Pressure Calculation of Intergranular Bubbles in UO_2

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Introduction

- **Inert gas atom** generated from nuclear fission reaction has very low solubility in UO_2 and **diffuses to the grain boundary** from inside the matrix.
- The formation of fission gas bubbles is the main cause of nuclear fuel swelling, and fuel pulverization due to rupture of grain boundaries caused by over-pressurization of intergranular bubbles during the transient accident
- As the experiments and calculation results show, the fission gas bubble is **over-pressured**, with pressure much higher than the capillary pressure.
- **Over pressurization factor was calculated based on the fission gas diffusion model and real microstructure of nuclear fuel.**

Calculation Method

- White et al. conducted microstructure analysis on intergranular bubbles present in the grains of nuclear fuel pellets of about 21 GWd/tU. [1] Among them, three pellets named 4000, 4004 and 4005 were used in this study.
- The Modified Forsbug-Massih model was used to calculate the amount of fission gas present in the grains of the nuclear fuel. [2]

$$\frac{dC}{dt} = D(t)\Delta_r C(r,t) + \beta(t)$$

C = gas concentration, D = diffusion constant, β = gas production, t = time, $\Delta_r = \frac{d^2}{dr^2} + \frac{2}{r}\left(\frac{d}{dr}\right)$

$$C(a,t) = \frac{b(t)\lambda N(t)}{2D}$$

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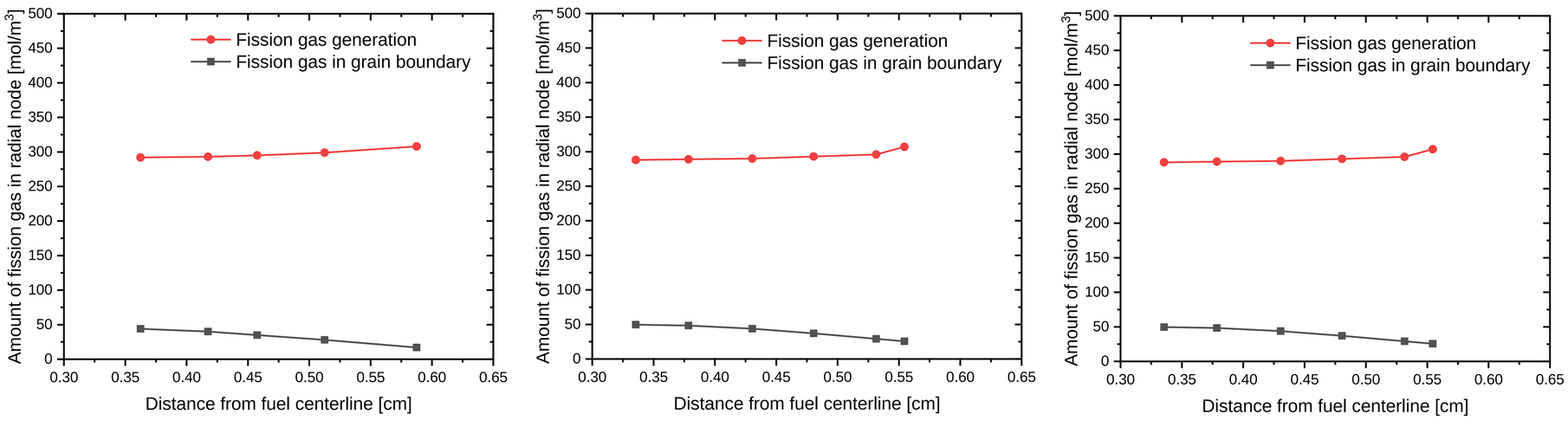
N = surface gas concentration, λ = resolution layer depth, a = hypothetical grain radius, b = resolution rate

- Based on the volume of bubbles in the SEM microstructure and the amount of fission gas calculated by the model, the pressure of the bubbles was calculated by applying to three different equations of states, and then compared with the capillary pressure.

