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Characterization and Basic Understanding of Radiation Damage
Mechanisms in Materials**

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Dimensional Changes and Pellet-Clad Interaction

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Joint ICTP-IAEA Workshop on

*The Training in Basic Radiation Materials Science and its
Application to Radiation Effects Studies and Development of
Advanced Radiation-Resistant Materials*

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Overview

- Fuel and clad mechanics
 - stresses and strains
 - contact forces and interactions
- fuel size changes
 - thermal expansion
 - densification
 - swelling
- Cladding creep
- Considerations for modelling
 - 1D/2D/3D



Introduction

- A purpose of fuel behaviour modelling is to predict mechanical loads in normal operation and transients
 - does the fuel rod fail?
- Stresses and strains are responsible for failure and occur because of
 - temperature gradients in the materials
 - different thermal expansion of fuel and cladding in contact with each other
 - irradiation induced geometry changes
 - clad creep-down, creep-out, growth
 - fuel densification and swelling
- Modelling in 1/1.5 D and 2/3 D (FEM)



Fuel & Clad Mechanics

- Practical approaches to “Fuel & Clad Mechanics” are governed by
 - complexity of the problem
 - many highly non-linear phenomena
 - complicated fuel-clad mechanical interaction
 - need for discretisation
 - incomplete knowledge on the state of the fuel
 - computer power limitations
- Whole rod usually treated in 1.5D
- Early attempts to apply FE techniques
 - limited to a few pellets (FEMAXI 1976)



Some equations for stresses and strains

1/1.5D fuel modelling codes typically employ an axi-symmetric “plain strain” formulation. It is better fulfilled for the cladding than the fuel.

- equilibrium condition

$$\frac{\partial \sigma_r}{\partial r} + \frac{\sigma_r - \sigma_t}{r} = 0$$
- compatibility condition

$$\frac{\partial \sigma_z}{\partial z} = 0$$
- compatibility condition

$$\varepsilon_r = \frac{\partial u}{\partial r} \quad \varepsilon_t = \frac{u}{r}$$
- compatibility condition

$$\varepsilon_z = \frac{\partial w}{\partial z} = C \quad (\text{plain strain})$$
- materials law (generalised Hooke's law)

$$\begin{pmatrix} \varepsilon_r \\ \varepsilon_t \\ \varepsilon_z \end{pmatrix} = \frac{1}{E} \begin{pmatrix} 1 & -\nu & -\nu \\ -\nu & 1 & -\nu \\ -\nu & -\nu & 1 \end{pmatrix} \cdot \begin{pmatrix} \sigma_r \\ \sigma_t \\ \sigma_z \end{pmatrix} + \begin{pmatrix} \varepsilon^i + \varepsilon_r^{cr} + \varepsilon_r^{pl} \\ \varepsilon^i + \varepsilon_t^{cr} + \varepsilon_t^{pl} \\ \varepsilon^i + \varepsilon_z^{cr} + \varepsilon_z^{pl} \end{pmatrix}$$



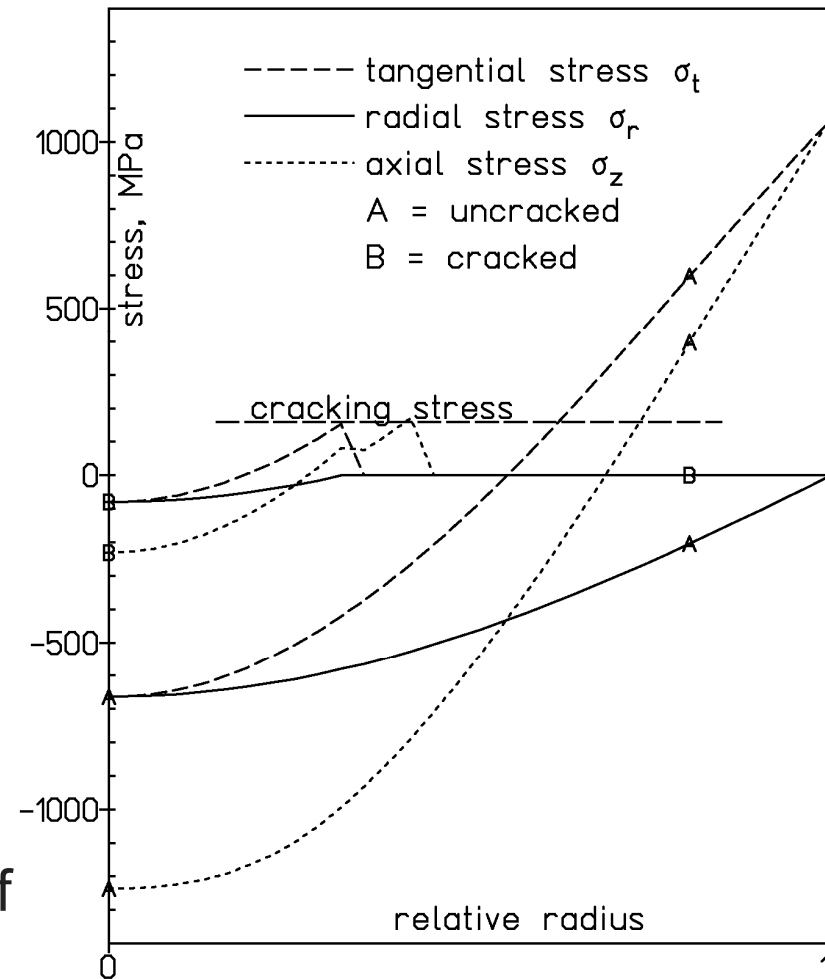
Symbols used

- r, t, z – directions (radial, circumferential, axial)
- σ - stress
- ε - strain
- ν - Poisson's number
- u - radial displacement
- w - axial displacement
- cr - creep
- pl - plastic
- i - isotropic ($\varepsilon^i = \varepsilon_{\text{thermal}} + \varepsilon_{\text{swelling}} + \varepsilon_{\text{densification}}$)



Fuel stresses → cracking

- Ceramic fuels crack easily due to the strong stresses caused by the (radial) temperature gradient
- The stress-strain equations are kept approximately valid by
 - introducing crack strains (e.g. Transuranus)
 - setting stresses to zero (e.g. Frapcon)
- If the fuel is cracked both radially and axially, the fuel displacement u is essentially free thermal expansion plus the contributions of swelling and densification



Contact situations

axially \ radially		sticking (contact)		sliding
		“open” gap pressure Δp	closed gap displacement Δu	
sticking	strain $\Delta \epsilon$		hard contact	
	displacement Δw	axially locked		
sliding		(no contact)		random stacking

- Many fuel modelling codes simplify by assuming either **no contact** (open fuel-clad gap) or **hard contact** (closed gap)
- Stress concentration in the cladding opposite of fuel cracks is not included in this matrix



Modelling Considerations (I)

- The pellet configuration is quickly affected by pellet cracking and fuel fragment relocation (see also lecture on temperature calculations)
- This should make the calculation of interaction(s) even more complicated, but on the other hand ...
- ... to calculate the slope of a pile of sand (or coal or boulders or ...) with some accuracy, we do not have to calculate and determine the interaction between all grains
 - Despite the differences, a single model describes the situation
- Can cracked fuel pellets within the cladding be treated like a pile of sand?



