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ARTICLE

A New Mechanistic and Engineering Fission Gas Release Model for a Uranium Dioxide Fuel

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A mechanistic and engineering fission gas release model (MEGA) for uranium dioxide (UO_2) fuel was developed. It was based upon the diffusional release of fission gases from inside the grain to the grain boundary and the release of fission gases from the grain boundary to the external surface by the interconnection of the fission gas bubbles in the grain boundary. The capability of the MEGA model was validated by a comparison with the fission gas release data base and the sensitivity analyses of the parameters. It was found that the MEGA model correctly predicts the fission gas release in the broad range of fuel burnups up to 98 MWd/kgU. Especially, the enhancement of fission gas release in a high-burnup fuel, and the reduction of fission gas release at a high burnup by increasing the UO_2 grain size were found to be correctly predicted by the MEGA model without using any artificial factor.

KEYWORDS: UO_2 , fission gas release, INFRA, diffusion, bubbles

I. Introduction

During the irradiation of a fuel in a reactor, fission products are generated and accumulated by fission reaction. Among them, noble gases, such as xenon and krypton, are insoluble in the fuel, and therefore, they are released out of the fuel. In uranium dioxide (UO_2) fuel, which is the standard fuel of a light water reactor (LWR), fission gas release is considered as one of the life-limiting parameters due to the increase in fuel rod internal pressure by the released fission gases. Therefore, their behavior has been of primary concern since the fuel was first irradiated in a reactor. Fission gases that remain in the fuel also influence fuel performance characteristics, such as the degradation of thermal conductivity,¹⁾ fission gas release during a transient, and rim microstructure formation.^{2,3)} The behavior of fission gases depends upon the irradiation conditions of the fuel, such as the temperature and fission rate. With the help of advanced electron microscopy technologies, such as scanning electron microscopy (SEM), electron probe microanalysis (EPMA) and transmission electron microscopy (TEM), the mechanisms and paths of the fission gas release out of the UO_2 fuel have almost been identified.^{4,5)} However, the satisfactory actual prediction of the fission gas release in the fuel rod during irradiation in the reactor whose conditions vary with time and space by fuel rod performance analysis codes has not been achieved yet.

This work is performed to develop a fission gas release model that is based upon its release mechanisms and practically applicable to a fuel performance analysis code. In real-

ity, during fuel irradiation, there exist variations in parameters, such as the temperature, fission rate and fuel microstructure with the time and space. Therefore, it is almost impossible to take them all into account in the prediction of the fission gas release. As such, engineering simplification according to the relative importance of different mechanisms and parameters could make the prediction of the fission gas release more efficient and reliable, and help to clarify the important parameters in the fission gas release behavior. The fission release model can be used to predict the fission gas release behavior practically and reliably under diverse conditions in both fuel irradiation histories and as-manufactured fuel data.

II. Modeling of a Fission Gas Release in UO_2 Fuel

1. Review of Fission Gas Release Mechanisms

The behavior of fission gas release in uranium dioxide fuel in an LWR has been studied for over fifty years and its mechanisms have almost all been identified. Among the mechanisms of fission gas release are the diffusion of fission gases out of the fuel, direct releases, such as recoil and knockout releases, and release by fuel cracking. Recoil release is the release of fission gases with a high kinetic energy right after fission near the external surface. Knockout release is the release of the fission gases near the external surface by collision with fission products or primary knock-on atoms.⁶⁾ During irradiation, fuel pellet cracking could occur by thermal tensile stress due to a steep temperature gradient. Fuel cracking increases the probability of fission gas release by diffusion and direct and recoil releases due to an increase in fuel surface to volume ratio.

Fission gas release during fuel irradiation by nondiffusion-

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al release, such as direct and recoil releases, may be less than 1%. Therefore, its effect on the fuel behavior is considered to be not significant. The diffusion of fission gases is the dominant fission gas release mechanism in the UO_2 fuel in an LWR under normal operation conditions. Fuel temperatures during normal irradiation conditions in an LWR are around 1,100–1,400°C at the center of the fuel and 400–600°C at the surface of the fuel pellet. It is less probable that the fuel temperature becomes higher than 1,600°C during the normal operation conditions. Therefore, the fuel temperature is not high enough for UO_2 grain growth that is known to occur at a temperature higher than 1,600°C. Key variables in the fission gas release may be the temperature, the diffusion coefficient of the fission gases, the production rates of the fission gases, and the grain size. The diffusion of the fission gases from inside the grain to the grain boundary can be affected by the traps inside the grain, such as the fission gas bubbles of nanometer size,⁷⁾ and the precipitates of the fission products.⁸⁾

Fission gas atoms generated by fission inside a UO_2 grain tend to diffuse to the grain boundary to form fission gas bubbles. The grain boundary can be simply classified into the grain face and the grain edge.⁴⁾ The grain face boundary is shared by two grains, while the grain edge boundary is shared by three grains and could behave like dislocation lines. The bubbles at the grain edge can easily grow along the line of the grain edge; thus, there is a high probability of the interconnection of the bubbles along the grain edge line by bubble growth. By the interconnection of the bubbles along the grain edge, the bubbles can grow to eventually touch the fuel external surfaces, which are called open bubbles and then the fission gases in these open bubbles are instantaneously released out of the fuel. The bubbles formed in the grain face boundary have a lenticular shape,⁴⁾ and they are found to be evenly distributed under normal irradiation conditions in an LWR. Since the grain face bubbles are less mobile than the grain edge bubbles, the grain face bubbles can have a higher internal pressure and may start to grow to achieve interconnection at a temperature higher than 1,600°C. In the postirradiation annealing tests at a high temperature, the fission gases in the grain face bubbles were found to grow and touch the grain edges to form more stable bubbles at the grain edges.⁹⁾ When the bubbles at the grain edge and grain face become open to the external surface, the fission gases in the open bubbles are released instantaneously. Then, the open bubbles may remain open during irradiation, and therefore, the fission gases that diffuse to the open bubbles later are instantaneously released out of the fuel. The open fraction of bubbles in the grain boundary increases with burnup. Therefore, the fission gas release can be enhanced at a high burnup due to the accumulation of the open bubbles or the open channels in the grain boundary.

