Investigation of High Burnup Structure Evolution in UO_2 nuclear fuel Using Potts Model based on Dislocation Density

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1. Introduction

A high burnup structure (HBS), which is observed in the periphery of a high burnup UO_2 fuel, has very unique microstructure. It consists of very small grains and large bubbles instead of original grains [1,2], and has the thresholds of burnup and temperature for the HBS evolution [3-5]. Although observations on the HBS have been carried out to explain the HBS evolution mechanism, some observations showed contradictory results. The grain size effect was investigated by observing the Xe depression in the HBS, which showed that the grain size dependency [6]. Authors concluded that the dependency resulted from the HBS nucleation on grain boundaries [6]. However, it did not explain the decreasing grain size dependency at the higher burnup and there was still a contradictory experimental observation that the HBS transformation did not always begin on the grain boundaries [7,8].

In this study, a computer simulation using the Potts model was implemented for investigating HBS evolution. Although Potts model in the early study [9] used the experimentally fitted parameters, the parameters for Potts model in this study established on theoretical backgrounds.

2. Potts model

Potts model defines a microstructure as two-dimensional triangular lattice with a periodic boundary condition. The initial microstructures having average sizes of 6.39, 7.94, 9.62, 15.22, or 21.51 μm were implemented. Each site has a spin, S_i, representing a site state and a grain's crystallographic orientation. We assume that the neighboring sites having a same spin belong to the same grain, and the perimeters of the sites with different spins are a grain boundary.

The total system energy, *G*, was calculated by

$$G = \sum_{i}^{M}\left[Hf(S_i) + \frac{J}{2}\sum_{j}^{nm}(1-\delta_{S_iS_j}) \right] \qquad (1)$$

where *J* is a constant related to a boundary energy, $\delta_{S_iS_j}$ the Kronecker delta function, S_i the spin at chosen site, and S_j the spin at nearest neighboring site [9]. For the two-dimensional triangular lattice, *nm* is 6. *H* is the stored energy per site due to an irradiation. The function *f(S)* is one for original grains and zero for HBS grains. The porosity in UO_2 fuel can be obtained by a linear fitting from the experimental data [10].

The HBS was simulated as follows: For the grain growth step, a grain site was randomly chosen and a new spin at that site was randomly chosen. The energy change, ΔG , was used for the change probability, *W*, which was determined from

$$W = \begin{cases} \exp(-\dfrac{\Delta G}{k_B T}) & for \quad \Delta E > 0 \\ 1 \quad for & \Delta E \le 0 \end{cases} \qquad (2)$$

where k_B is the Boltzmann constant, *T* the simulation temperature [9]. For the bubble migration step, a bubble site and a nearest neighbor site, which was not a bubble, were exchanged. Then, the change probability was calculated.

The parameters used in this paper are summarized as follows:

$$J = \begin{cases} \gamma_{GB} S & \text{for grain boundary} \\ \gamma_P S & \text{for bubble surface} \end{cases}$$

where $\gamma_{GB} = \gamma_m \dfrac{\theta_i}{\theta_m}\left[1 - \ln\left(\dfrac{\theta_i}{\theta_m}\right)\right]$ [11].

$H = U_{dis} \cdot \rho_N \cdot A$ [12]

where $U_{dis} = \dfrac{Gb^2}{4\pi(1-\upsilon)} \ln\dfrac{r_1}{r_0} + \dfrac{Gb^2}{8\pi(1-\upsilon)^2}$,

$$\rho_N(t) = \frac{C_1}{C_2}\left[\frac{1-\exp(\sqrt{C_1C_2}\,t)}{1+\exp(\sqrt{C_1C_2}\,t)}\right]^2 + \rho_0 \text{ [13]},$$

$$C_1 = \left[\frac{\pi \nu_l D_i c_i^2}{\sqrt{2}\Omega^{\frac{5}{3}}}\right]^{\frac{1}{2}},$$

$$C_2 = \frac{\nu_l \left[f(\upsilon)/\pi \right]^{\frac{1}{2}}}{C_A C_\rho}.$$

3. Results and discussion

Fig.1 shows the effect of initial grain size on the HBS fraction at 923K. The HBS fractions sharply increase at 60 GWd/tM and the HBS is fully developed at 64 GWd/tM in all initial grain sizes. This threshold burnup for the HBS evolution agrees with the observed results [1,2,7]. The abrupt HBS fraction change means a change of the HBS evolution mechanism at 60 GWd/tM.

Below 60 GWd/tM the HBS grains are nucleated on the intergranular bubbles since the combination of grain boundaries and the bubbles' surfaces induces a high energy state, which makes the HBS evolution easy. Above 60 GWd/tM, however, intragranular bubbles can also contribute to the HBS nucleation as shown in Fig. 2. This nucleation site addition seems to weaken grain size dependency on the HBS evolution as the previously mentioned experiment [6].

Fig. 3 shows the temperature dependency on the HBS evolution. The simulated threshold temperature is 1400~1473K, which agrees with the observed result [5].

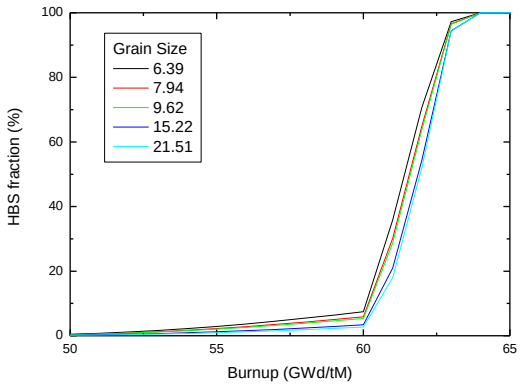

Fig. 1. Effect of grain size on HBS fraction at 923K

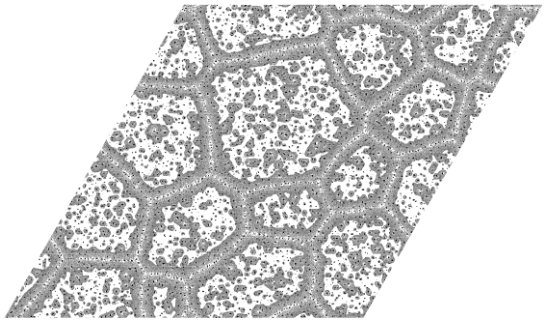

Fig. 2. Microstructures at 62GWd/tM

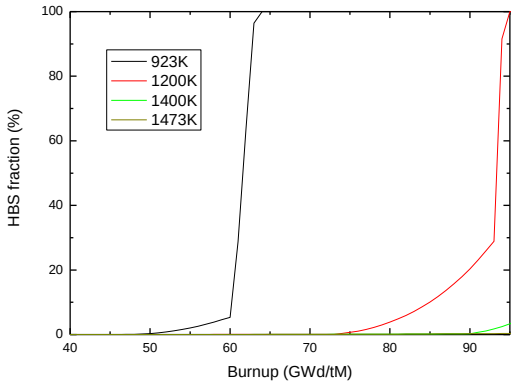

Fig. 3. Effect of temperature on HBS fraction

3. Conclusions

The Potts model, based on theoretical dislocation density, successfully simulated the main characteristics of HBS. It reproduced the thresholds of burnup and temperature for the HBS evolution. It also made the snapshots of the evolving HBS microstructure with time, which could explain why the contradictory experimental results existed.

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