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Preliminary Study of Fission Gas Bubble Growth and Interconnection using FDM

Dong-Hwa Lee *, Jang Soo Oh, Hyo Chan Kim
LWR Fuel Technology Research Division, Korea Atomic Energy Research Institute,
111 Daedeok-Daero 989 Beon-gil, Yuseong-gu, Daejeon, Korea
**Corresponding author: donghwalee@kaeri.re.kr*

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1. Introduction

Fission gas behavior in UO_2 fuel is important for fuel performance, as the diffusion of Xe within fission gas bubbles affects both fuel swelling and the amount of fission gas released into the fuel rod plenum[1,2].

Fission gas release (FGR) occurs in the three stages [1]. First, fission gas atoms move from grain to grain boundary. Second, gas bubbles form, grow, and connect on the grain face, linking with grain edge bubbles. Third, the gas moves through the interconnected grain edge tunnels to reach free surfaces for release.

Most fission gas release model [3,4,5] used for fuel performance calculations typically rely on partial differential equations (PDEs) to model transport of gas atoms to grain boundary that occurs in stage one. In stage two, bubble interconnection is modeled as threshold for gas that has reached the grain boundary. Fission gas exceeding this threshold is immediately released. And then, stage three is not considered by assuming that the transport of fission gas to free surfaces through grain edge tunnels in instantaneous. These modes overly simplify the real behavior of fission gas within the fuel. Therefore, these models have limited accuracy and applicability under different conditions, such as higher burnup or accident tolerant fuel (ATF). Improving the representation of fission gas bubble evolution, both within grain and grain boundary, is therefore important for achieving higher accuracy in fuel performance analysis.

KAERI have been developing microcell UO_2 fuel[6] as an ATF. In order to enhance the accuracy of predicting the fission gas release of the ATF, foundational research was conducted using a microstructure model to implement the growth and connection of fission gas bubbles. Diffusion equation is implemented using Finite Difference Method (FDM) to employ the diffusion of fission gas inside the grain. Bubble and grain boundary was described as distinct region compared to grain region, in order to demonstrate the growth and interconnection of bubble.

In this paper, we introduce a preliminary study of fission gas diffusion and growth-interconnection of bubble. A simple FDM based code was developed and its simulation result is presented and discussed.

2. Methodology

In this section, we discuss the methodology of describing fission gas diffusion and bubble growth-interconnection.

To solve problem using FDM, solution domain is discretized using uniform mesh. While density of fission gas is stored inside each mesh, bubble should be described using different domain compared to grain domain. Therefore, the solution domain is decomposed into three domains: gain, bubble, and grain boundary.

First, diffusion equation is solved inside grain domain to calculate distribution of fission gas. Next, amount of fission gas, absorbed to each bubble, is calculated. Then, pressure inside each bubble is evaluated and decide amount of 'bubble growth'. Finally, bubble growth direction is calculated and bubble domain is set again.

2.1 Diffusion of fission gas inside grain

We assume that fission gas freely diffuses inside the grain. Transient diffusion equation is:

$$\frac{dC}{dt} = \nabla \cdot (D\nabla C - \boldsymbol{v}C) + R \quad (1)$$

where, C is the density of fission gas, t is the time, D is the diffusivity, $\boldsymbol{v}$ is the advection velocity, and R is the source/sink of the gas. Note that, by changing the value R of each domain, production of fission gas inside grain can be described.

2.2 Bubble growth and interconnection

Bubble is described using bubble domain, and assumed to be growing larger. There are three steps in calculating bubble growth.

First step is to calculate amount of fission gas absorbed to bubble domain. It can be obtained by investigating sink boundary condition, which are bubble domain, while calculating diffusion equation inside grain domain.

Next step is to find the fission gas pressure inside each bubble. Diffusion equation inside bubble domain is calculate until it reaches equilibrium. Note that, amount of fission gas absorbed to bubble domain is imposed as source boundary condition. Once the fission gas density of each bubble is obtained, internal pressure of each bubble can be calculated using ideal gas law.

Finally, bubble growth is applied and domain is set again. Internal pressure of each bubble gives amount of bubble growth, while grain boundary gives preference of bubble growth direction.

In order to decide direction of bubble growth, filtering scheme on domain is applied. Internal pressure of all domains is blurred using filter (i.e. Gaussian, Shepard), while pressure inside grain domain is assumed to be 0, and pressure inside grain boundary is assigned to be constant. Among the blurred cells of mesh, the cells with high fission gas pressure are selected as next bubble domain, and its numbers are already calculated on previous step.