In addition to noble gases, such as xenon and krypton, volatile gases, such as iodine and cesium, whose boiling temperatures are 184 and 669°C, respectively, can contribute to the nucleation, growth and interconnection of bubbles, during the irradiation of which, the temperature is higher than their boiling temperature.¹⁰⁾ At a temperature higher

than 1,600°C, grain growth can occur in a UO_2 pellet. A grain grows with the movement of the grain boundary. As the grain boundary moves, fission gases in contact with the moving grain boundary are swept and precipitated into the bubbles at the grain boundaries. This mechanism is called grain boundary sweeping. The fission gas bubbles in the grain boundary could be destroyed by collision with the fission fragments or the primary knock-on atoms.¹¹⁾ The destruction or resolution probability of the fission gas bubbles may depend upon the bubble size and fission rate. Even though the bubbles at the grain boundary are destroyed by the fission fragments, there may be a high probability that the fission gases in the destroyed bubbles return to the grain boundary to form bubbles again due to a short traveling distance. Therefore, the net effect of a fission gas bubble resolution at the grain boundary would be similar to a decrease in the effective diffusion coefficient of fission gases. During the recombination of the displaced atoms in the lattice structure near the fission spikes, the displaced fission gas atoms may be more easily concentrated to form bubbles in the grain boundary, so that there could be a biased fission gas bubble precipitation or nucleation in the grain boundaries.

Fission gas release could increase during the power or temperature transients. During a slow power transient, fission gases are released by the enhanced diffusion due to a high temperature. During fast transients, such as a fast power ramp and a reactivity-induced transient, in which the power increases very fast, in less than a second, the fission gases in the grain boundary bubbles are released by the intergranular and intragranular crackings of the fuel. The cracking or separation of the grain boundaries could occur at a low stress when the fission gas bubbles exist at the grain boundaries. Therefore, the amount of released fission gases during a fast transient could be proportional to the inventories of the fission gases in the grain boundary bubbles and the extent of grain boundary separation.

At a burnup higher than 70 MWd/kgU, the fuel microstructure is found to be transformed to the rim microstructure where the fuel grains are very finely divided by diameters of less than 1 μm and the fission gas bubbles in the rim microstructure region are found to be larger than the finely divided grains.^{2,3,12)} The fission gas bubbles are not randomly but uniformly distributed; thus, there is a lower probability of bubble interconnection. Therefore, it is less probable that the fission gases in the bubbles in the high-burnup structure region are released by the bubble interconnection network during a normal operation. However, during fast transients, such as a reactivity-initiated accident (RIA), the fission gases in the high-burnup structure region could be released by grain boundary separation or cracking through the grains.^{13,14)}

2. Modeling of Fission Gas Release

The possible mechanisms of fission gas release were briefly reviewed in section II.1. For the modeling of the fission gas release to be used in the fuel performance analysis code, it is desirable that the relative importance of each mechanism is estimated to derive the dominant mechanisms that need to be primarily modeled. It is not practical to try to con-

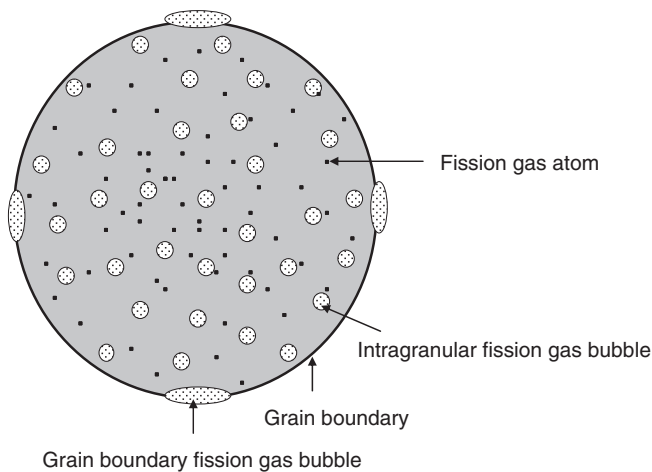


Fig. 1 Fission gas behavior in a single grain

sider all the possible mechanisms since some of them cannot be determined separately.

The purpose of the fission gas release modeling is to predict the fuel behavior that could affect the fuel integrity and safety, and also to guide fuel design improvements. Therefore, the fission gas release model needs to predict correctly the phenomena identified through the fuel irradiation tests, such as a high fission gas release at a high power, a low fission gas release for a large grain pellet and an enhanced fission gas release at a high burnup.

For the case of a fission gas release less than 1% at a burnup lower than about 40 MWd/kgU-rod average under normal LWR operation conditions, the diffusional fission gas release processes may not be fully developed enough; thus, nondiffusional fission gas releases, such as the direct and recoil releases helped by pellet cracking, may be the primary mechanisms of the fission gas release. For the case of a fission gas release of 1–5% at a burnup lower than about 60 MWd/kgU-rod average, the diffusional release could have occurred locally in high-temperature regions, such as the fuel center. For the case of a fission gas release higher

than 5% at a burnup higher than about 60 MWd/kgU-rod average, the diffusional fission gas release may considerably progress in the fuel. Therefore, a fission gas release by diffusion is the dominant mechanism in the UO_2 fuel under normal LWR irradiation conditions. The processes in the diffusional fission gas release include fission gas generation inside a fuel grain, diffusion to grain boundaries, the formation of fission gas bubbles at the grain boundaries, the interconnection of the bubbles by growth at the grain edge and grain face, the instantaneous release of fission gases from open bubbles, the formation of open channels through which fission gases are released, and the accumulation of the open channels with burnup. The following are the simplified illustrations of the fission gas release processes by diffusion, which are applied in a new mechanistic and engineering fission gas release model, or MEGA model.

Figure 1 illustrates the behavior of the fission gases inside the grain assumed to be spherical. Fission gas atoms diffuse to the grain boundary and form a fission gas bubble there. Inside the grain, there exist very small bubbles of nanometer size, which are formed with the help of the displacement and recombination of the lattice atoms along the fission fragment track. They could hinder the diffusion of the fission gases by absorbing them. The concentration of these bubbles inside the grain becomes in equilibrium by the continuous nucleation and destruction of the bubbles during irradiation. Inside the grain, the effects of the nanosize bubbles and fission products precipitating upon the diffusion of the fission gases cannot directly be determined in the experiments, and therefore, such effects need to be determined by an indirect way, *i.e.*, by fitting the model prediction to the fission gas release data base.

