Timothy Bowles

NE 533 Test 3

1. $\varepsilon_{total} = ?$ $\quad \alpha_{th} = 10\times10^{-6}$ $\quad \dot{F} = 6\times10^{13}\ \frac{fiss}{cm^3 s}$ $\quad T_f = 1600K$ $\quad T_{ref} = 500K$ $\quad \Delta\rho_0 = 0.015$

$b_D = 5\,MWD/kgU \approx 0.005\,FIMA$ $\quad \rho(UO_2) = 10.97\ \frac{g}{cc}$, $\quad t = 300$ days

$\varepsilon_{th} = \alpha\Delta T = (10\times10^{-6})(1600-500) = 0.011$

ε_D: $\beta = \frac{\dot{F}t}{N_u}$; $N_u = 10.97\frac{g}{cc}\cdot\frac{1mol}{270g}\cdot\frac{6.022\times10^{23}}{1mol}\cdot\frac{1U}{1UO_2} = 2.447\times10^{22}\frac{U}{cc}$

$\Rightarrow \beta = \frac{(6\times10^{13}\frac{fiss}{cc\,s})(300\cdot24\cdot3600)}{2.447\times10^{22}\,U/cc} = 0.063555$

$T > 750°C \Rightarrow C_D = 1$

$\varepsilon_D = \Delta\rho_0\left(\exp\left(\frac{\beta\ln(0.01)}{C_D\beta_D}\right)-1\right) = 0.015\left(\exp\left(\frac{(0.063555)\ln(0.01)}{(1)(0.005)}\right)-1\right) = -0.015$

$\varepsilon_{sFP} = 5.577\times10^{-2}\rho\beta = 5.577\times10^{-2}(10.97)(0.063555) = 0.03888$

$\varepsilon_{gFP} = 1.96\times10^{-28}\rho\beta(2800-T)^{11.73}\exp(-0.0162(2800-T))\exp(-17.8\rho\beta)$

$= 1.96\times10^{-28}(10.97)(0.063555)(2800-1600)^{11.73}\exp(-0.0162(2800-1600))\exp(-17.8(10.97)(0.063555))$

$= 2.643\times10^{-6}$

$\varepsilon_{total} = \varepsilon_{th}+\varepsilon_D+\varepsilon_{sFP}+\varepsilon_{gFP} = 0.011-0.015+0.03888+2.643\times10^{-6} = \boxed{0.0348826 \text{ or } 3.49\%}$

2. Tdal crewp: RXA, $\sigma_m = 85MPa$, $T = 650K$, $LHR = 200\frac{W}{cm}$, $t = 200$ day

$A_0 = 3.14\times10^{24}$ $\quad G = 4.2519\times10^{10} - 2.2185\times10^{7}T$, $\quad n = 5$, $\quad Q = 2.7\times10^5$, $\quad C_0 = 1.654\times10^{-24}$ $\quad C_1 = 0.85$

$C_2 = 1$ $\quad R = 8.314\frac{J}{mol\,K}$

$\dot{\varepsilon}_{ss} = A_0\left(\frac{\sigma_m}{G}\right)^n\exp\left(\frac{-Q}{RT}\right) = 3.14\times10^{24}\left(\frac{85000000\,Pa}{4.2519\times10^{10}-2.2185\times10^{7}(650)\,Pa}\right)^5\exp\left(\frac{-2.7\times10^5\frac{J}{mol}}{(8.314)(650)}\right)$

$= 1.593\times10^{-10}\ \frac{1}{s}$

$\dot{\varepsilon}_{ir}$: $\phi = 5\times10^{11}\,LHR = 5\times10^{11}(200) = 1\times10^{14}\ \frac{n}{cm^2 s}$

$\dot{\varepsilon}_{ir} = C_0\phi^{C_1}\sigma_m^{C_2} = (1.654\times10^{-24})(1\times10^{14})^{0.85}(85\,MPa)^1 = 1.1167\times10^{-10}\ \frac{1}{s}$

$\varepsilon_{tot} = (\dot{\varepsilon}_{ss}+\dot{\varepsilon}_{ir})t = (1.593\times10^{-10}+1.1167\times10^{-10})(200\times24\times3600) = \boxed{0.00468 \text{ or } 0.468\%}$

