

4. Thermomigration-Induced Surface Instability in Metallic Fuel

4.1 Introduction

Post-irradiation metallography of the AFC-3A Rod 4 specimen [1, 2] shows an irregular fuel surface containing deep, surface-connected cavities separated by protruding regions of fuel (Figure 4.1). Several of the cavities have relatively sharp profiles, and some of the intervening protrusions are also locally sharp. This morphology differs from the comparatively uniform outward displacement that might be expected from swelling alone.

We believe that thermomigration-driven surface diffusion may offer an explanation for the formation of the observed surface pores. Imagine a fuel surface with an initial sinusoidal perturbation and note that a surface protrusion reduces the local helium-gap thickness and is therefore likely to be cooler than an adjacent depression. Because uranium tends to migrate from hotter to colder regions, this temperature variation could drive material from depressions toward protrusions, thus amplifying the original perturbation. The objectives of this study are to first develop a benchmark problem to ensure that the finite element implementation described in Section 3 can be correctly applied to an external fuel surface and then to use the verified capability to simulate surface evolution in the AFC-3A fuel specimen.

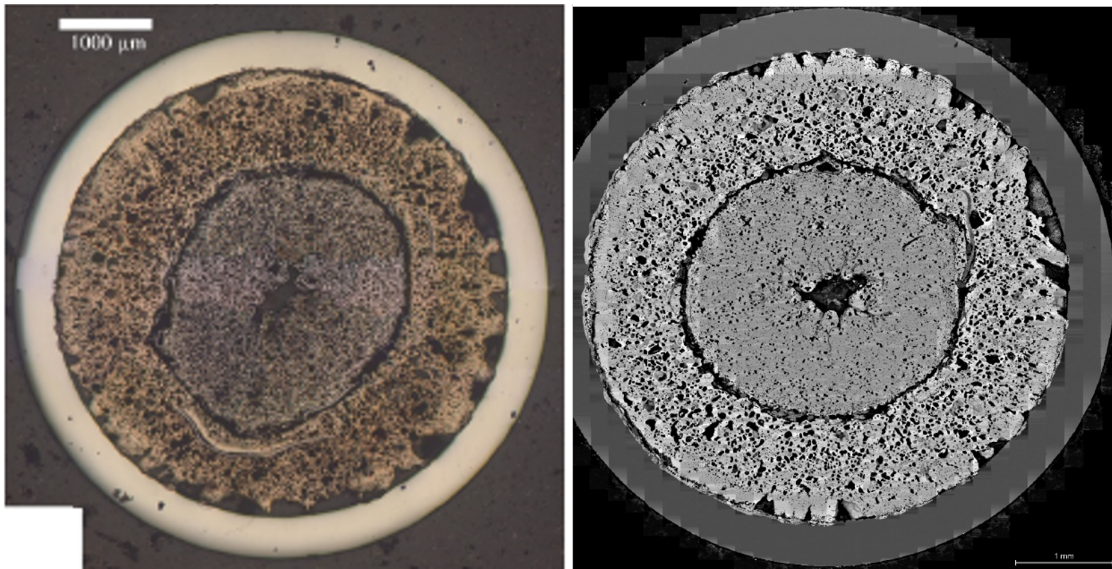


Figure 4.1: Two post-irradiation images of the AFC-3A Rod 4 specimen [1, 2]. The fuel surface contains deep surface-connected cavities and intervening protrusions, including several relatively sharp features.

4.2 Gas Gap Benchmark

The finite element implementation was first tested using the idealized gas gap problem shown in Figure 4.2. A volumetrically heated solid having a small sinusoidal surface perturbation is separated from an isothermal outer boundary by a gas gap. The analytic solution assumes locally one-dimensional heat transfer normal to the surface, with lateral heat conduction ne-

glected. The finite element model uses a correspondingly anisotropic thermal conductivity so that the numerical and analytic problems are directly comparable.