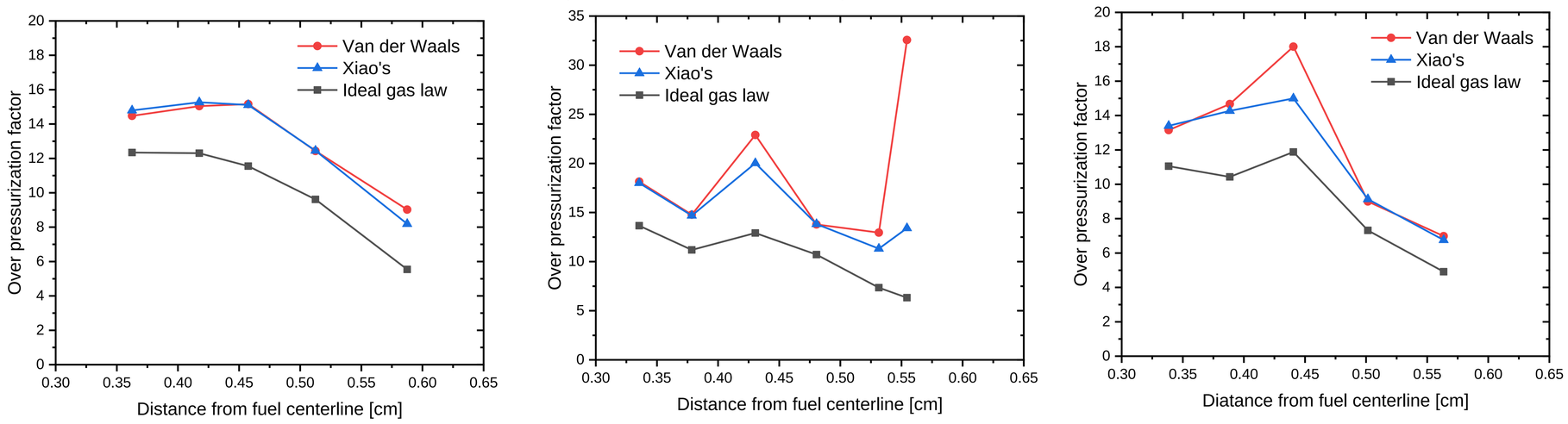
Calculation Result

❖Calculated amount of fission gas in pellet 4000, 4004, 4005



- Burnup is higher in outside part of the nuclear fuel and the fission gas production is high.
- Diffusion from the grain inside to the boundary is smaller in fuel outside part due to the relatively low temperature
- The amount of fission gas in grain boundary tends to decrease overall toward the outside of the nuclear fuel.

❖Over pressurization factor in pellet 4000, 4004, 4005



- Ideal gas law, Van der Waals, Xiao's equation of state [3] were used.
- It was investigated how many times the calculated pressure had a value of the capillary pressure.
- In the case of the Van der Waals equation, there is a tendency to estimate the pressure very high when calculating small volumes. Therefore, the pressure at the outermost part of the 4004 pellet tended to increase significantly.

- As the result of the calculation with the most reliable Xiao's equation of state, calculated by molecular dynamic simulation, the overpressurization factor tends to decrease toward the outside of the nuclear fuel.
- the reason for over pressurization is that the rate at which the fission gas diffuses into the intergranular bubble is faster than the rate at which the bubble expands due to the pressure driven diffusion of UO_2 outward by the bubble pressure.
- This difference in diffusion rate will of course be larger as the temperature increases, and thus the over-pressurization will be greater in the hot area. Therefore, it has a larger over-pressurization factor in the center of the fuel.

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[1] White et al. A Summary of Swelling Data Obtained from the AGR/Halden Ramp Test Programme
[2] K. Forsberg, A.R. Massih, Diffusion theory of fission gas migration in irradiated nuclear fuel UO2, J. Nucl. Mater. 135 (1985) 140–148.
[3] H.X. Xiao, C.S. Long, A modified equation of state for Xe at high pressures by molecular dynamics simulation, Chinese Phys. B. 23 (2014).

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