3. FG release: $t = 60$ day; $T = 1500K$; $\dot{F} = 3\times10^{13}\ \frac{fiss}{cc\,s}$ $\quad$ A) $a_1 = 10\mu m$ (10×10^{-4} cm) $\quad$ B) $a_2 = 25\mu m$ (25×10^{-4} cm)

A) $\tau = D\frac{t}{a^2}$; $D = D_1+D_2+D_3$ $\quad k_b = 8.6173\times10^{-5}\ \frac{eV}{K}$

$D_1 = 7.6\times10^{-6}\exp\left(\frac{-3.03eV}{k_bT}\right) = 5.01675\times10^{-16}\ \frac{cm^2}{s}$

$D_2 = 1.41\times10^{-18}\exp\left(-\frac{1.19eV}{k_bT}\right)\sqrt{\dot{F}} = 7.754\times10^{-16}\ \frac{cm^2}{s}$

$D_3 = 2.0\times10^{-30}\dot{F} = 6\times10^{-17}\ \frac{cm^2}{s}$

$D = 5.01675\times10^{-16}+7.754\times10^{-16}+6\times10^{-17} = 1.337075\times10^{-15}\ \frac{cm^2}{s}$

$\Rightarrow \tau = 1.337075\times10^{-15}\left(\frac{(60\times24\times3600)s}{(10\times10^{-4}cm)^2}\right) = 0.00693$ $\quad (< \pi^{-2}\approx 0.1)$

$f = 4\sqrt{\frac{Dt}{\pi a^2}} - \frac{3}{2}\frac{Dt}{a^2} = \boxed{0.1775}$ or $\boxed{17.75\%}$

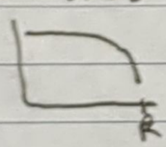
$a = 25 \times 10^{-4}$ cm

B) $\tau = 1.337675 \times 10^{-15} \cdot \frac{60 \times 24 \times 3600}{(25 \times 10^{-4})^2} = 0.001109 < \pi^{-2} \approx 0.101$

$f = 4\sqrt{\frac{Dt}{\pi a^2}} - \frac{3}{2}\frac{Dt}{a^2} = \boxed{0.07349 \text{ or } 7.349\%}$

4. U^{4+} is the typical charge state in UO_2 because O^{2-} is usual oxygen state. This changes as fission products build up and change electronegative system state. U^{3+}, U^{4+}, U^{5+}, and U^{6+} are viable states and form U_4O_9, U_3O_8, UO_3. O/M increases w/ burnup.

5. Oxygen concentration decreases with radius and drops sharply at the fuel/cladding interface. ZrO_2 is more favorable than the ~~[illegible]~~ same compound.



Mo is a fuel additive to help stabilize ~~[illegible]~~ O/M ratio in fuel. It functions as a oxygen sink for oxygens released after a Uranium fission. ~~[illegible]~~ Slows O/M increase w/ burnup.

6. Melting temperature, thermal conductivity, and creep vary as a function of stoichiometry in UO2.

7. Fission product types:

Soluble oxides (Y, La, rare earths): Dissolution cation sublattice. Chemically inert w/ FPs.

Insoluble oxides (Zr, Ba, Sr): Form insoluble oxides in fluorite lattice. Take O place in lattice.

Metals (Mo, Ru, Pd, Tc): Form metallic precipitates, cause swelling

Volatiles (Br, Rb, Te, I, Cs): Gas at interior, solid at exterior, some are corrosive.

Noble gas (Xe, Kr): insoluble, form voids + decrease thermal conductivity.

8. Fission gas release:
Stage 1: Produce FG from fission + diffuse to GB or form intergranular gas bubble (size limited num)
Stage 2: Gas bubbles nucleate on GB, bubbles grow + interconnect
Stage 3: Gas travels through interconnected bubbles to free surface

9. Creep is material deformation at stresses below the yield stress that happen over time caused by defect diffusion. Thermal creep, or Bulk diffusion (Nabarro-Herring Creep), is defect diffusion at high temperatures.