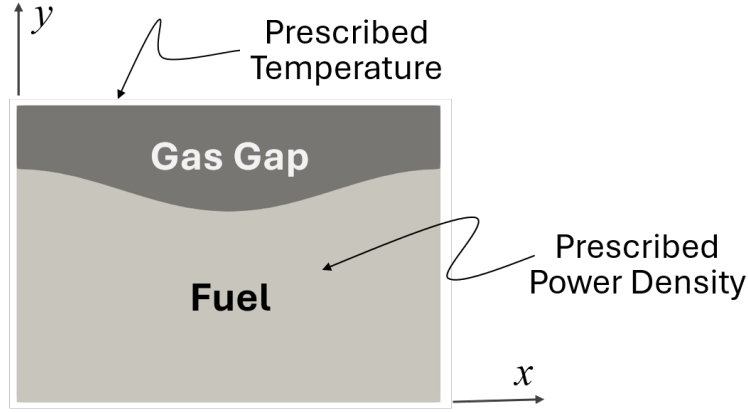


Figure 4.2: Schematic of the gas gap boundary value problem used to benchmark thermomigration-driven surface instability. A small sinusoidal perturbation of the fuel surface produces a spatial variation in gas gap thickness and fuel-surface temperature.

For a small-amplitude sinusoidal perturbation having initial amplitude A_0 and wavelength λ , the analytic solution for the perturbation amplitude is

$$A(t) = A_0 \exp(\omega t), \quad (4.1)$$

where

$$\omega = \Omega B_T \frac{q'''(H_s - H_g)}{\kappa_{\text{gas}}} k^2, \quad (4.2)$$

$$B_T = M_s \frac{Q^*}{T_{\text{ref}}}, \quad (4.3)$$

$$k = \frac{2\pi}{\lambda}. \quad (4.4)$$

where T_{ref} is the nominal fuel surface temperature. The quantities appearing in the solution are defined in Table 4.1.

Figure 4.3 compares the analytic solution with the finite element calculation. For the reference uranium calculation, the analytic and finite element growth rates differ by about 0.55 percent. The comparison provides a direct verification that the calculated surface-temperature variation is converted correctly into thermomigration-driven surface flux and surface motion.

Table 4.1: Definitions of quantities used in the analytic gas gap solution.

Symbol	Definition	Symbol	Definition
$A(t)$	Surface-perturbation amplitude	A_0	Initial perturbation amplitude
ω	Exponential growth rate	Ω	Atomic volume
B_T	Thermomigration coefficient	M_s	Surface mobility
Q^*	Heat of transport per atom	T_{ref}	Nominal fuel surface temp
q'''	Volumetric heat-generation rate	κ_{gas}	Gas thermal conductivity
H_s	Nominal solid thickness	H_g	Nominal gas-gap thickness
k	Perturbation wavenumber	λ	Perturbation wavelength

