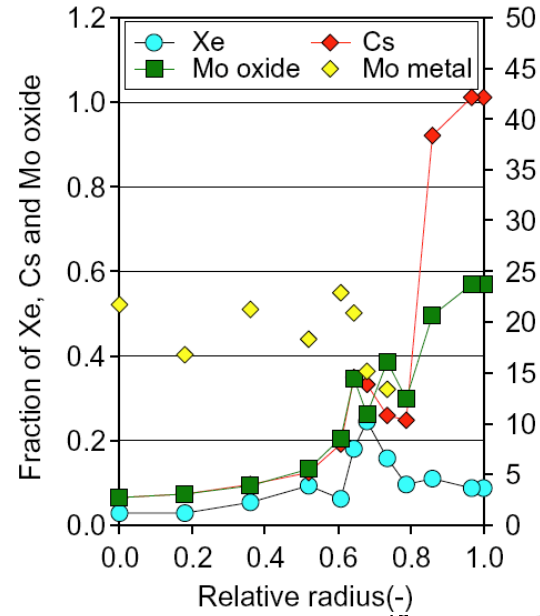
Fig. 4. Radial Pu distribution of XD1071 obtained from PIE (initial O/M = 1.955, initial Pu = 30 wt%).

Ref: Ishii and Asaga, JNM, 2001

In addition to columnar grain & axial pore restructuring, there is rim-structure and FP segregation in FBR MOX







Ref: Maeda, Tanaka, Asaga, Furuya, JNM, 2005

Heat capacity and thermal conductivity are functions of starting composition and burn up

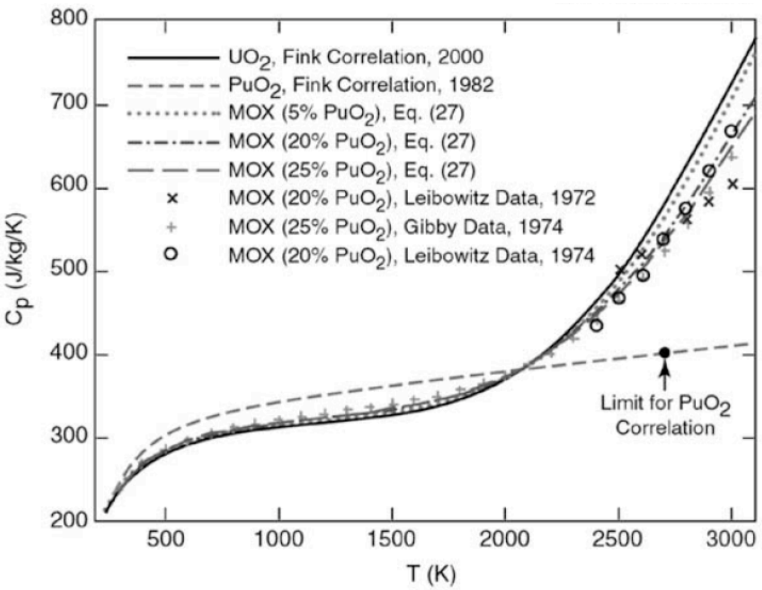


Fig. 8. Comparison of data and correlations for heat capacity of MOX.