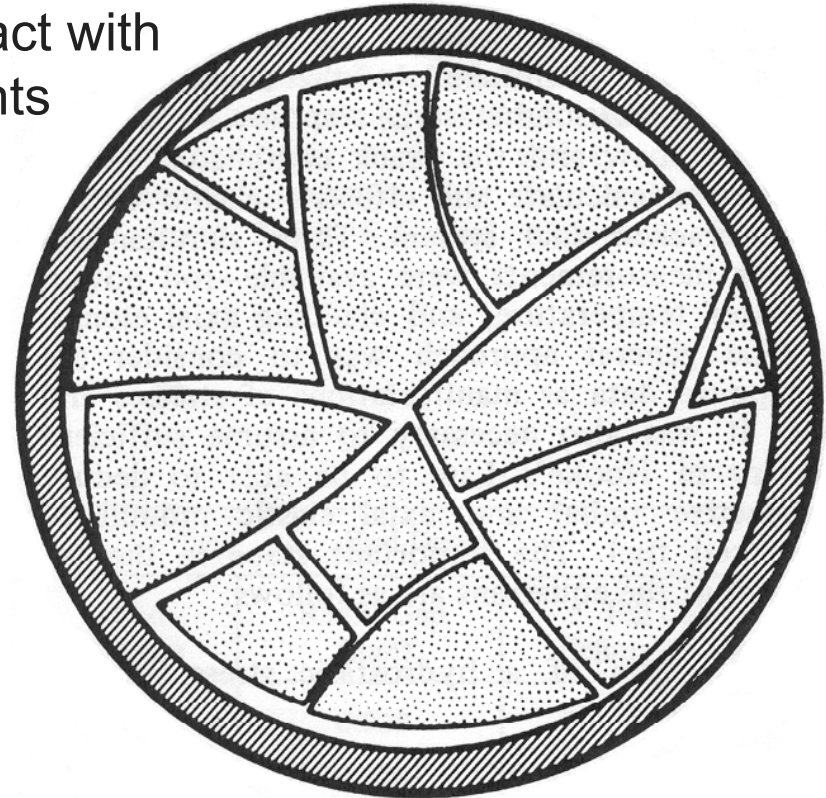
Modelling Considerations (II)

- Williford et al. proposed a crack compliance model
- Fuel and cladding are always in contact with each other, as observed in experiments
- The surfaces with roughness d interact with each other via contact stresses σ

$$\frac{1}{2} \operatorname{erfc}\left(\frac{d}{R\sqrt{2}}\right) = \frac{\sigma}{\sigma + H}$$

d = crack width, R = roughness,
 H = Meyer hardness

- The model allows a unified treatment of thermal and mechanical behaviour
- Suitable for the high burnup situation with bonded fuel



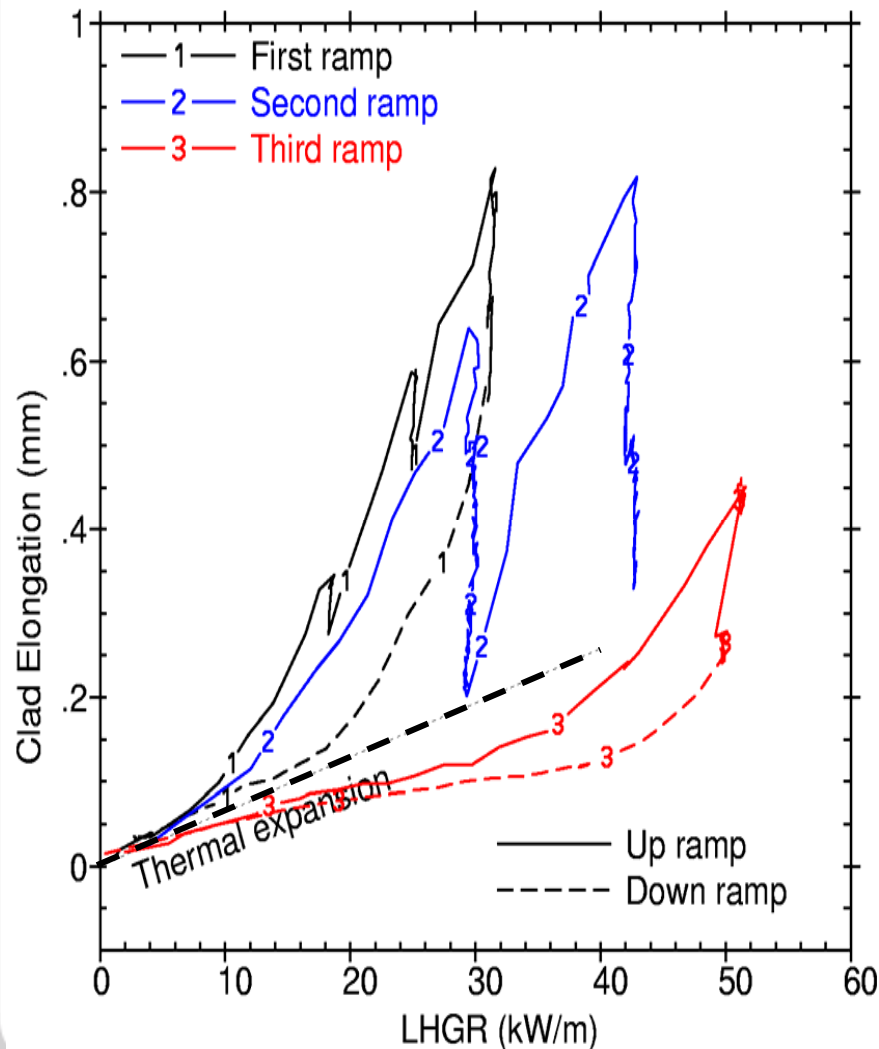
PCMI in practice

- experimental observations -

- Onset of interaction – fresh fuel
- Random stacking
- Development of onset of interaction with burnup
- Axial ratcheting
- PCMI at high burnup, bonded fuel



