Microstructural Simulations of Fission Gas Bubbles Generation and Grain Recrystallization in the High Burnup Structure of UO_2

Faris B. Sweidan[a], Ho Jin Ryu[a*]
[a] *Department of Nuclear and Quantum Engineering, KAIST, Yuseong-gu, Daejeon 34141, Republic of Korea*
**corresponding author: hojinryu@kaist.ac.kr*

1. Introduction

The microstructure of UO_2 nuclear fuel experiences severe irradiation damage. The periphery side of the fuel experiences significantly higher damage compared to the center of the fuel as it is enriched relative to the rest of the fuel by resonance neutrons which are absorbed by ^{238}U at the surface. This leads to excessive fission damage and the growth of fission gas bubbles. This localized unique damage is referred to as the rim structure or the High burnup Structure (HBS) region [1-4].

It has been experimentally observed that the temperature and the local burnup thresholds for the formation of the HBS range between 1000-1200 °C and 60-80 MWD/kgU, respectively [1, 5, 6]. However, due to the lack of in-situ microstructural characterization techniques during the reactor operation, the mechanism of the HBS formation is not fully known.

Mesoscale simulations have played a significant role in revealing the mechanism of microstructural phenomena that occur in materials. Kinetic Monte Carlo (kMC) [1, 8, 9, 10] and Phase-Field [11-13] simulations have been separately applied to understand the formation mechanism of the HBS of UO_2. However, in this study, a hybrid model that combines elements of the phase-field model, as well as the kMC Potts model, is used to simulate fission gas bubbles generation and grain recrystallization in the high burnup structure of UO_2. Compared to the reported studies, this study considers the effect of fission gas bubble pressure and the radial burnup and temperature profiles in the simulations.

2. Model Description

The hybrid phase-field Potts model is developed by Homer et al. [14]. This model combines Monte Carlo Potts methods and with the Cahn–Hilliard equation-based phase-field model. To apply this model to the HBS, The grains are assigned to one phase while the pores and bubbles are assigned as a second phase. Thus, the HBS is evolved if the system energy of the HBS is lower than that of the original structure in an irradiated UO_2. Therefore, the total system energy, E, is defined as the following equation [1, 2]:

$$E = \sum_{i}^{M}\left[Hf(S_i) + \frac{J}{2}\sum_{j}^{n}(1-\delta_{S_iS_j})\right] \quad \dots (1)$$

where E is the total energy of the system, H is the stored irradiation energy, f(S_i) has a value of one for the original grain sites and zero for the HBS grain sites, J is the boundary energy, δ_{SiSj} is the Kronecker delta function, M the total number of lattice sites, S_i is the site, n is the number of neighboring sites and is equal to 8 for 2D simulations, and S_j the nearest neighboring site.

Then, the standard Metropolis algorithm is applied to determine the probability of accepting the event based on the energy calculated in Equation 1. The probability is calculated by the following equation [1, 9, 14]:

$$P = \begin{cases} 1, & \Delta E \leq 0 \\ e^{\left(-\frac{\Delta E}{k_B T}\right)}, & \Delta E > 0 \end{cases} \quad \dots (2)$$

where k_B is the Boltzmann constant and T the simulation temperature.

The relationship between burnup (Bu) and porosity (P) in HBS is reported in [1] and it is obtained by a linear fitting from the experimental data in [4] as follows:

$$P(\%) = \begin{cases} 0.06 \cdot Bu, & Bu \leq 60 \\ -6.6 + 0.17 \cdot Bu, & 60 < Bu \leq 100 \\ 4.4 + 0.06 \cdot Bu, & Bu > 100 \end{cases} \quad \dots (3)$$

where P(%) is the porosity and Bu is the burnup in MWd/kgU. More details about the model are reported in [1, 14]. It is important to mention that the aim of using this model is to generate the amount of fission gas bubbles that correspond to a certain burnup, as reported in [1]. All the simulations were done using the open-source Stochastic Parallel PARticle Kinetic Simulator (SPPARKS) package developed by Sandia National Laboratories [15].

3. Preliminary Results

Before applying the fission gas bubble generation and grain recrystallization model, Potts grain growth model was used to generate the initial microstructure of UO_2. Grain growth was terminated when the average grain size reached 10 μm, similar to the grain size of fresh UO_2 fuel. Fig. 1 shows the initial microstructure obtained from Potts model.

After applying the modified model to the initial microstructure presented in Fig. 1. The simulation was conducted until the local burnup reached 110 MWd/kgU at a temperature of 923 K, which is the typical temperature of the HBS region in UO_2 fuel. The recrystallized grains size and the fission gas bubbles at that burnup are shown in Fig. 2. The average size of the recrystallized grains in the simulation is 180 nm, which matches the results reported in [1, 3, 4].

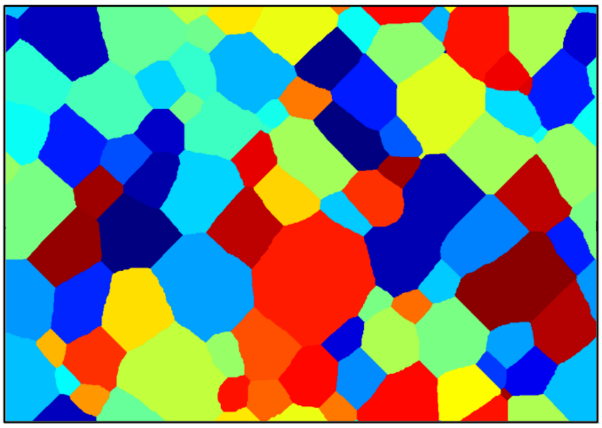

Fig. 1. Initial microstructure of the UO_2 rim region

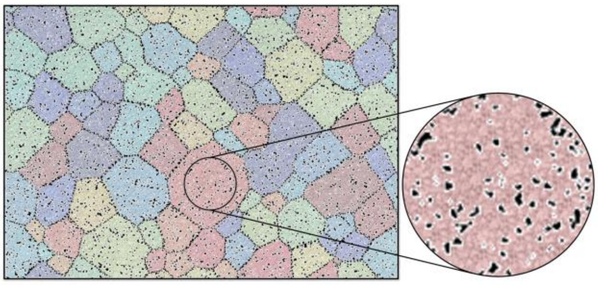

Fig. 2. Recrystallized Grains and fission gas bubbles rim region of in irradiated UO_2

However, in the current simulation results, the fission gas bubble average size is less than the experimental measurements. Improvements are necessary to be applied to take into account the growth of the fission gas bubble size due to the overpressurization resulting from the presence of fission gases.

4. Conclusions

The hybrid Potts phase-field model was utilized to simulate the evolution of the high burnup structure in the rim region of UO_2 nuclear fuel. These simulations represent the fission gas bubble generation and grain recrystallization that occur in that region. The results show that the original UO_2 grains are fully consumed by the recrystallized grains at a burnup of 110 MWd/kgU. In addition, recrystallized grains size shows good agreement with other simulation results [1] as well as experimental measurements [3, 4]. These simulation methods allow for the prediction of the mechanisms that occur under irradiation and that are observed experimentally.

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