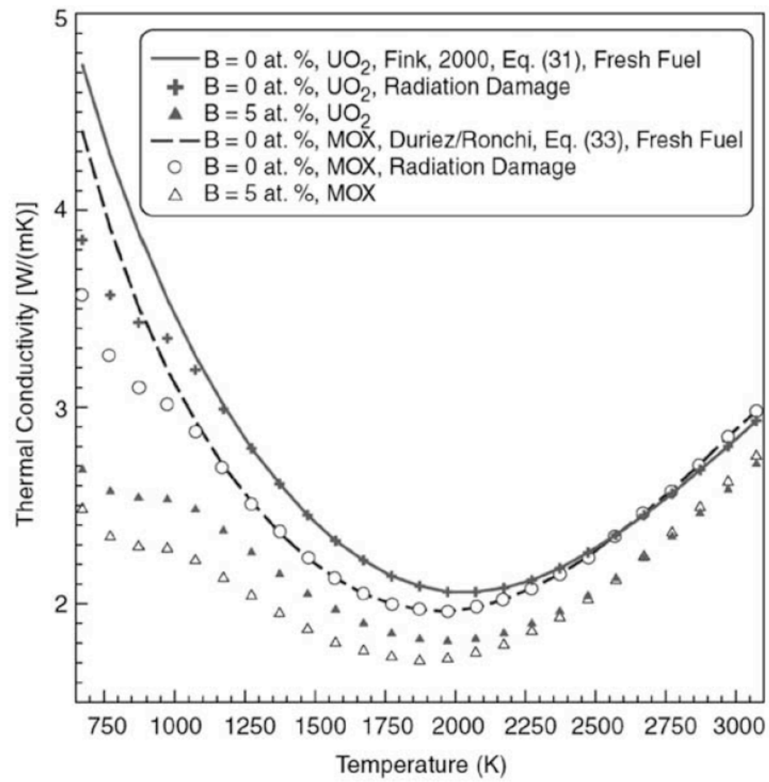
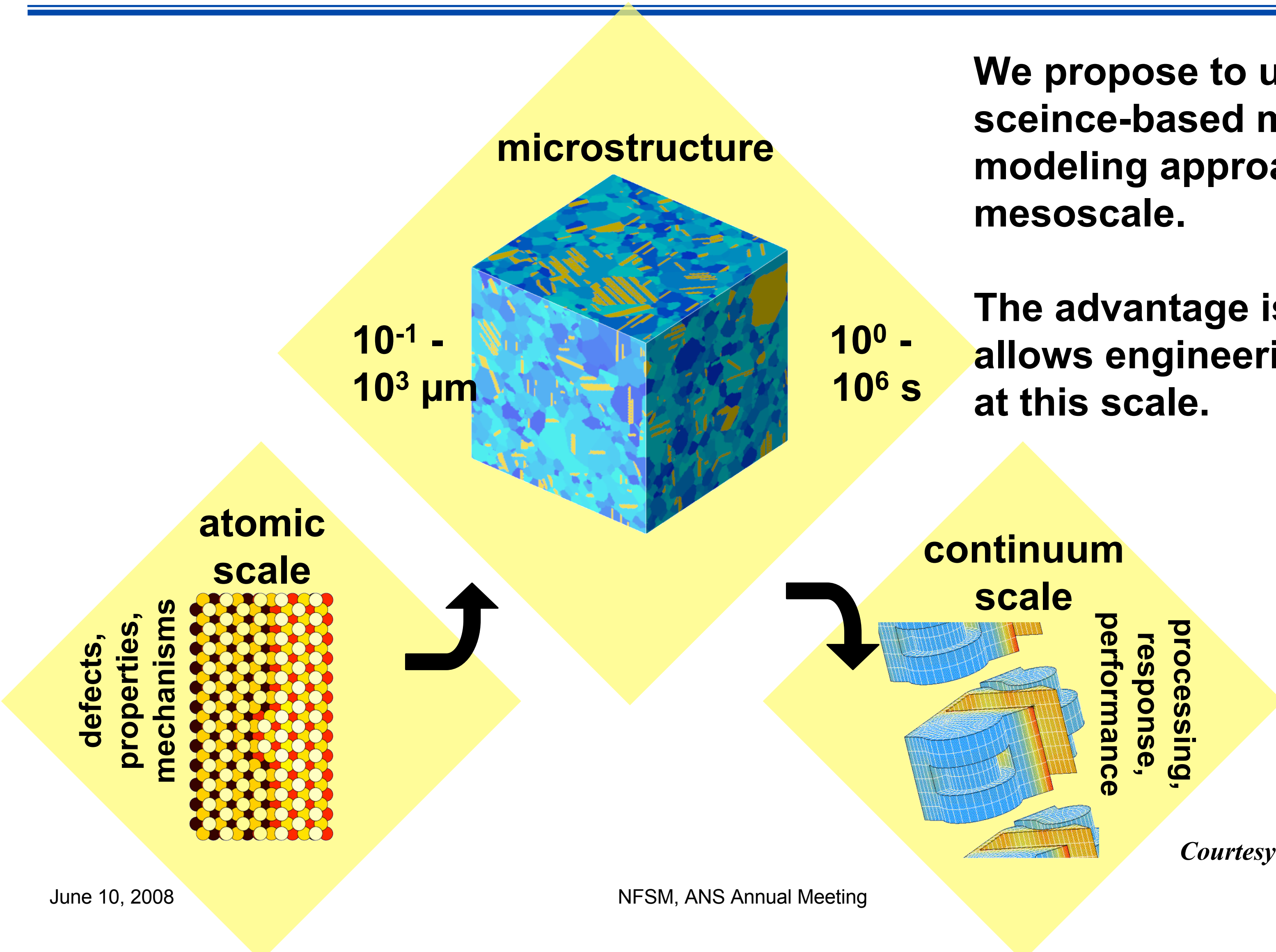