PCMI: Onset of interaction – fresh fuel



The experimental observations are difficult to reconcile with predictions of models assuming a concentric arrangement of fuel and cladding and a dividing gap:

- First power ramp: very early onset of interaction
- Following power ramps: shift of PCMI onset to higher power
- Relaxation of axial strain during power holds (sliding, densification, creep)
- Continuation of elongation when power increases (strong contact)

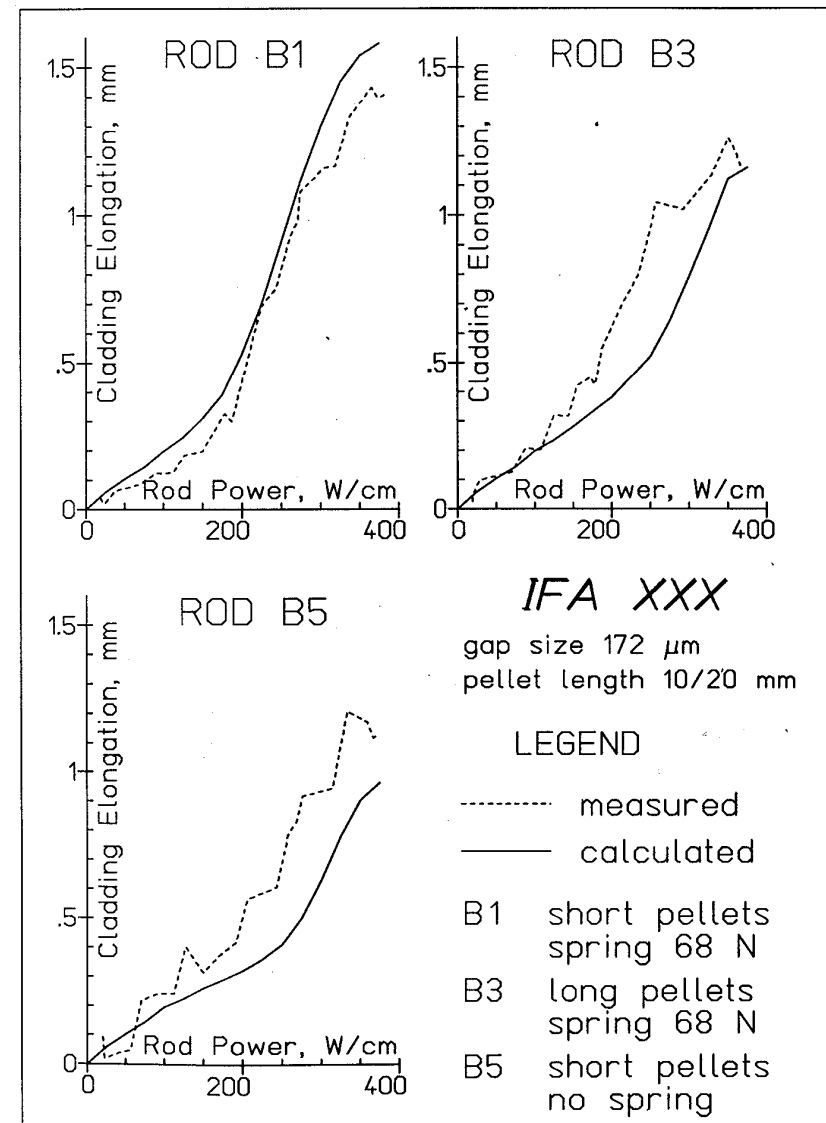


Random stacking

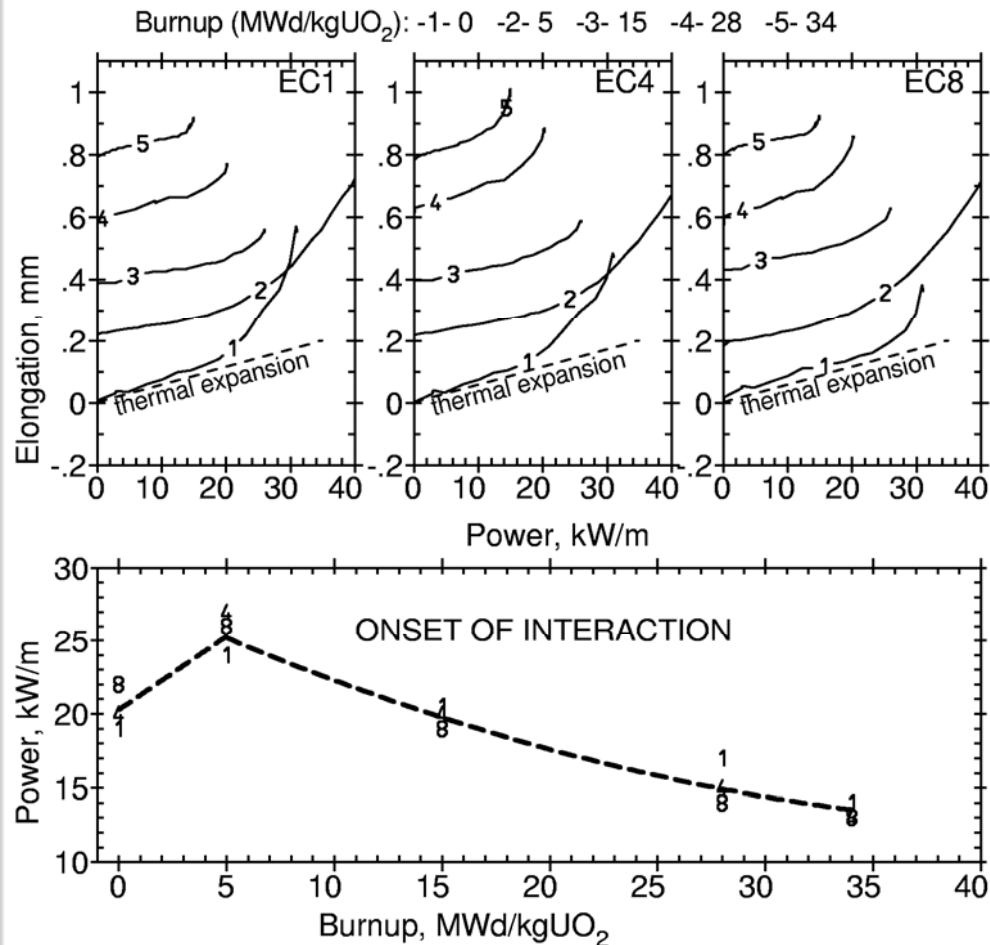
The fuel stack has no stability in itself. Pellets are eccentrically located, and some touch the cladding at one side. This “random stacking” causes PCMI from the beginning, even if the pellet-clad gap is nominally open.