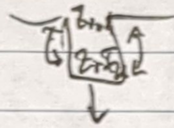
10. Zr cladding benefits include: High corrosion resistance, high Thermal conductivity, cheap. Helps retain FPs, maintain core geometry, and contain pellets

11. Loops form on the pyramid plane (a), causing growth in a and contraction in c plane.

12. Stage 1: cladding contracts from water pressure and gets longer.
2: Partial clad/fuel contact presses out at contact causing ~~elongating~~ w/ fuel growth
3: Full clad/fuel contact, cladding expand out ward + contracts in length dimension

13. Time: Build environment + ZrO_2 breach on internal
Corrosive environment: I Shane to Zr cladding + corrosive material
~~T~~ Tensile stress: Crack from fuel apply stress after clad/fuel contact from creep
Susceptible material: Zr metal exposed.

14. ZrI_4 gas move to surface + corrode Zr metal. ZrO_2 formed w/ expose Zr. Pits on the metal until thin ligament left and the ductile tear creates failure. ~~Bth~~ PCI lead after pinhole failure.

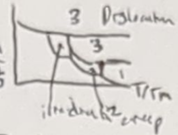
 cyclic degradation.

NE533 TEST 2 CRIB SHEET

Grain boundary: Energy level, nucleation + misorientation; (name, orientation, rotation, alignment)
texture: orientation of all grains, no preference = no texture
size: initial LWR size = 10 μm; effects: Fission gas release, swelling, creep, thermal cond.
Grain boundary diffusion: faster than bulk diffusion: More space; effect creep
segregation: impurity atoms prefer GBs
GBs impede dislocation motion: Hall-Petch effect $\sigma_y = \sigma_0 + \frac{k_y}{\sqrt{d}}$
GBs migrate to reduce energy: $v_{GB} = M_{GB}(P_d - P_r)$ (mobility; driving force; resisting pressure)
$M_{GB} = M_0 e^{-\frac{Q}{k_B T}}$ $\frac{m^4}{Js}$; $k_B = 8.6173e{-5}$ eV/K; $M_0 = 4.6e{-9}$ $(\frac{m^4}{Js})$; $Q = 2.77$ eV (UO_2)
$P_d = \frac{2\gamma_{GB}}{R}$; $v = M\frac{2\gamma_{GB}}{R}$; $D(t)^2 - D_0^2 = 2M\gamma_{GB}t$
$\frac{dD}{dt} = k\left(\frac{1}{D} - \frac{1}{D_m}\right)$; $k = 2M_{GB}\gamma_{GB}$; $D_{m,UO_2}^{\mu m} = 2.23e3\exp\left(\frac{-7620}{T}\right)$
Solute drag: GB migration impeded by pores, precipitates; solute atoms
Irradiation can accelerate grain growth
Fuel densification: T + irradiation help; $\varepsilon_D = \Delta\rho_0\left(\exp\left(\frac{\beta\ln(0.01)}{C_D\beta_D}\right) - 1\right)$
β (FIMA); $\beta_D = 5\frac{MWD}{kgU} \approx 0.005$ FIMA; $C_D = 7.235 - 0.00860(T-25)$ $T < 750C$
$\Delta\rho_0$ = total densification possible $= 1$ $T \geq 750C$
$\beta = \frac{\dot{F}t}{N_u}$; FIMA to MWD/kgU $\times 950$
UO_2 is ionic compound; U^{3+}, $\overbrace{U^{4+}, U^{5+}, U^{6+}}^{\text{most stable}}$; U_4O_9, U_3O_8, UO_3; lattice accomodate FPs
hypo (UO_{2-x}); hyper (UO_{2+x}); extra O in lattice sites; Fabout 2
FP formation shift ox state to ~~stay~~ O^{2-}; $\Delta\bar{G}_{O_2} = 2\mu_{O_{2,sys}} - G^\circ_{O_2}$
Mo/MoO_2 additive provide O sink as U fissioned; low O near cladding
Stoichiometry impacts: Melt, conduct, creep, Fission gas release, grain growth, chemical reactions
Most fuel codes ignore stoichiometry
O/M ratio changes during operation; UO_2 is cubic fluorite structure
Fission products: [concentrations change over time]
Soluable oxides (Y, La, rare earth) dissolve in cation sublattice [dissolved]
Insoluable oxides (Zr, Ba, Sr) form insoluble oxides in fluorite lattice [grey]
Metals (Mo, Ru, Pd, Tc) form metallic precipitates [white]
Volatiles (Br, Rb, Te, I, Cs) gas at interior, solid at exterior [void]
Noble gas (Xe, Kr) insoluble; form inter- or intra-granular voids [void]
O/M increase w/ Burnup
FPs Segregate to GBs + voids; interact w/ cladding: Te corrosive; Sr, Cs, Pu, Am Bond; Cs, Cd, I SCC;