Fig. 13. Effect of radiation damage and burnup, *B*, on the recommended Eqs. (31) and (33) for the thermal conductivity of stoichiometric 95% dense UO_2 and MOX fuels.

Ref: Carbajo, Yoder, Papov and Ivanov, JNM, 2001

Although we describe & understand fuel behavior at mesoscale, we model as continuum at macroscale.



We propose to use a sceince-based materials modeling approach at the mesoscale.

The advantage is that it allows engineering of fuels at this scale.

Courtesy of E.A. Holm

FRAPCON, A LWR Fuels Code

- **FRAPCON iteratively calculates as functions of time and fuel rod specific power**
  - fuel and cladding temperature,
  - rod internal gas pressure,
  - fuel and cladding deformation,
  - release of fission product gases,
  - fuel swelling and densification,
  - cladding thermal expansion and irradiation-induced growth, cladding corrosion, and
  - crud deposition

Bernal et al. NUREG/CR-6534, Vol. 2

Although we describe & understand fuel behavior at mesoscale, we model as continuum at macroscale.

Thermal models in FRAPCON

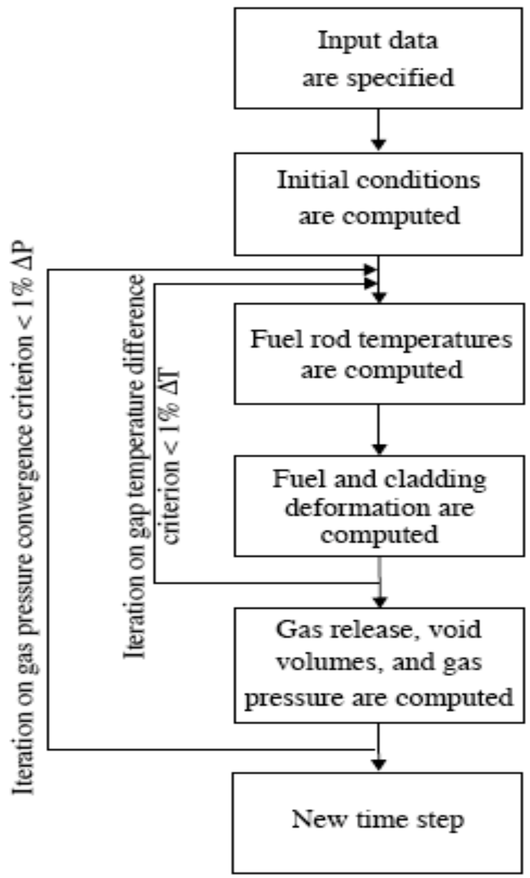


Figure 2.1 Simplified FRAPCON-3 Flow Chart

$$T_b(z) = T_{in} + \int_0^z \left[\frac{4q''(z)}{C_p G D_e}\right] dz$$

Coolant temperature

$$T_W(z) = T_b(z) + \Delta T_f(z) + \Delta T_{cr}(z) + \Delta T_{ox}(z)$$

Clad surface temperature

$$\iint_S k(T,\bar{x})\vec{\nabla}T(\bar{x}) \bullet \hat{n}\,ds = \iiint_V S(\bar{x})\,dV$$