Interaction due to random stacking depends on

- Pellet length (L/D) → shorter pellets means more friction interfaces
- Hold-down spring force → stronger friction force against alignment
- Stack length → longer fuel columns are less randomly stacked which means weaker interaction



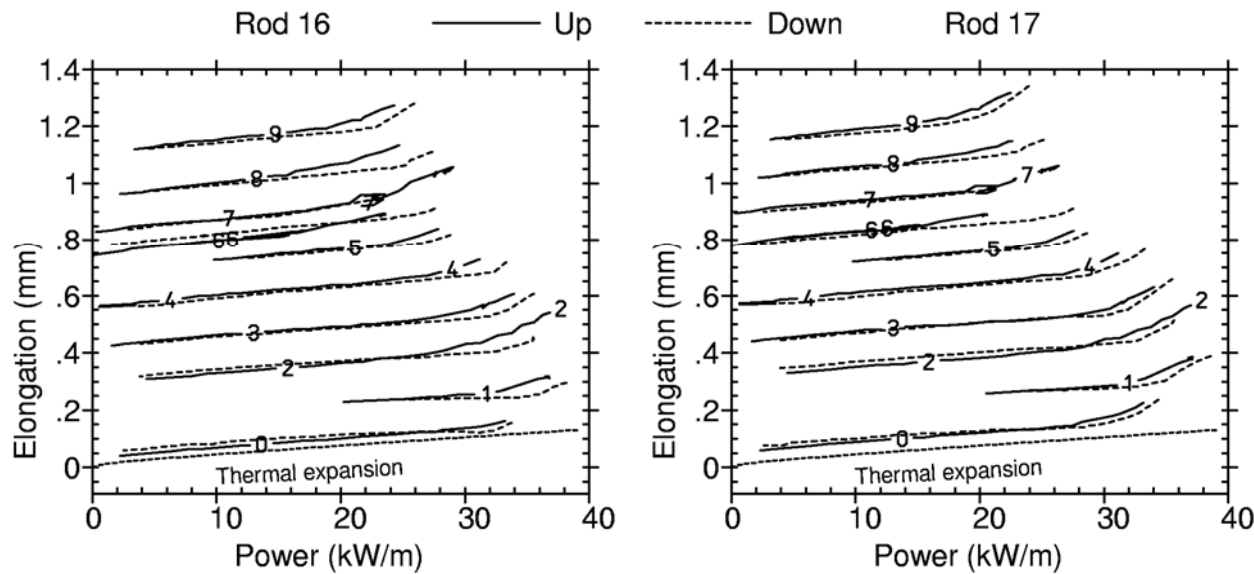
PCMI: Development of onset of interaction Fuel-clad accommodation



- The onset of interaction moves to lower power with increasing burnup and decreasing power
- The accommodation of fuel and cladding to each other result in small 'interaction tails' as long as power does not exceed previously reached levels.
- Consequences for conditioning/deconditioning of fuel, e.g. after stretch-out

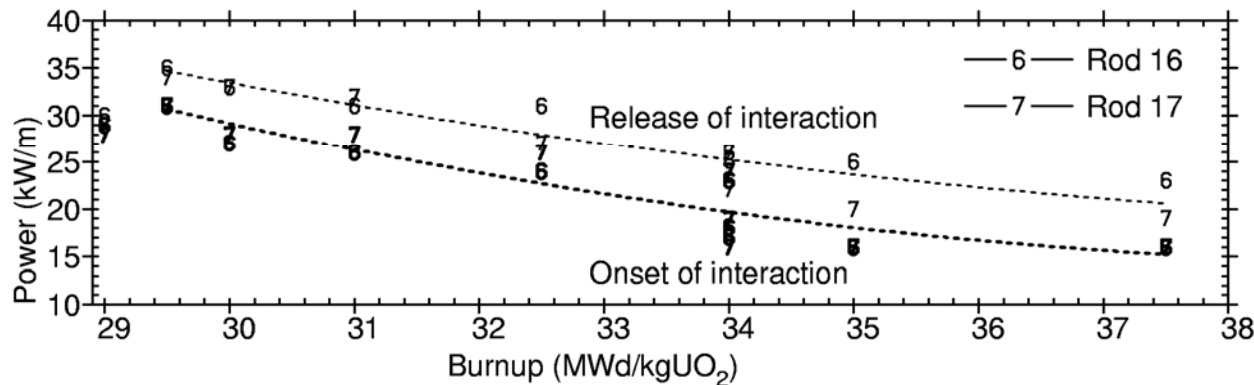


PCMI: Axial ratcheting



Burnup
MWd/kgUO₂

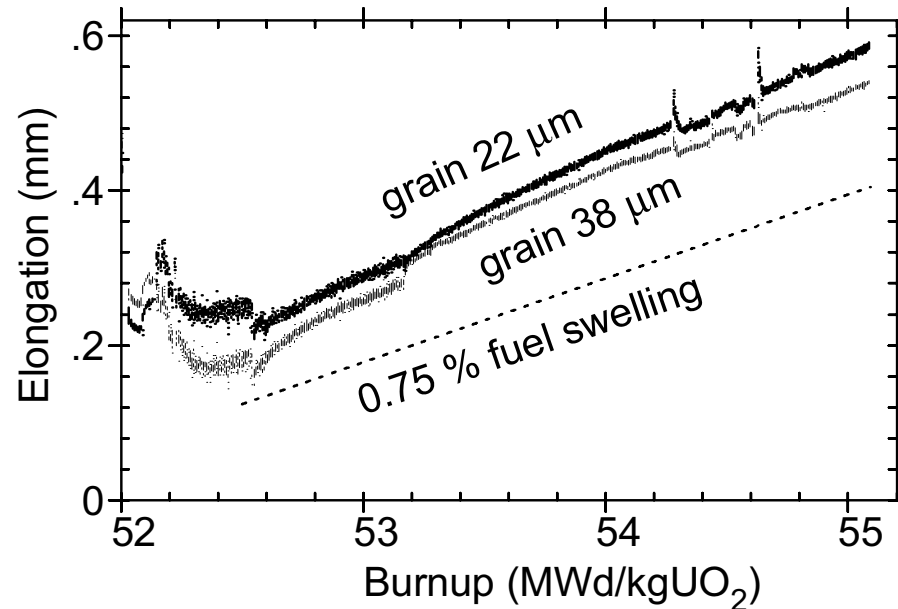
-0- 29.0
-1- 29.5
-2- 30.0
-3- 31.0
-4- 32.5
-5- 34.0
-6- 34.0
-7- 34.0
-8- 35.0
-9- 37.5