Filter blurring system provide a random smooth growth of bubble, while grain boundary value imposes preference of bubble growth direction along the grain boundary. It should be pointed out that bubbles grow not only along the grain boundaries, but also along grain interiors.

3. Result & Discussion

We introduce a simple simulation result of bubble growth. As illustrated in Fig. 1, circular bubbles are initially located on grain boundaries randomly, and all grain domain acts as fission gas source. Therefore, both fission gas creation and diffusion are imposed inside grain domain.

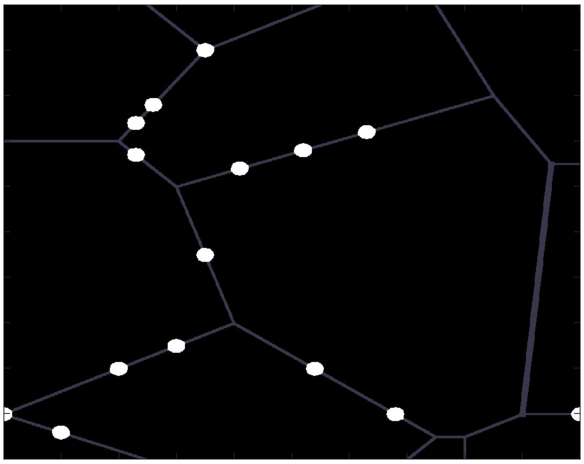
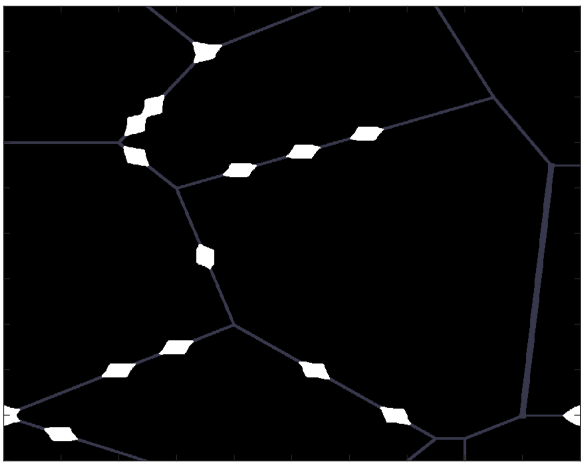


Fig. 1. Schematic illustration of microstructure and bubble.



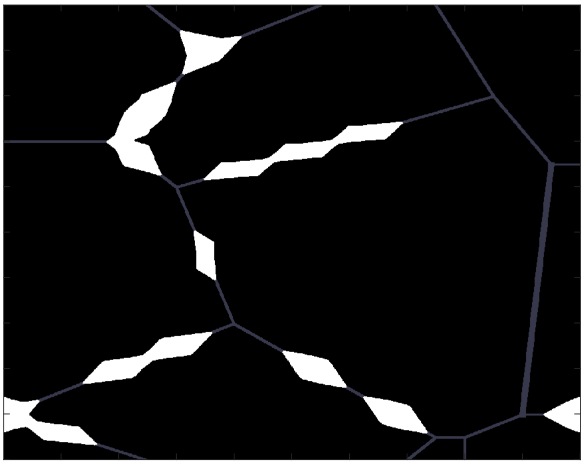


Fig. 2. Bubble growth and interconnection along time.

Fig. 2. shows the bubble growth and interconnection. Bubble grows mostly along the grain boundary, having diamond shape. Interconnection between bubbles are automatically achieved.

4. Conclusions

Preliminary study of microstructure-based fission gas diffusion and growth of bubble is achieved. Diffusion equation is implemented using FDM to solve diffusion inside grain and bubble. Creation of fission gas in grain and its diffusion is automatically achieved. Microstructure and bubble can be arbitrary assigned. Temperature or time dependent diffusivity and fission gas creation rate can be assigned.

The new approach can describe the interactions of various microstructure changes that occur within the fuel pellet during irradiation by using mechanistic models that define the physics of the phenomena. For this reason, it is expected to more accurately predict the growth and connection of fission gas bubbles in fuel pellet the evaluate FGR reduction effect caused by microcells in microcell UO2 pellet, which are candidates for ATF.

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