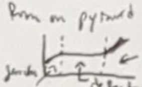
Fission Gas Release:
Stage 1: Produced from fission + diffuse to GB; intergranular bubble on GB surfaces
2: Gas bubbles nucleate on GB, grow + interconnect
3: Gas travels through interconnected bubbles to free surface
Also, particle recoil + knockout at low temp + pellet fracture during transients
FG release reduces thermal cond; ↑ pressure; Post irradiation anneal + In-pile release
Booth model: 1 stage; sphere grain: $\dot{c}_g = k_g + \nabla\cdot D\nabla c_g$; $\dot{c}_g = k_g + D\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_g}{\partial r}\right)$
PIA: $J_a = -D\left(\frac{\partial c_g}{\partial r}\right)_a$; $f = \frac{4\pi a^2\int_0^t J_a dt}{4/3\,\pi a^3 C_g^0} = \frac{3}{aC_g^0}\int_0^t J_a dt$
$\tau = D\frac{t^2}{a}$ ⇒ $f = 6\sqrt{\frac{Dt}{\pi a^2}} - 3\frac{Dt}{a^2}$ $\tau < \pi^{-2}$; $f = 1 - \frac{6}{\pi^2}e^{-\pi^2\frac{Dt}{a^2}}$ $\tau \geq \pi^{-2}$
In pile: $\dot{c}_g = y\dot{F} + D\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_g}{\partial r}\right) - \lambda c_g$; $\dot{F} = q N_u \sigma_{F235}\phi_{th}$; $f = \frac{3}{ay\dot{F}t}\int_0^t J_a dt$
$f = 4\sqrt{\frac{Dt}{\pi a^2}} - \frac{3}{2}\frac{Dt}{a^2}$ $\tau < \pi^{-2}$; $f = 1 - \frac{0.0662}{Dt/a^2}\left(1 - 0.93\exp\left(-\pi^2\frac{Dt}{a^2}\right)\right)$ $\tau \geq \pi^{-2}$
total gas prod $= y\dot{F}t$; $y = 0.3017$
Forsberg-Massih model (Stage 1+2): overpredicts gas release b/c neglects GB bubble percolation
Gas diffusivity: $D = D_1 + D_2 + D_3$ $\frac{cm^2}{s}$; $D_1 = 7.6e{-6}\exp\left(-\frac{3.03eV}{k_B T}\right)$
$D_2 = 1.41e{-18}\exp\left(-\frac{1.19eV}{k_B T}\right)\sqrt{\dot{F}}$; $D_3 = 2.0e{-30}\dot{F}$; $D_{eff} = \left(\frac{\Gamma r}{\Gamma r + \Gamma t}\right)D$
Fuel size + shape change: Thermal expansion, densification, swelling, irradiation creep
densification first 5-10 MWd/kgU
Swelling: solid swelling, gaseous swelling, high burnup swelling
$\varepsilon_{sfp} = (5.577e{-2})\rho\beta$; ρ = current UO_2 density $\left(\frac{g}{cm^3}\right)$; β = Burnup in FIMA
$\varepsilon_{gfp} = 1.96e{-28}\rho\beta(2800-T)^{11.73}\exp(-0.0162(2800-T))\exp(-17.8\rho\beta)$
T < 1000K FG stay in GBs; T = 1000K-1700K micro swelling + diffusion
$\varepsilon_{total} = \varepsilon_{th} + \varepsilon_D + \varepsilon_{sfp} + \varepsilon_{gfp}$
creep: defect diffusion; thermal or irradiation driven
$\dot{\varepsilon} = \frac{C\sigma^m}{D_{gr}^b}e^{-\frac{Q}{k_B T}}$