The slight mismatch between release and onset of interaction causes axial ratcheting and elongation peaks



PCMI: high burnup behaviour



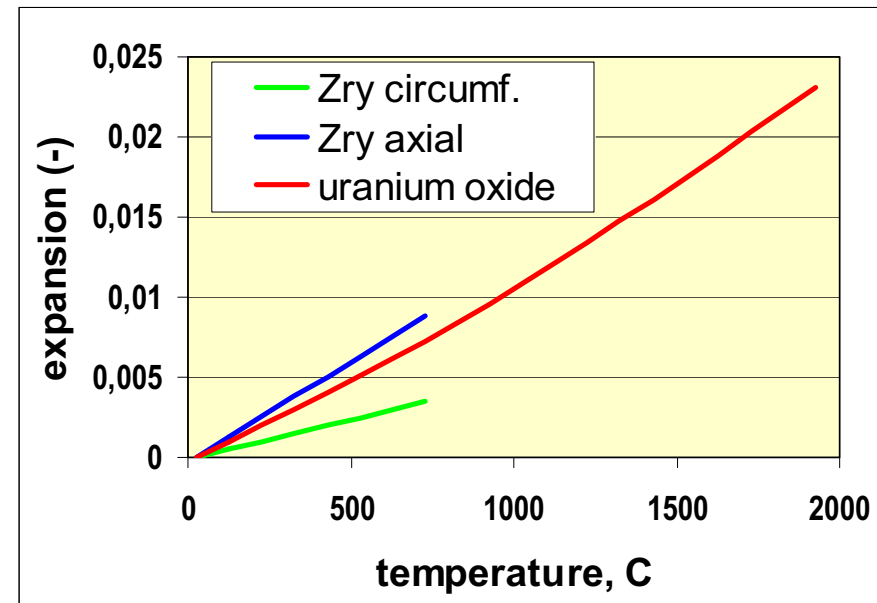
Cladding elongation response of re-instrumented PWR fuels (61 MWd/kgU) with different grain sizes during steady state periods.

- **Permanent elongation**
Clad elongation increase reflects fuel swelling
- **Ratcheting**
Elongation peaks associated with shut-down / start-up (release/onset mismatch)
- **Relaxation**
Initial relaxation of high power elongation. Stress caused by ratcheting is relaxed by fuel creep within a few days

Thermal expansion

(equations see temperature lecture)

- Thermal expansion occurs instantaneously and is the main cause of PCMI in
 - semi-rapid power changes, e.g. control rod withdrawal and reactor start-up
 - very rapid power changes, e.g. reactivity insertion accidents
- Uranium oxide expands more than Zircaloy (circumferentially)
- The fuel gets much hotter than the cladding
- → PCMI due to thermal expansion



Fuel densification

- UO_2 pellets are produced by pressing of powder and sintering at high temperature (1600–1700 °C)
- The fuel pellets have a small amount of porosity (3 - 5%) after the sintering
- Some of the porosity is removed as a result of irradiation, leading to densification of the fuel
- This has led to problems in the “early days”, but is well under control in today’s routine fuel fabrication
- Most research on densification from about 1970 - 1985
 - H. Assmann, H. Stehle; Thermal and in-reactor densification of UO_2 : mechanisms and experimental results; NEaD 48 (1978)
- Densification affects the gap size and thus the fuel temperature



Densification model

- UO₂ in-reactor densification and thermally activated sintering depend on:

- burnup
- density
- pore size distribution
- grain size
- temperature
- O/U-ratio

$$\frac{\Delta V}{V} = -p_{0,0}(1 - e^{-a \cdot B}) - \sum_i p_{0,i} \left(1 - \left(1 - \frac{b \cdot B}{d_i}\right)^3\right)$$

$p_{0,0}$ = init. fine porosity fraction, diam. < 0.1 μm

$p_{0,i}$ = init. coarse porosity fract. i , diam. > 0.1 μm

d_i = diameter of coarse porosity class i ($d > 0.1$)

B = burnup; a, b = constants

- According to theory, mechanisms controlled by temperature are effective only for $T > 1300^\circ\text{C}$



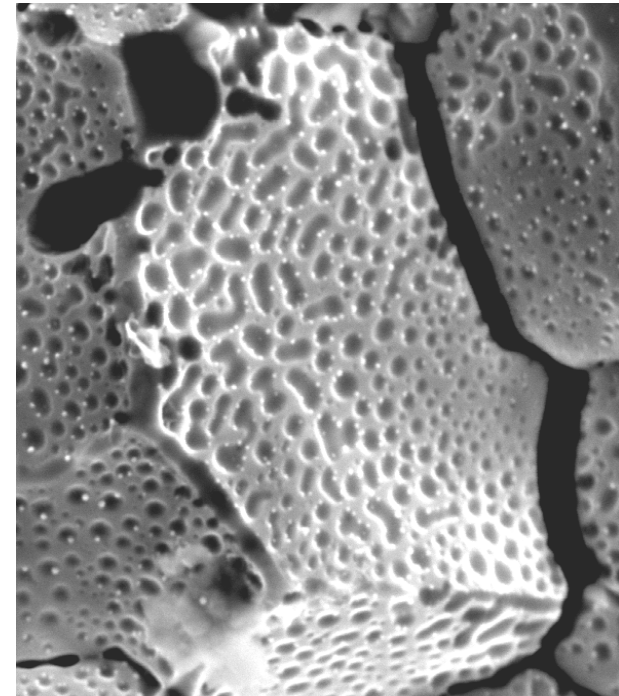
Fuel swelling

- Swelling is due to the inclusion of solid fission products in the matrix and accumulation of fission gas in pores (effective at high T)
- theoretically, the solid fission product swelling rate is
 - 0.13% $\Delta V/V$ per 10^{26} fissions/ m^3 (0.037% per MWd/kg) if the fuel completely utilized the vacancies created during irradiation
 - 0.54% $\Delta V/V$ per 10^{26} fissions/ m^3 (0.153% per MWd/kg) if none of the vacancies are used
- Swelling measured in-core is often between these values in the range 0.5-1.0%/MWd/kg and includes the effect of gaseous fission products (Xe, Kr)