Heat conduction in Fuel pellet

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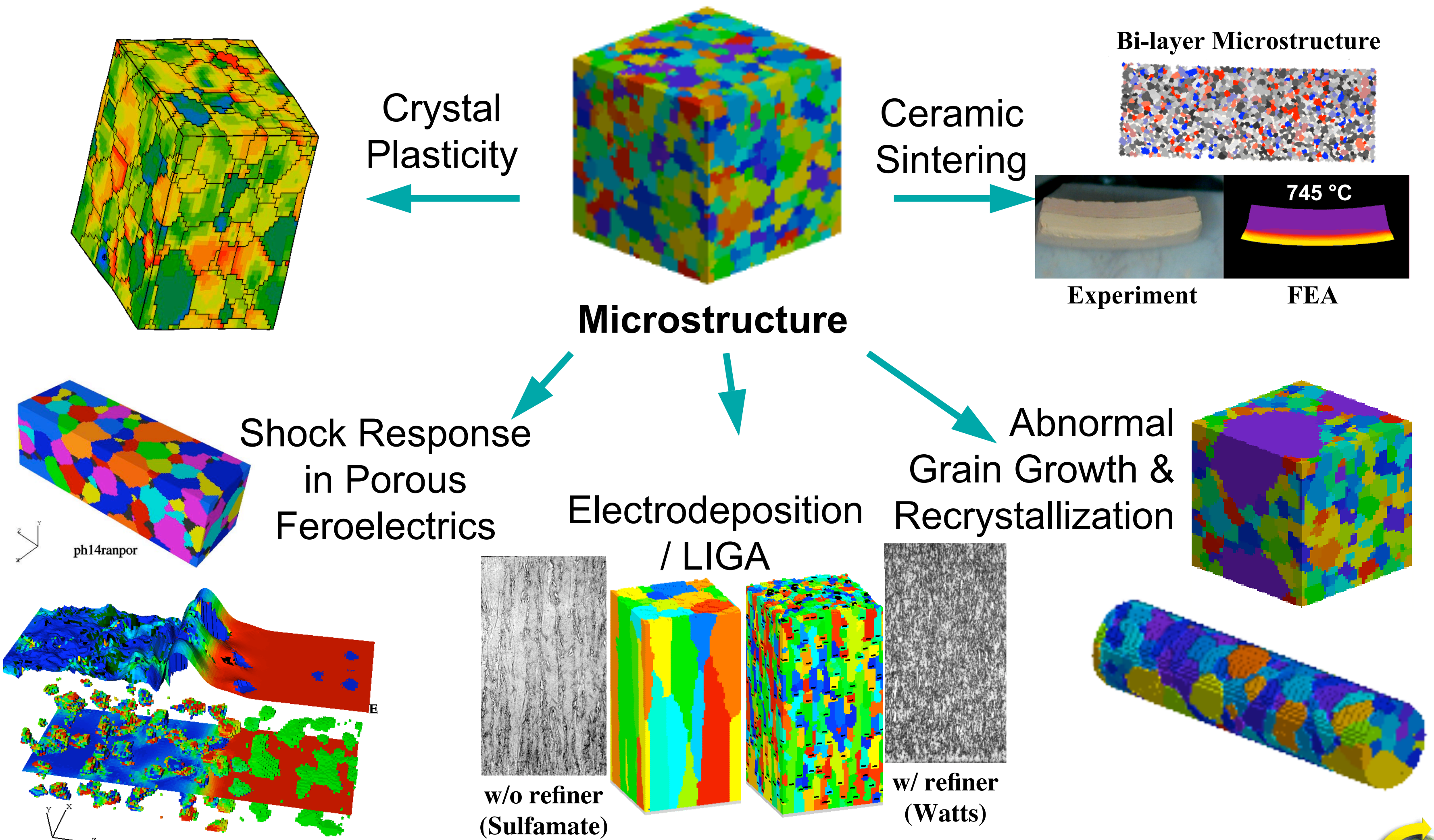
Ref NUREG/CR-6534, Vol. 2

Materials models have been developed to simulate a wide range of microstructural evolution processes.