Bulk diffusion (Nabarro-Herring creep): high T; m=1, b=2, Q=self diff — Bowes
GB diffusion (Coble creep); m=1, b=3; Q = GB diff; diff along GB to elongate
Dislocation creep (Power law creep): dislocation glide under high stress; dislocations climb to defects to avoid obstacles; m = 4-6; b = 0; Q = self diff

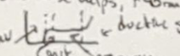


$\dot{\varepsilon} = \rho_d^m b v_d$; ρ = density of mobile dislocations; b = burgers vector; v_d = dislocation velocity

Fracture: increase gap reduction, reduce thermal cond; increase avenues for FG release
empirical + semi-empirical + mechanistic cracking model
$\sigma_{frac} = G^{-m}\sigma_{frac,ms}$; $m = 0.04-0.05$; $10\mu m \to 100\mu m$ σ_{frac} decreases by 10%.
Fracture strength 10x in compression than tension
Cladding: contain fuel, FP, fragments, heat transfer, shape
Zirc alloy: Pro: σ_{abs}↓, corrosion resistance, mechanical props, ↑ thermal cond; Con: hydride embrittlement
Anisotropic anisotropies lead to creep + growth; corrosion under high-T steam
Pure Zirc spalled; Alloys Sn, Nb, Fe, Cr, Ni, O
Zircaloy: α HCP to 863C; β BCC; tubes formed SRA or RXA
$v(T) = \frac{kE_p}{2E_d} = \frac{k(T-M)}{2E_d}$ 8x displacements per atom
Interstitial loops form on pyramid plane (a), shrink on outer axis (c)
Irradiation growth



Irradiation growth temp dependent
Zirc creep: $\sigma_m = \left[\frac{1}{2}\left((\sigma_{11}-\sigma_{22})^2 + (\sigma_{22}-\sigma_{33})^2 + (\sigma_{33}-\sigma_{11})^2 + 6(\sigma_{12}^2 + \sigma_{23}^2 + \sigma_{31}^2)\right)\right]^{1/2}$
$\dot{\varepsilon}_{ss} = A_0\left(\frac{\sigma_m}{G}\right)^n\exp\left(-\frac{Q}{RT}\right)$; $A = 3.14e24\frac{1}{s}$; $G = 4.2519e10 - 2.2185e7T$ Pa
$n = 5$; $Q = 2.7e5\frac{J}{mol}$
$\dot{\varepsilon}_{ir} = C_0\phi^{C_1}\sigma_m^{C_2}$; ϕ = fast flux = $3e11 \times LHR\frac{n}{cm^2 s}$; $C_1 = 0.85$, $C_2 = 1$; C_0 = SRA 3.557, RXA 1.654, PRXA 2.714, ZIRLO 2.846 $\times 10^{-24}$
Creep: a) coolant pressure → b) local contact c) all contact
Hydrides = 0.2% growth for 0.1% H; Irradiation hardening
high stress "swept away" loops ⇒ clean channel ↓ effective ductility
Fatigue: S-N curve; lower life less than 10^4; 2x, 20x design factors
Pellet Cladding Interaction: chemical + mechanical; Fuel swell, clad shrink, fuel crack → clad crack w/ SCC
corrosion from I, Cd, Cs near FG on fuel crack; $ZrI_4 \rightleftarrows Zr + 2I_2$
Low dose helps, ↑ grain size helps, pellet hour glass hurts; ↑ Power ↑ fuel cracks



; cause oxide flaw + FP; inter- and intra-granular cracks possible
Pinhole crack: release corrosive gas + create oxide to close hole; operate smooth to avoid
Sn for corrosion, but now use Nb