Gaseous fuel swelling

- The fission products xenon and krypton (noble gases) are virtually insoluble in the UO_2 fuel matrix
- By diffusion, they accumulate in inter- and intra-granular bubbles
- Gas atoms in bubbles occupy more space than the atoms they originated from
- Consequently, the fuel volume is increased \rightarrow gaseous fuel swelling
- Correlations are highly empirical

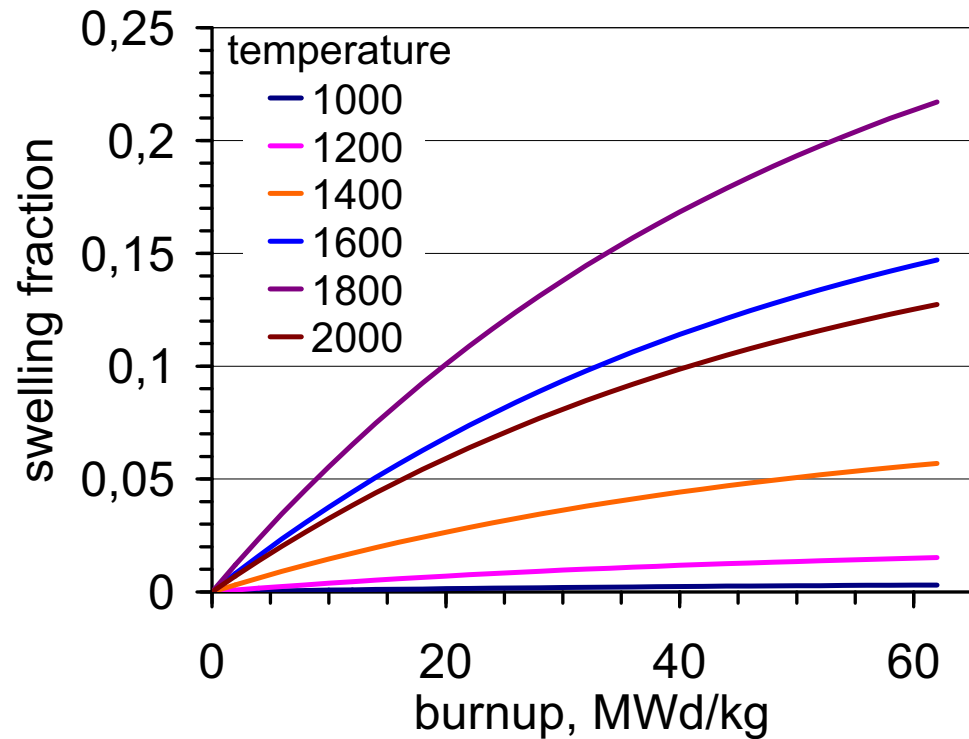


Gaseous fuel swelling - MATPRO

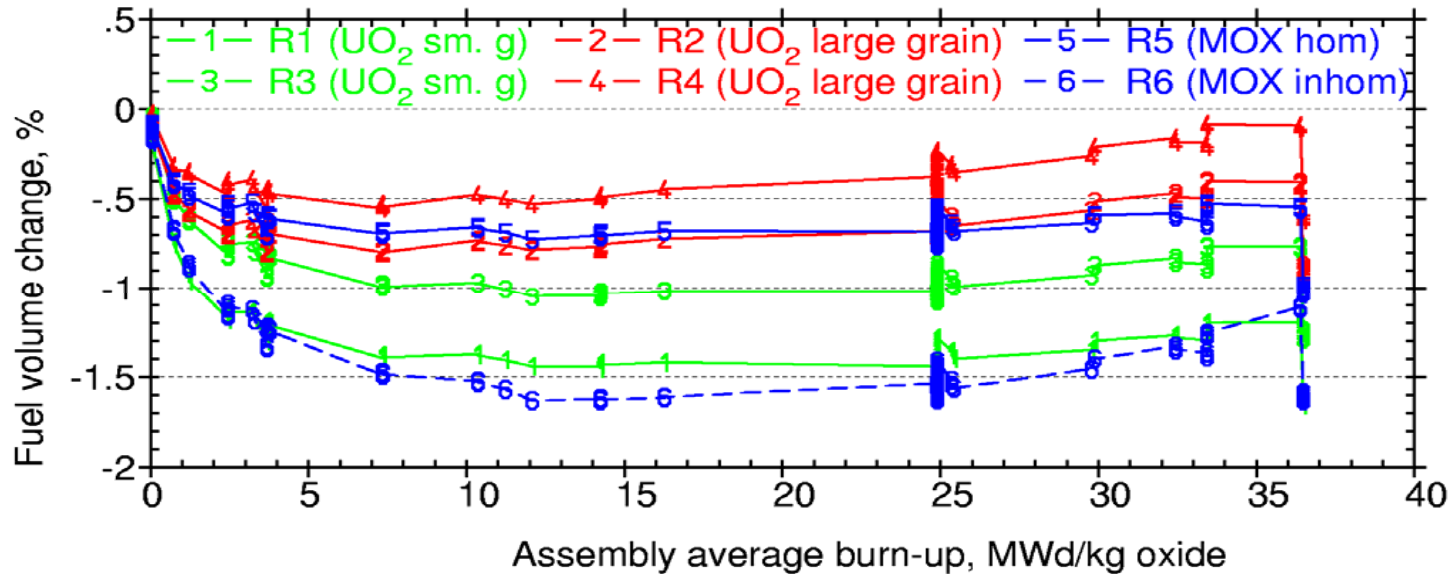
$$\Delta S_g = 2.5 \cdot 10^{-31} \Theta^{11.73} e^{-0.0162\Theta} e^{-0.0227B} \Delta B$$

$$\Theta = 2800 - \min(T + 273, 2800)$$

- The potential for gaseous fuel swelling increases with burnup
- It is significant for temperatures $>1500^\circ\text{C}$
- Reduced at very high T because of fission gas release