Figure 2 shows the state at which the fission gas bubbles are formed at the grain edge, but they are not interconnected as yet, such that a diffusional fission gas release has not occurred. **Figure 3** illustrates the state at which there are some cases of bubble interconnection at the grain edge and gases in some of the grain edge bubbles near the external surface are released. It can be around 1% fission gas release. This

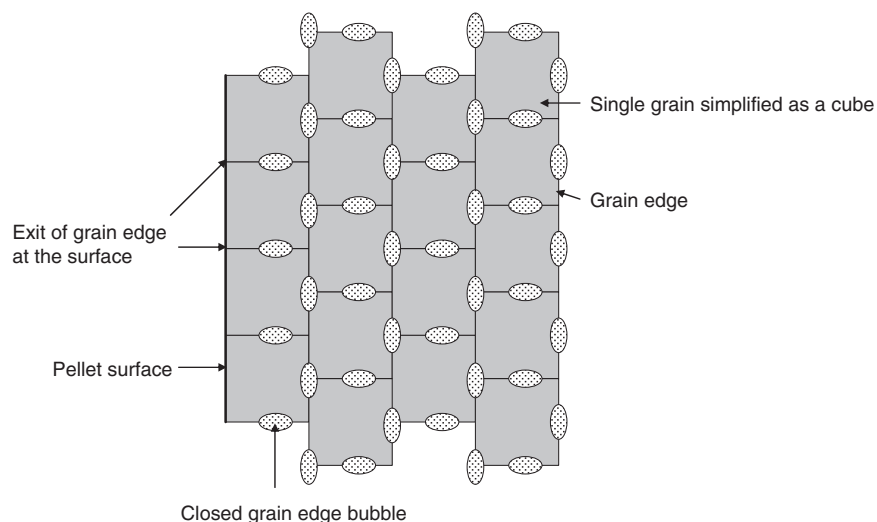


Fig. 2 Formation of fission gas bubbles at the grain edge

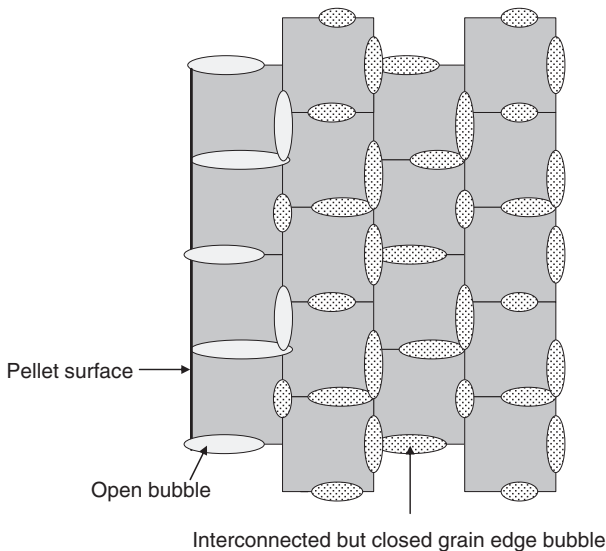


Fig. 3 Grain edge bubbles at a low fission gas release state

is greater than the amount of the fission gases released by nondiffusional release mechanisms, such as those of the direct and recoil releases.

Figure 4 illustrates the effect of pellet cracking on the fission gas release. Fuel pellet cracking induced by a thermal tensile stress could influence the fission gas release by introducing a new free surface and subsequently by opening the closed fission gas bubbles in the grain boundary, which exist in a closed state before the pellet cracking. Therefore, the pellet cracking may be one of the primary causes of the disagreement between the measured and predicted fission gas releases in the low and medium burnup ranges. Preventing the pellet cracking could reduce the fission gas release.

Figure 5 illustrates the bubbles in the grain face and at the grain edge. The fission gas bubbles in the grain face have a lenticular shape and are uniformly distributed in the grain face. The bubbles at the grain edge can be elongated along

the grain edge line. The fuel in Fig. 5 is supposed to be in a state similar to that in Fig. 2.

Figure 6 shows the state at which all the fission gas bubbles at the grain edge are interconnected and all the fission gases inside them are released. This can be found after a postirradiation annealing test of the fuel at a temperature probably higher than 1,600°C.⁹⁾

Figure 7 shows the state at which the bubbles in the grain face are interconnected with each other and also with the grain edge bubbles. The fission gases at the grain edge and in the grain face bubbles that are interconnected with the grain edge bubbles are released. This can be found in a postirradiation annealing test at a temperature probably higher than 1,800°C.⁹⁾ Fractional fission gas release may be higher than 40%.

Based upon the above diffusional fission gas release processes in a UO_2 fuel, the MEGA model was developed. The schematic diagram of the MEGA model is shown in **Fig. 8**. The MEGA model considers only the diffusional fission gas release. The other mechanisms, such as direct release, pellet cracking and grain growth, were not explicitly considered in the MEGA model.

The diffusion of the fission gases from inside the grain to the grain boundary is calculated first. This diffusional release can be obtained by solving the time-dependent diffusion equation as shown below.⁸⁾

$$\frac{\partial C(r,t)}{\partial t} = D_{\text{eff}}(t) \left(\frac{\partial^2 C(r,t)}{\partial r^2} + \frac{2}{r} \frac{\partial C(r,t)}{\partial r} \right) + p(t) \quad (1)$$

Here, r is the radial position in the grain sphere, t is time, D_{eff} is the effective diffusion coefficient of the fission gases, $C(r,t)$ is the concentration of the fission gases in the grain, and $p(t)$ is the production rate of the fission gases in the grain.