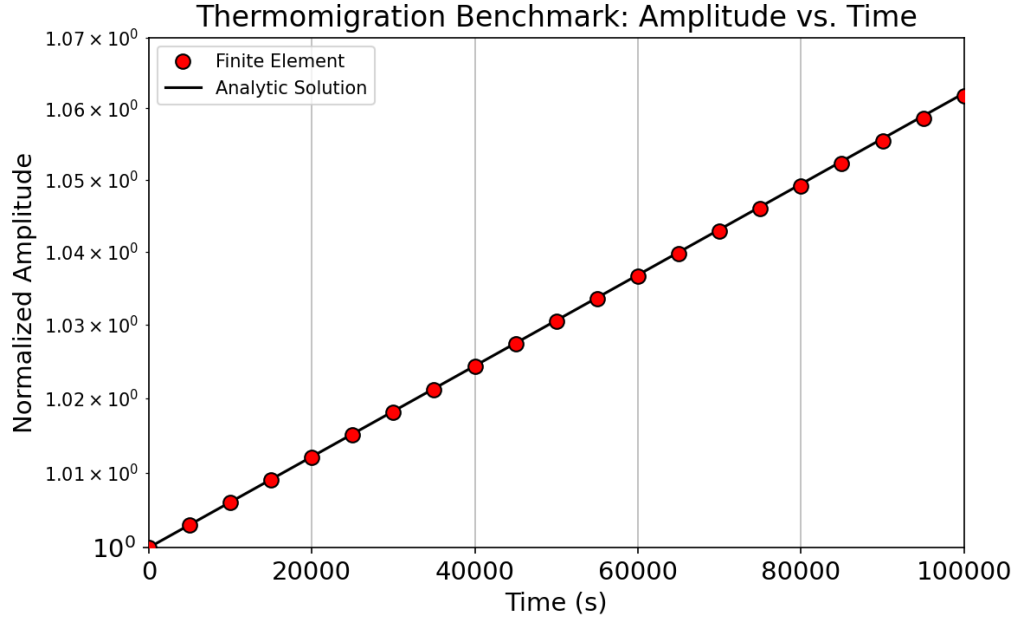


Figure 4.3: Comparison of finite element and analytic predictions of the growth in perturbation amplitude over time for the gas gap benchmark.

4.3 Simulations of Surface Pore Formation

The verified capability was then applied to an annular helium-bonded fuel geometry with an initially perturbed outer fuel surface. In these initial simulations, the perturbation to the fuel surface caused the helium gap thickness to vary as

$$t_{\text{gap}} = t_0 + \delta \cos(m\theta), \quad (4.5)$$

where the nominal helium gap thickness t_0 was assumed to be $50 \mu\text{m}$, the perturbation to the gap size δ was assumed to be $5 \mu\text{m}$, and the number of wavelengths over the full circumference (m) was taken to be 16. In addition, the fuel itself was assumed to behave as a linear elastic solid. The substantial change in fuel geometry shown below is produced almost entirely by surface-diffusion-driven transport of material along the fuel outer surface.

Figure 4.4 shows the predicted evolution of the fuel surface over a period of 84 days. Although

the initial perturbation was sinusoidal, by the time fuel contacts the cladding, sharp peaks have formed on the fuel surface separated by wide, cusp-like valleys. Once contact has been established, the character of the solution changes as local compressive stresses develop and stress-driven surface diffusion begins to contribute to redistribution of material along the fuel surface. These stresses cause the initially sharp peaks to flatten and conform to the cladding. As the simulation progresses, the peaks broaden into plateaus and the initial depressions narrow and deepen, producing surface morphologies qualitatively similar to those observed in the AFC-3A Rod 4 metallography.