Densification & swelling



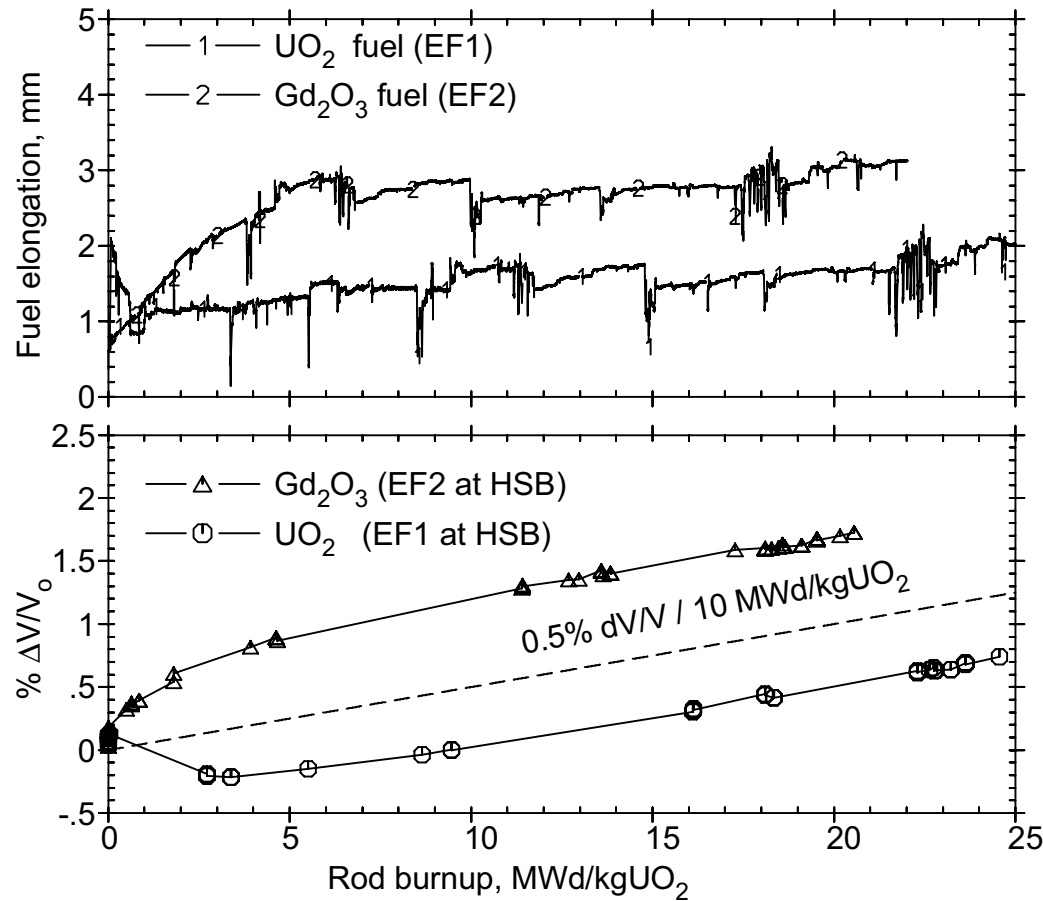
Numerous experiments address fuel densification and swelling. The primary instrument is the fuel stack elongation detector. Densification information can also be derived from rod pressure measurements.

The data of the example stem from a disk fuel irradiation and show a dependence on

- grain size (small vs. large grain)
- irradiation temperature
- fuel fabrication (for MOX fuel)



Densification and swelling as measured with a fuel stack elongation detector (EF)



Swelling of UO₂ and Gd-UO₂ fuel derived from fuel stack length change

UO₂ and (U,Gd)O₂ fuel comparison

- Irradiation of production line UO₂ and Gd-UO₂ fuel, 8 w/o gadolinia
- No densification is observed for Gd-UO₂ fuel
- Both fuel types show a swelling rate of about 0.5% ΔV/V



Clad creep-down

- In water cooled reactors, the cladding is initially in compressive state
- The resulting creep-down of the cladding contributes to closing the fuel-cladding gap
- A typical steady state creep equation has the form

$$\varepsilon = f(\sigma, \phi, t) \cdot \exp(-Q / RT)$$

σ = stress; t = time

ϕ = fast neutron flux



Empirical steady state creep correlations

$$\varepsilon_s = A \cdot \sigma^m \cdot \varphi^n \cdot \exp(-Q/RT) \cdot t$$

$$\varepsilon_s = A \cdot \sinh(B \cdot \sigma) \cdot (\varphi \cdot t)^p \cdot \exp(-Q/RT)$$

A, B = constants

m, n, p = constants

(n, p ≤ 1; m > 1)