The fuel grain is assumed as a sphere and the assumed boundary condition is that the fission gas concentration at the grain boundary is always zero, which is reasonable, considering that the fission gas atoms diffusing to the grain

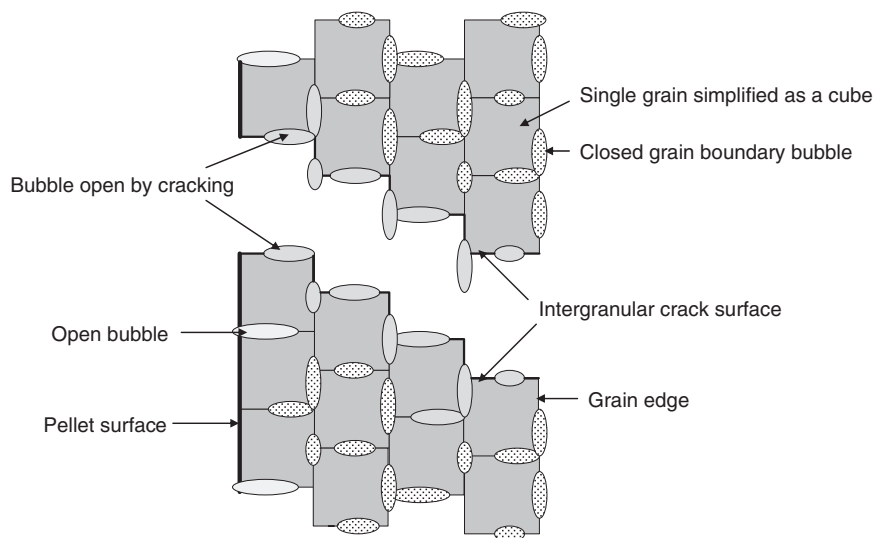


Fig. 4 Fission gas release by pellet cracking

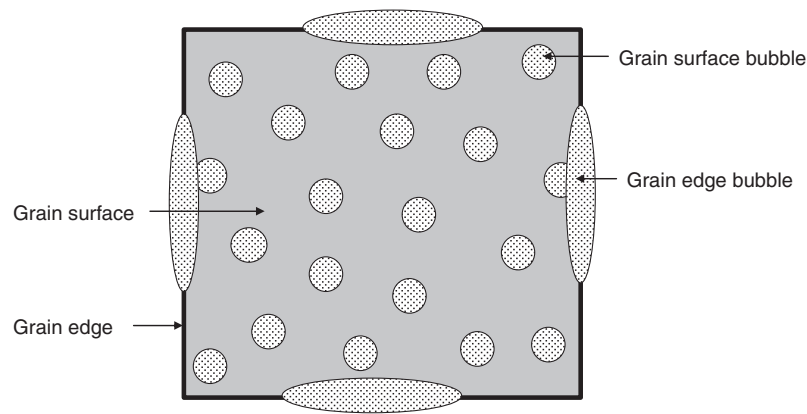


Fig. 5 Grain surface bubbles at a low fission gas release state

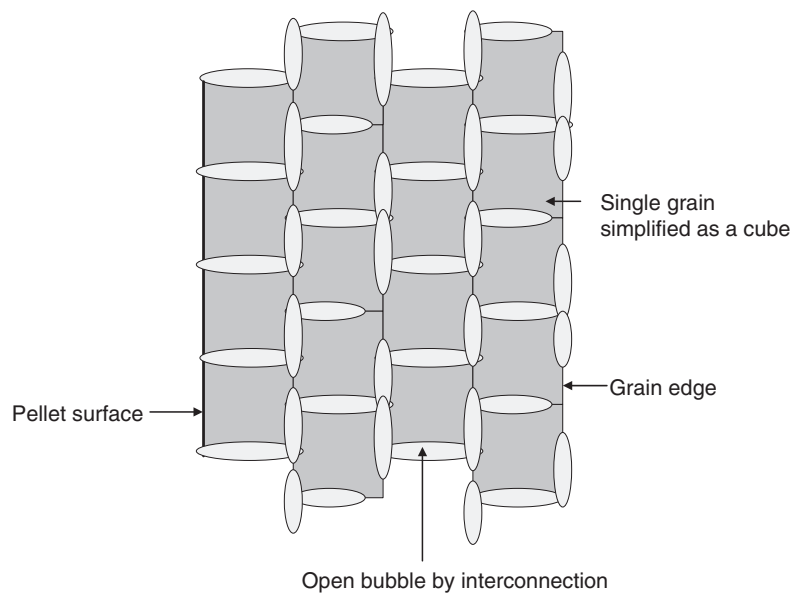


Fig. 6 Fully interconnected grain edge bubbles at a high fission gas release state

boundary are easily nucleated as or absorbed by the fission gas bubbles at the grain boundary. Hindering of the fission gas diffusion inside the grain by the fission gas bubbles of nanometer size and the fission product precipitates can be considered using the effective fission gas diffusion coefficient.⁸⁾ Then, Eq. (1) can be solved using the ANS 5.4 solution scheme^{14,15)} that gives the analytical solution, therefore saving a lot of computing time to solve the time-dependent differential equations when time-varying variables, such as the temperature, diffusion coefficient and fission gas generation rate, are assumed to be constant in a fixed time step and to change by a step in the next time step.

The grain boundary can be divided into the grain face and grain edge.⁴⁾ The fission gas bubbles at the grain edge can grow easily along the grain edge line to be interconnected with the neighboring grain edge bubbles, and then finally, they could become open to the external surface.

The effect of the bubble interconnection at the grain edge on the fission gas release can be estimated by the following simple method. When a UO_2 grain is assumed as a cube whose length is l and the total length of the grain edges in

a cube is $12l$, the number of grain edge exits per unit fuel external surface area is $2/l^2$ and the number of grains per unit fuel volume is $1/l^3$, as shown in Fig. 2. Then, the total length of the grain edges per unit fuel volume is $6/l^2$. By assuming an effective linear range near the grain edge where all the fission gases in the grain are released to the grain edge to form the grain edge bubbles as x , an effective volume is postulated as that of a cylinder with radius x centered along the grain edge line. Then, the effective volume per unit fuel volume is $6\pi(x/l)^2$. Also, by assuming the length of the grain cube that is equivalent to the grain size to be $10\text{ }\mu\text{m}$ and the effective range from the grain edge to be $1.0\text{ }\mu\text{m}$, the fraction of the effective volume is 0.19. Therefore, a fission gas release up to 19% could be accounted for by a diffusional release through the grain edge bubble interconnection from the fuel in an effective range.