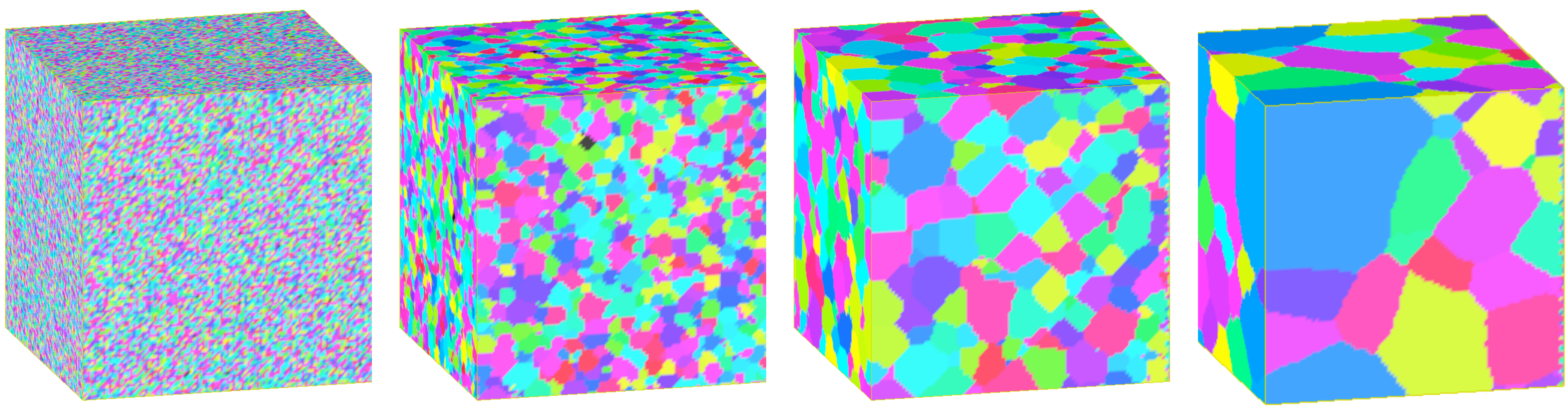
Grain growth in a thermal gradient

Thermal gradient is simulated by changing the mobility of the grain boundaries as a function of temperature.