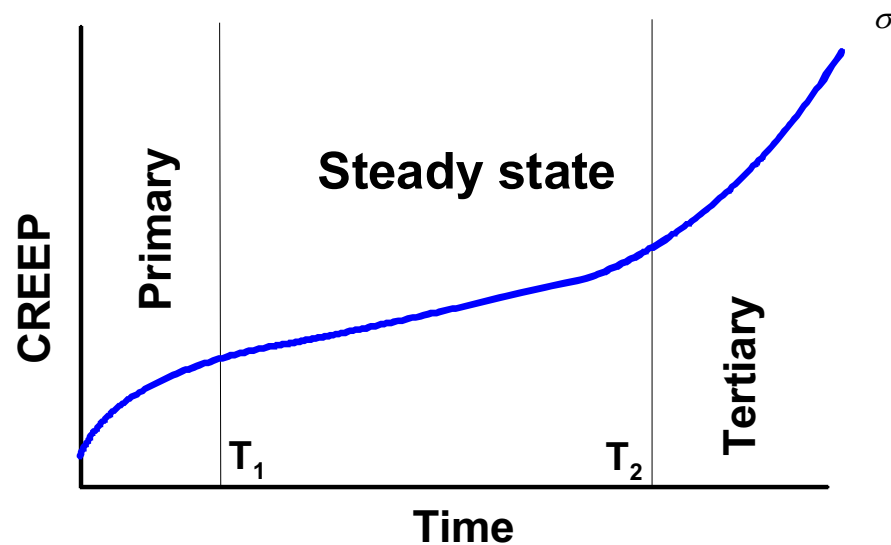
σ = stress

φ = fast neutron flux

T = temperature

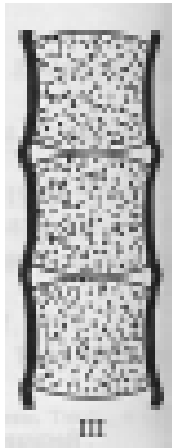
Q = activation Energy

t = time

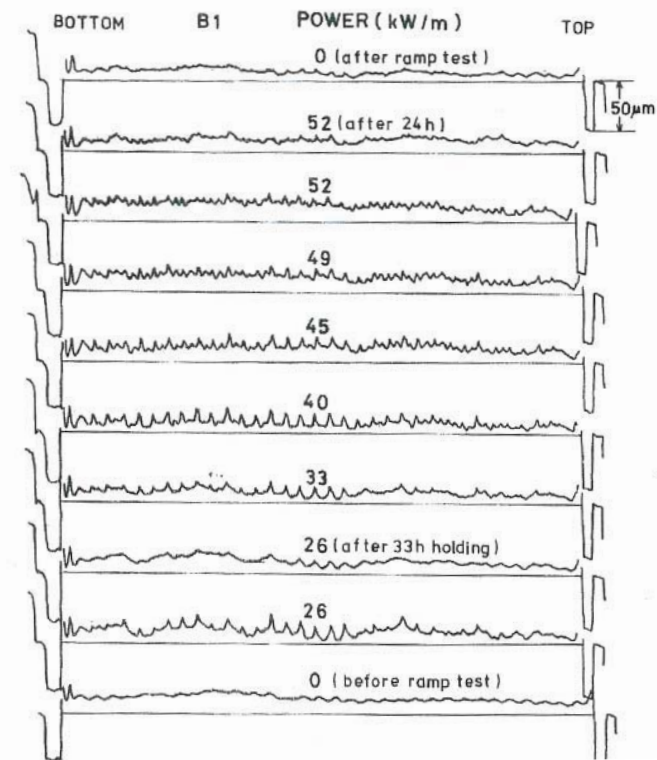
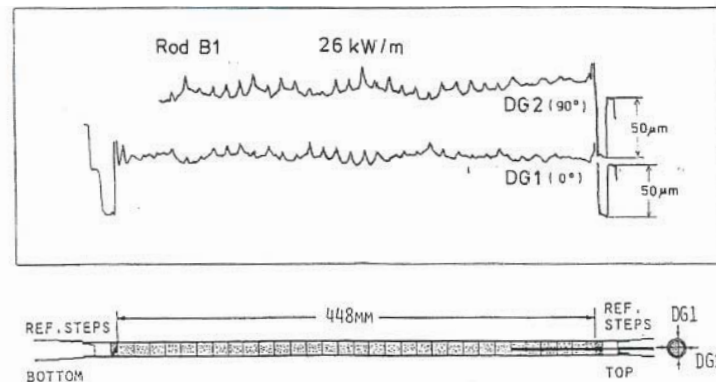


Ridge formations from PCMI

- Ridges at pellet-pellet interfaces caused by the hour-glass shape of the fuel pellet under its temperature gradient
- Ridging reduced during hold periods at power due to fuel creep

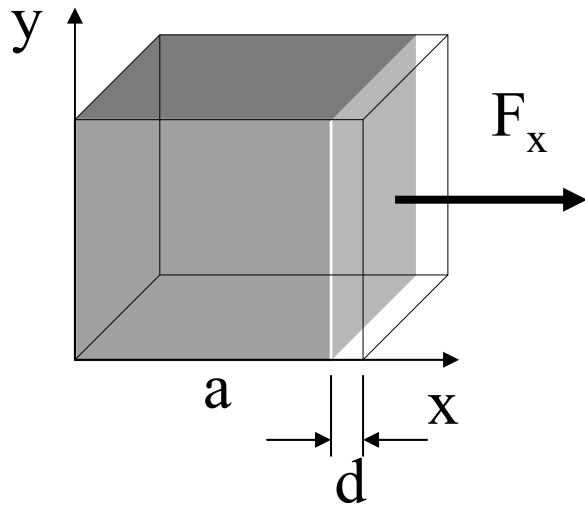


The figure shows data from rig with diameter gauge for measurement of cladding diameter change during power ramp



Strain energy density

(for improving failure predictions)



Force F_x acting on cube with length a , causing stress $\sigma_x = F_x/a^2$, (elastic) displacement d in x direction and strain $\epsilon_x = d/a$

Work $W = \frac{1}{2} F_x d$

Strain energy $U = \frac{1}{2} \sigma_x a^2 \epsilon_x a = \frac{1}{2} \sigma_x \epsilon_x a^3$

General, with shear stresses and strains

Strain energy density $u = \frac{U}{V} = \frac{1}{2} \sigma_x \epsilon_x a^3 / a^3 = \frac{1}{2} \sigma_x \epsilon_x$

$u = \frac{1}{2} (\sigma_x \epsilon_x + \sigma_y \epsilon_y + \sigma_z \epsilon_z + \tau_{xy} \gamma_{xy} + \tau_{yz} \gamma_{yz} + \tau_{xz} \gamma_{xz})$



Critical strain energy density correlation

- The critical strain energy density (CSED) at which failure occurs, is claimed to be a material property
- In reality, it depends on a number of parameters
- The following correlation was developed by CIEMAT based on work by Rashid (Anatech/EPRI) and experimental results from the French PROMETRA program on irradiated Zry-4 cladding

$$\text{CSED} = 43.77 - 203.61x - 126\dot{\epsilon} + 0.00194T \quad [\text{MPa}]$$

x = oxide layer thickness, 15 – 130 μm

T = clad temperature, 553 – 753 K

$\dot{\epsilon}$ = clad strain rate, 0.01 – 5 s^{-1}



Modelling Considerations

Codes must consider all the aspects, and more, shown in this presentation

- cladding
 - thermal expansion, creep, thermo elasticity, plasticity, growth,...
- fuel
 - thermal expansion, densification, cracking and relocation (contact force and crack pattern), fission product swelling, creep, gaseous swelling, fission gas release (PCI failure),...
- relative movement between pellet and cladding: no contact, frictional sliding, sticking
- additionally for PCI failure modelling (ramp tests, RIA)
 - local stresses, crack initiation, fission product release, crack propagation (SCC)



Modelling PCMI

- 1 ½ D codes
 - axi-symmetric 1D model (radial dependence only) does not allow direct calculation of ridge formation
 - axial length (z direction) is divided into nodes
 - axial coupling of nodes
- 2D – 3D codes
 - more rigorous description of the geometry, but ...
 - restricted to a few pellets (2D: axi-symmetric r-z)
 - special coupling elements
- Goals
 - Calculation of dimensional changes during irradiation
 - PCI failure probability / limits
 - Operational constraints?





The END