The interconnection of the fission gas bubbles at the grain edge where three grains are interfacing is dominant, while the interconnection of the fission gas bubbles in the grain face where two grains are in contact is not significant at a temperature below about $1,600^\circ\text{C}$.¹⁷⁾ Therefore, the fission

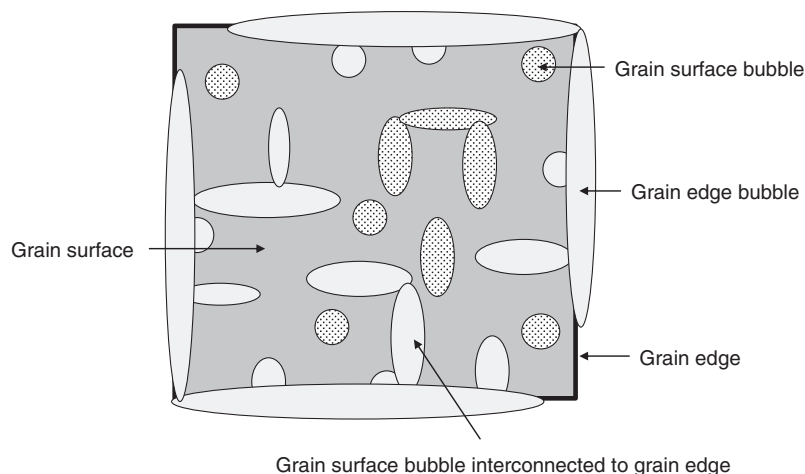


Fig. 7 Grain surface bubbles at a very high fission gas release state

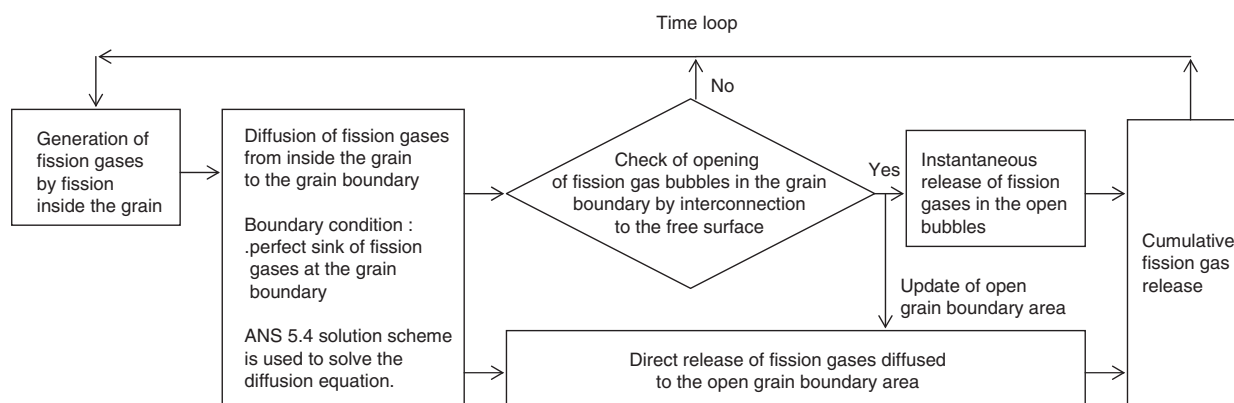


Fig. 8 Schematic diagram of the MEGA model

gas bubbles at the grain edge play a major role in a fission gas release under the normal irradiation conditions of an LWR fuel. Postirradiation annealing experiments show a much higher probability of bubble interconnection at the grain edge than in the grain face.⁹⁾ It can be assumed that at a certain concentration of the bubbles or fission gases at the grain edge, a certain fraction of the bubbles at the grain edge are open to the external surface and a certain fraction of the grain edge surface is open to the external space; therefore, the open grain edge could act as an open channel, such that the fission gases that directly diffuse to the open channel later on are instantaneously released to the external space.

In the MEGA model, the above behavior of a fission gas bubble in the grain boundary is simplified as follows. At a critical concentration of the fission gases in the grain boundary, a certain fraction of the grain boundary bubbles is assumed to be interconnected with each other and then open to the external surface to release the fission gases in those bubbles. It is assumed that a certain fraction of the grain boundary area becomes open to the external surface and remains open at the critical concentration of the fission gases in the grain boundary. Later, when the fission gas concentration at the grain boundary reaches the critical value again, the same process is repeated, as shown in Fig. 8.

Among the parameters that affect a fission gas release, the diffusion coefficient, the critical concentration of the fission gases in the grain boundary open to the external surface by bubble interconnection, fractions of both the open fission gas bubbles and the open grain boundary area in the grain boundary at the critical concentration, and the resolution of the fission gas bubbles in the grain boundary by the fission fragments could have a combined effect on the fission gas release. Except for the diffusion coefficient, the other parameters cannot be directly obtained by experimental measurement. There have been many attempts to analytically derive these parameters, such as the critical concentration of the fission gases in the grain boundary, and the fraction of the bubbles and the fractional surface area covered by the open bubbles at the critical concentration.^{4,18,19)} However, the ideal percolation theory such that spherical fission gas bubbles of the same size are randomly generated in the grain boundary cannot be applied since the grain size of the UO_2 fuel is not uniform and the fission gas bubbles in the grain face and at the grain edge are not of the same size and shape. Therefore, the above three parameters, such as the critical concentration of the fission gases in the grain boundary, the fraction of the open grain boundary fission gas bubbles at the critical concentration and the fraction of the open grain

boundary areas at the critical concentration are eventually derived by a comparison of the MEGA model predictions with the measured fission gas release data base.