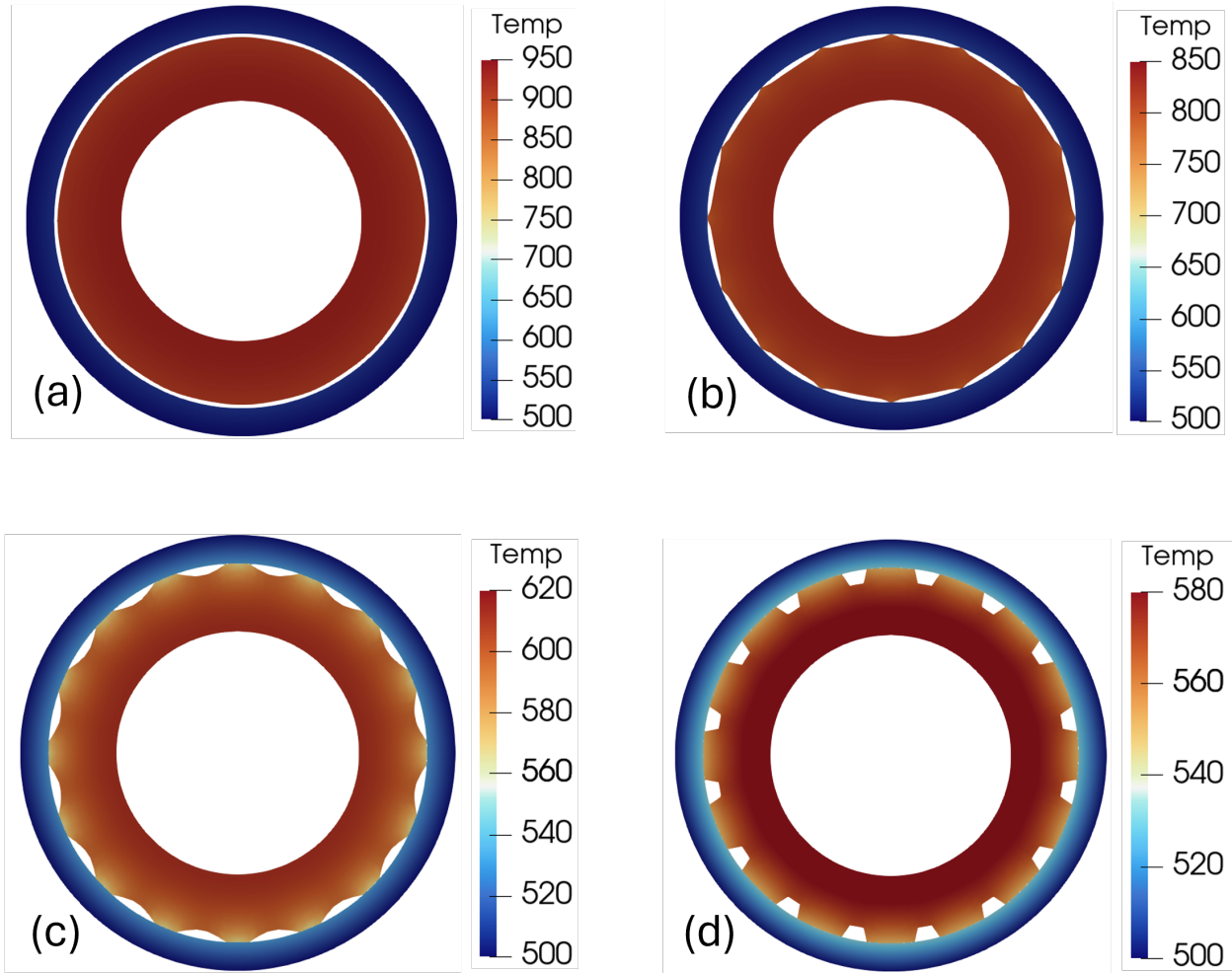


Figure 4.4: Representative HeavyMetal simulation of thermomigration-driven surface evolution in annular, helium-bonded metallic fuel (a) time = 0+ days; (b) time=28 days; (c) time=58 days; (d) time=84 days. The initially small surface perturbations grow into pronounced cavities and protrusions as material is redistributed along the fuel surface. Also note that the temperature contour levels are different for each time and that the peak fuel temperatures drop substantially as more of the fuel contacts the cladding.

Significant work remains before these calculations can be used for engineering analysis. Important next steps include incorporating fuel creep and swelling, improving the expressions for surface diffusivity, and ensuring that the models used here remain consistent with other microstructural observations such as pore migration. Nonetheless, these initial analyses have met their intended goal, which was to assess the hypothesis that thermomigration-driven surface diffusion contributes to surface-pore formation. The calculations show that initially small perturbations can evolve into pronounced surface cavities and protrusions qualitatively similar to those observed in AFC-3A Rod 4. Although these results do not conclusively establish thermomigration as the cause of the observed morphology, the current results, together with the lack of plausible alternative explanations, provide support for the hypothesis and indicate that thermomigration-driven surface diffusion warrants continued investigation.

References

- [1] J. M. Harp, L. Capriotti, and F. Cappia, *Baseline Postirradiation Examination of the AFC-3C, AFC-3D, and AFC-4A Experiments*, INL/EXT-18-51447, Rev. 0, NTRD-FUEL-2018-000120, Idaho National Laboratory, September 2018.
- [2] T. Yao, Y. Tang, and F. Xu, *Quantitative Insight to Fission Gas Pores Distribution in Irradiated Annular U-10Zr Metallic Fuel Using Machine Learning*, INL/CON-24-76767, Rev 0, Idaho National Laboratory, March 2024.