$$P = M(T)\exp\left(\frac{-\Delta E}{k_B T_s}\right) \quad \Delta E>0$$

$$P = M(T) \quad \Delta E\leq 0$$

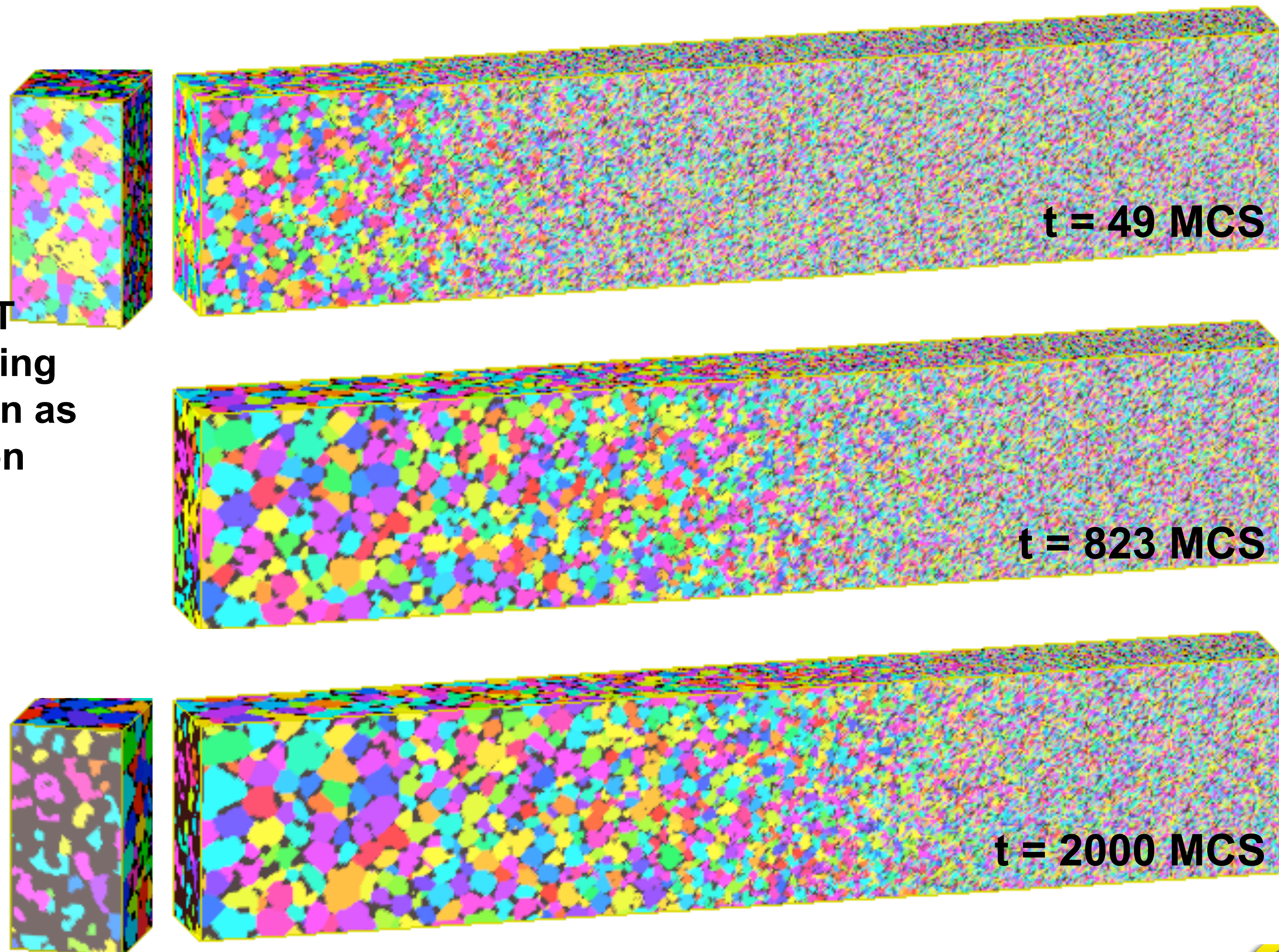
$$M = M_o \exp\left(\frac{-Q}{k_B T}\right)$$



In a thermal gradient, grain growth scales linearly with the mobility; kinetics and grain size distributions are locally normal.

Grain growth & bubble migration in a thermal gradient

- Start with random distribution of grains and pores.
- Applied linear T gradient assuming surface diffusion as bubble migration mechanism.
- Grains & pores coarsened more in the high temp. region with net pore migration to hot region.



Thermal conduction

Basic phonon scattering model :

$$K(T) = \frac{1}{3}\int S(\omega)v^2(\omega)\tau(\omega)d\omega,$$

$S(\omega)$ is the specific heat, $v(\omega)$ is the phonon velocity, $\tau(\omega)$ is the phonon relaxation time.

If more than one process is scattering phonons

$$\frac{1}{\tau(\omega)} = \sum_i \frac{1}{\tau_i(\omega)}.$$

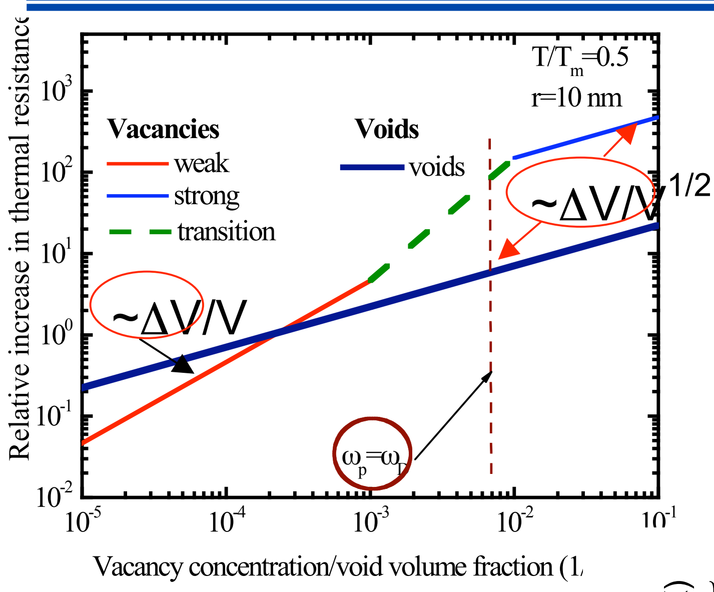
$$\frac{1}{\tau_i} = \frac{\Gamma_i \Omega}{4\pi v^3}\omega^4,$$ **Impurities**