III. Validation and Verification of the MEGA Fission Gas Release Model

A fission gas release data base includes the fuel manufacturing, fuel irradiation and postirradiation examination data. Uncertainties or errors can be introduced into these data generation steps. There are also uncertainties in the fuel behavior itself, such as that in the fuel temperature estimation, due to a variation in fuel thermal conductivity, fuel relocation and fuel gap conductance. To validate the MEGA fission gas release model, fission gas release data bases with their reliability qualified by many users would be desirable. The primary objective of the MEGA fission gas release model is to predict the fission gas release up to a high burnup at which the diffusional fission gas release process considerably progresses, such that the fractional fission gas release must be higher than several percent to become an important parameter for the fuel in-pile behavior. Actually, a fission gas release less than 5% may not have a significant effect on fuel rod integrity, when considering that the current fuel rod is designed to maintain its mechanical integrity up to a fission gas release higher than 10% at a burnup of 60 MWd/kgU. The data base in which the fractional fission gas release is less than 1% can be affected by statistical scattering characteristics, such as the cracking of the fuel pellet, as-manufactured open porosity in the fuel, and the variation in fuel temperature due to relocation by the cracking of the pellet. Therefore, this data base is not adequate for validating diffusional fission gas release models, such as the MEGA model.

First, through the sensitivity analysis of the parameters in the MEGA model, the relative importance of the parameters can be evaluated. The known parameters in the fission gas release can be the diffusion coefficient of the fission gases, the grain size, the production rate of the fission products, and the temperature. The unclear parameters may be the shape and size of the fission gas bubbles in the grain boundary, the critical concentration of the fission gases at which a certain fraction of the fission gas bubbles at the grain boundary become open to the external space through the interconnection of the bubbles, the fractions of both the open fission gas bubbles and the open area in the grain boundary at a critical concentration of the fission gas bubbles, and the resolution probability of the fission gas bubbles in the grain boundary. The key parameters were selected for the sensitivity analysis of the MEGA model. They are the diffusion coefficient of the fission gas, the temperature, the fuel grain size, the critical concentration of the fission gases at the grain boundary for the opening of the fission gas bubbles to the surface by interconnection, and the fractions of the open fission gas bubbles and the open grain boundary at the critical concentration.

The MEGA fission gas release model was inserted into the fuel performance analysis code INFRA.²⁰⁾ **Figure 9** is the representative high-power and high-burnup PWR fuel rod

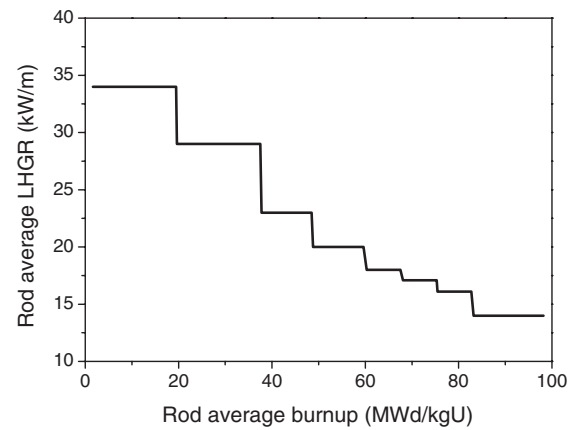


Fig. 9 High-power and high-burnup fuel rod power history

Table 1 Reference parameters in the MEGA model

| Parameter | Value |
|---|--------------------|
| Critical concentration of the fission gases in the grain boundary [atoms/m ²] | 4×10^{20} |
| Fraction of the open grain boundary fission gas bubbles at the critical concentration | 0.016 |
| Fraction of the open grain boundary areas at the critical concentration | 0.0016 |

power history used in the sensitivity analysis.²¹⁾ The optimized parameters in the MEGA model used in the reference calculations, such as the critical concentration of the fission gases in the grain boundary and the fractions of both the fission gas bubbles and the grain boundary area in the grain boundary to be open at the critical concentration, are given in **Table 1**. For the diffusion coefficient of the fission gases, the diffusion coefficient derived by Turnbull *et al.*²³⁾ is used in the reference calculations. Due to the variations in the size and shape of the fission gas bubbles and UO₂ grains, the values of such parameters cannot be determined analytically, as explained in section II.2. Therefore, they were derived by a comparison of the MEGA model prediction with the measured fission gas release data. In the MEGA model, the resolution of the fission gases in the grain boundary into the grain by fission fragments is not explicitly considered. The effects of volatile fission gases, such as iodine and cesium, which could exist as a gas state during fuel irradiation, on fission gas bubble behaviors, such as nucleation, growth and interconnection, are also not taken into account explicitly in the MEGA model. By considering the difficulty in quantifying the fission gas bubble resolution, it can be said that the effective diffusion coefficient and the other parameters shown in Table 1, which were derived based upon the measured fission gas release data base, could implicitly consider the effects explained above.

Figure 10 compares the effects of the diffusion coefficient on the fission gas release. By changing the diffusion coefficient by a factor of two, the fission gas release could vary by 30–40%. **Figure 11** compares the different diffusion co-