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1. Change grain size: T = 1800K, $\gamma = 1.5\frac{J}{m^2}$, t = 100hr, $D_0 = 5\mu m$
$M_{GB} = M_0\exp\left(-\frac{Q}{kT}\right)\frac{m^4}{Js}$; $M_0 = 4.6\times10^{-5}$ $Q = 2.77eV$ ⇒ $M_{GB} = 8.07\times10^{-17}\frac{m^4}{Js}$
$D = \sqrt{2M\gamma t} - D_0 = \sqrt{2(8.07\times10^{-17})(1.5)(100\times3600)} - 5\times10^{-6} = 1.46\times10^{-5}$ m or 14.6 μm
2. Densification: t = 60 day; $\Delta\rho_0 = 0.01$; T = 1400K; $\dot{F} = 4\times10^{13}\frac{fiss}{cm^3 s}$
$\varepsilon_0 = \Delta\rho_0\left(\exp\left(\frac{\beta\ln(0.01)}{C_D\beta_D}\right) - 1\right)$ $C_D = 1$ $T > 750C$ $\beta_0 = 5\frac{MWD}{kgU} = 0.005$ FIMA
$\beta = \frac{\dot{F}t}{N_u}$; $N_u = 10.97\frac{g}{cc}\cdot\frac{1\,mol}{270g}\cdot\frac{6.022\times10^{23}}{1\,mol}\cdot\frac{1U}{1UO_2} = 2.447\times10^{22}\frac{U}{cc}$ ⇒ $\beta = 0.0085$
$\beta > \beta_0$ $\varepsilon_D = -0.01$; beyond process step
3. Triple gas release: $\dot{F} = 5\times10^{13}\frac{fiss}{cc\,s}$ T = 1450K t = 100 day a = 10 μm
$D = D_1 + D_2 + D_3$; $D_1 = 7.235e{-16}\frac{cm^2}{s}$; $D_2 = 7.289e{-16}\frac{cm^2}{s}$; $D_3 = 1\times10^{-16}\frac{cm^2}{s}$; $D = 1.05e{-15}$
$\tau = \frac{Dt}{a^2} = \frac{(1.05e{-15})(100\times24\times3600)}{(10\times10^{-4})^2} = 0.101$ (cm →)
$f = 4\sqrt{\frac{Dt}{\pi a^2}} - \frac{3}{2}\frac{Dt}{a^2} = 0.368$ or $\boxed{36.8\%}$
4. Zr creep: T = 600K, LHR = 250 $\frac{W}{cm}$; σ_m = 200MPa, SRA, 3 yrs
$R = 8.314\frac{J}{K\,mol}$
$\dot{\varepsilon}_{ss} = 1.48\times10^{-10}\frac{1}{s}$; $\dot{\varepsilon}_{ir} = 4.43\times10^{-10}\frac{1}{s}$
$(\dot{\varepsilon}_{ss} + \dot{\varepsilon}_{ir})(3yr) = 0.056$ or 5.6% strain
5. Total change in volume: $\dot{F} = 2e13\frac{fiss}{cc\,s}$ T = 1400K $T_{ref} = 300K$ $\Delta\rho_0 < 0.01$
$\beta_0 = 5\frac{MWD}{kgU}$ $\alpha_F = 11e{-6}\frac{1}{K}$ $N_u = 2.45e22\frac{U}{cc}$ t = 14 day
$\varepsilon_{total} = \varepsilon_{th} + \varepsilon_D + \varepsilon_{sfp} + \varepsilon_{gfp}$
$\varepsilon_{th} = \alpha\Delta T = (11\times10^{-6})(1400-300) = 0.0121$
$\varepsilon_D = \Delta\rho_0\left(\exp\left(\frac{\beta\ln(0.01)}{C_D\beta_D}\right) - 1\right)$; β = ? = FIMA: $\frac{\dot{F}t}{N_u} = 9.87\times10^{-4}$
C_D: $T > 750$ ⇒ $C_D = 1$
$\varepsilon_D = 0.01\left(\exp\left(\frac{(9.87\times10^{-4})\ln(0.01)}{(1)(0.005)}\right) - 1\right) = -0.006$
$\varepsilon_{sfp} = 5.577e{-2}\rho\beta = 5.577e{-2}(10.97)(9.87\times10^{-4}) = 5.98\times10^{-4}$
$\varepsilon_{gfp} = 0.002$
$\varepsilon_{total} = 0.0121 - 0.006 + 5.98e{-4} + 0.002 = 0.008$ or 0.8% swell