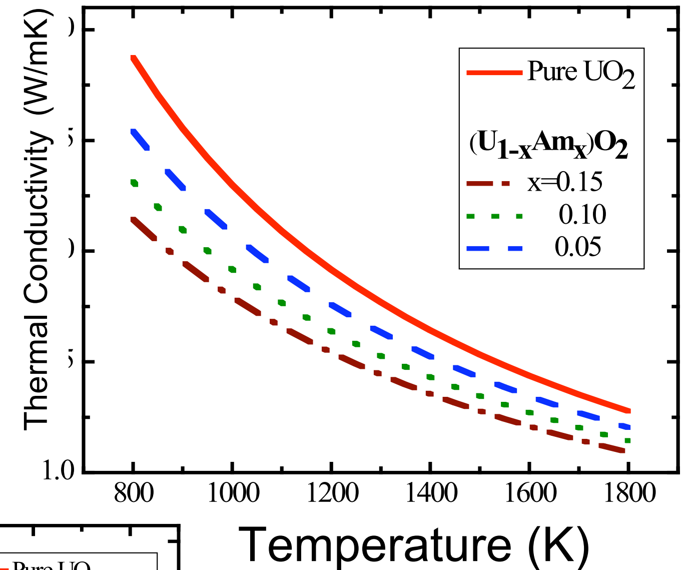
$$\frac{1}{\tau_v} = \frac{9C_v \Omega}{4\pi v^3}\omega^4,$$ **Vacancies**

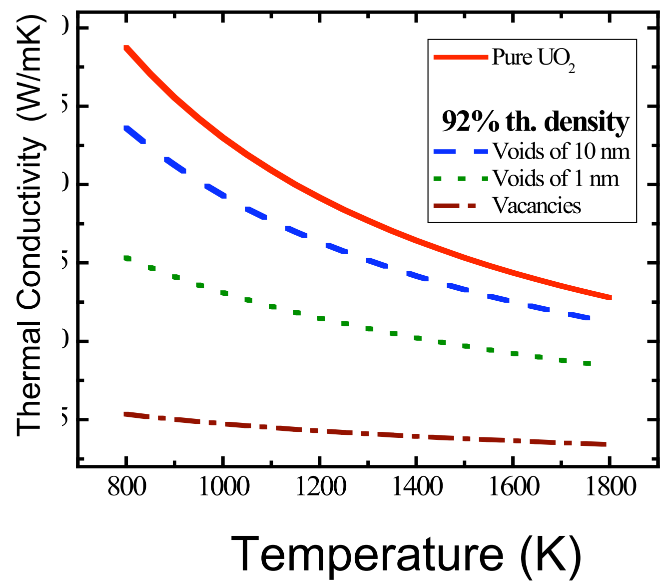
$$\frac{1}{\tau_{void}} = \pi r^2 N v.$$ **Voids / precipitates**

Work of L. Snead

Thermal conductivity for various fuel states







Work of L. Snead

Conclusions

- **We propose that the new generation of fuels performance and fabrication codes be**
  - Science-based
  - Materials models integrated at the microstructural mesoscale
  - Provide chemical composition, microstructure and other physics-based state variables as a function of irradiation history.
- **Such a capability will fundamentally improve our ability to design and license advanced fuels**
  - Fuels can be engineered at the microstructural scale
  - The number of experiments for design and qualification will be greatly reduced
  - Better, more robust fuels can be engineered