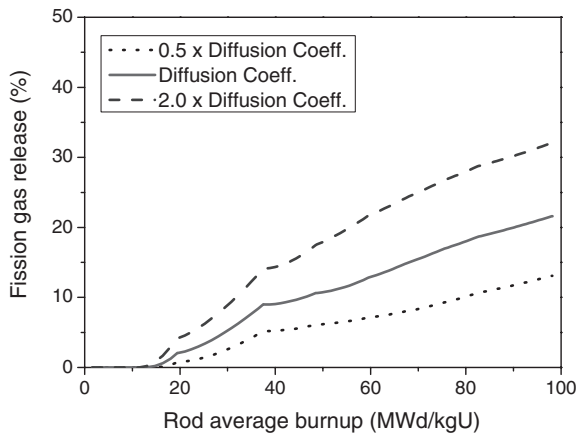


Fig. 10 Effect of the diffusion coefficient on the fission gas release

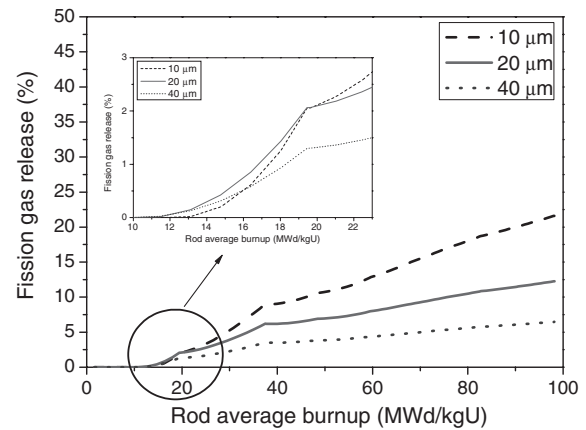


Fig. 13 Effect of the grain size on the fission gas release

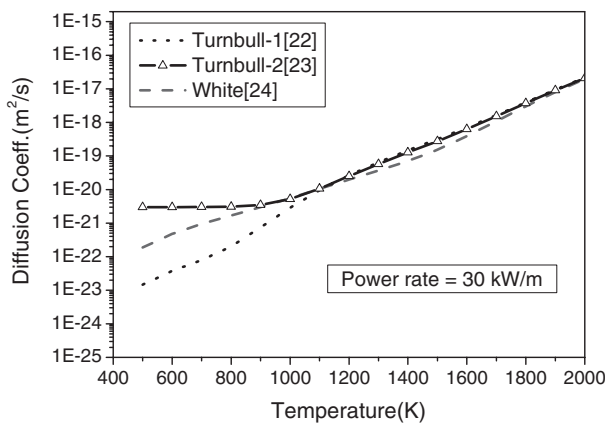


Fig. 11 Diffusion coefficients of the fission gas in UO_2

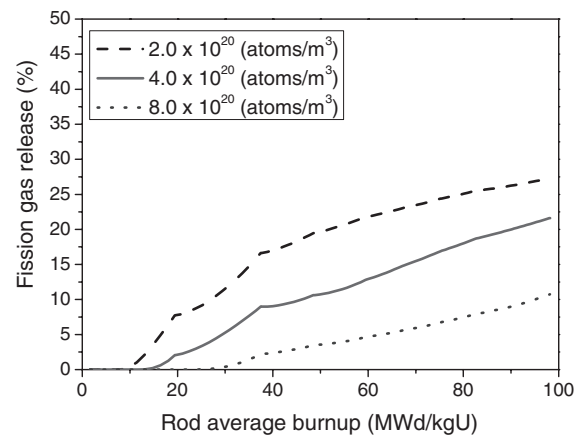


Fig. 14 Effect of the critical concentration of the fission gases on the fission gas release

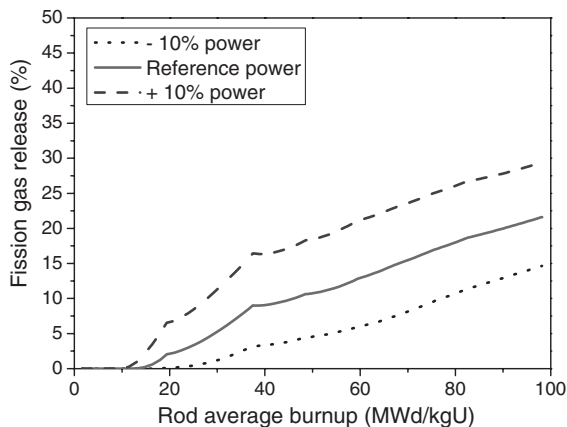


Fig. 12 Effect of the power level on the fission gas release

efficients of the fission gases.^{22–24}) There is a large difference in the low temperature at which the irradiation-induced diffusion makes a dominant contribution. In the MEGA model, the Turnbull-2 model²³⁾ is used. **Figure 12** shows the effect of the fuel temperature or power level on the fission gas release, which directly affects the diffusion coefficient of the fission gases.

Figure 13 shows the effect of the UO_2 grain size. By increasing the grain size by two times, the fission gas release at a high burnup can be reduced by about 30–40%. In a low burnup, less than about 15 MWd/kgU, there is not much grain size influence on the fission gas release, and even the larger grain fuel gives a slightly higher fission gas release, which is sometimes found in the fuel irradiation tests,^{25,26)} since the fission gas concentration per unit grain boundary area increases faster with burnup for a larger grain fuel. Therefore, bubble interconnection occurs earlier. It is notable that grain volume corresponding to a unit grain boundary area is larger for a larger grain, while the grain boundary area corresponding to a unit grain volume is smaller for a larger grain. **Figure 13** shows that the MEGA model correctly predicts that the unique behavior of fission gas release with burnup depends upon the grain size.

Figure 14 shows the effect of the critical concentration of the fission gases in the grain boundary on the fission gas release. By lowering the critical concentration, the fission gas release by fission gas bubble interconnection starts at a lower burnup. **Figure 15** shows the effect of the fraction of the open fission gas bubbles at the critical concentration, which is instantaneously released out of the fuel. The fission gas re-

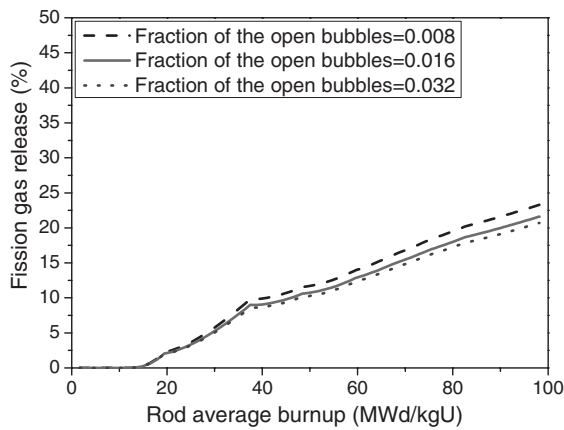


Fig. 15 Effect of the open bubble fraction on the fission gas release

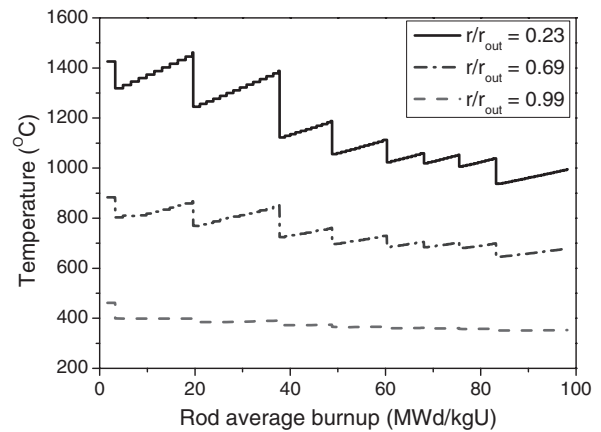


Fig. 18 Variation in fuel temperature with burnup

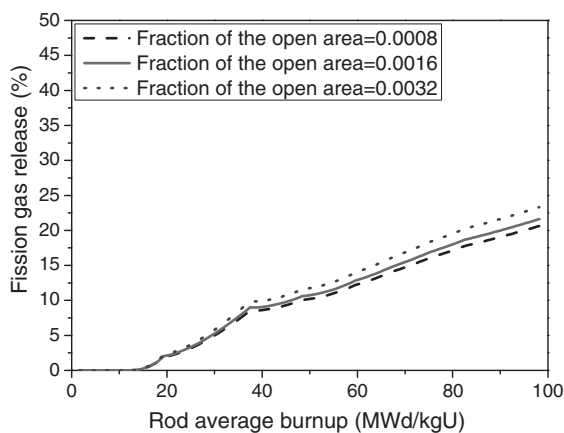


Fig. 16 Effect of the grain boundary open area fraction on the fission gas release

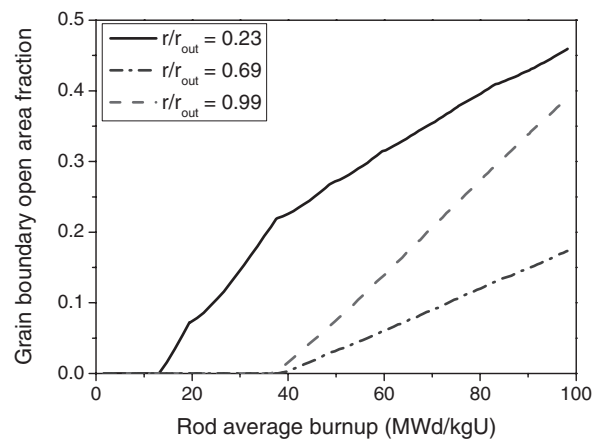


Fig. 19 Variation in grain boundary open area fraction with burnup

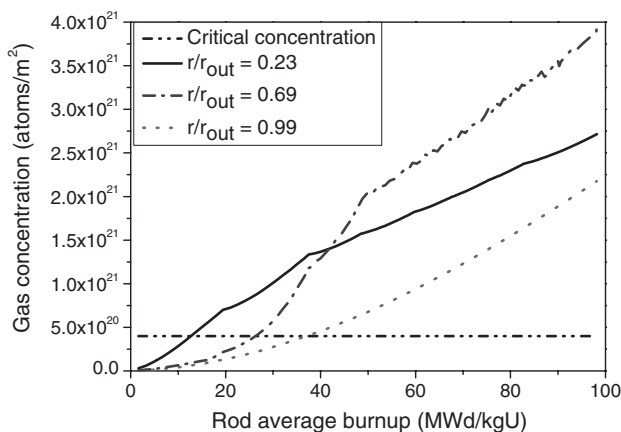


Fig. 17 Variation in fission gas concentration in the grain boundary with burnup

lease increases with this fraction. **Figure 16** shows the effect of the fractional open grain boundary area at the critical concentration of the fission gases at the grain boundary. Both the amount of released fission gases and the enhancement at a high burnup due to the accumulation of the open channels

depend upon this fraction. **Figures 17–19** show the variations in fission gas concentration in the grain boundary, temperature and fractional grain boundary area open to the external surface with the burnups in the fuel center, midradius and periphery regions. In the high-temperature fuel center region, fission gas release occurs earlier due to the rapid diffusional movement of the fission gas atoms. At the pellet periphery, athermal diffusion of fission gases is enhanced due to a high fission density. Through the sensitivity analysis of the key parameters in the fission gas release, it was verified that the MEGA model correctly predicts the effects of the key parameters on the fission gas release, which are generally known from the fuel irradiation tests.

Figure 20 compares the prediction of the MEGA model in the INFRA code for the measured fission gas release data with the burnup,²⁰⁾ showing that the MEGA model could predict the fission gas release quite well up to a high burnup without any artificial factors, such as a burnup enhancement factor. Even though the power level of the fuel rods is low at a high burnup as shown in **Fig. 21**, the fission gas release is still enhanced in **Fig. 20**, which is due to the accumulation of the open grain boundary area with the burnup in the MEGA model.

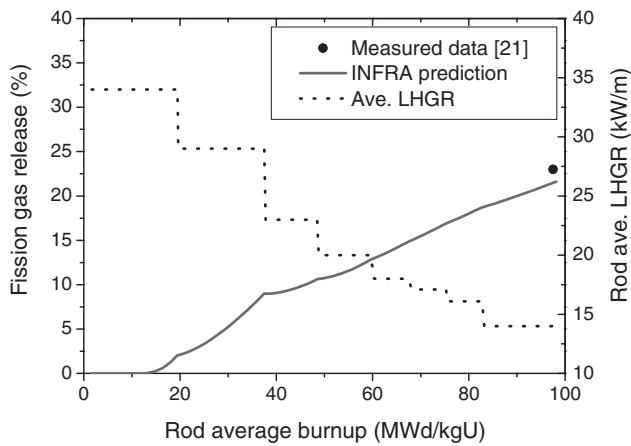


Fig. 20 Comparisons of the MEGA fission gas release prediction with the measured data from PWR²¹⁾

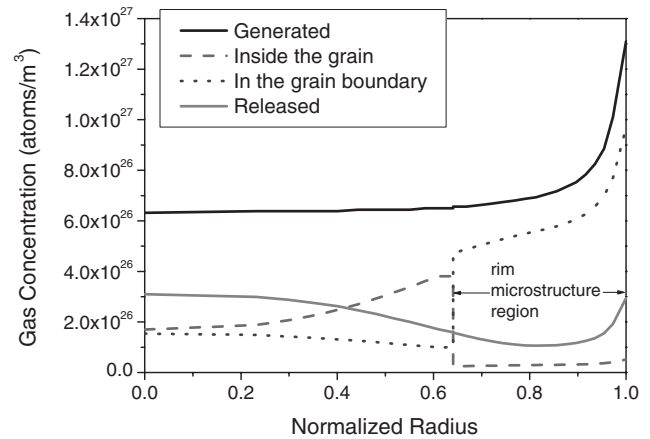


Fig. 23 Radial distribution of the fission gases at 94 MWd/kgU

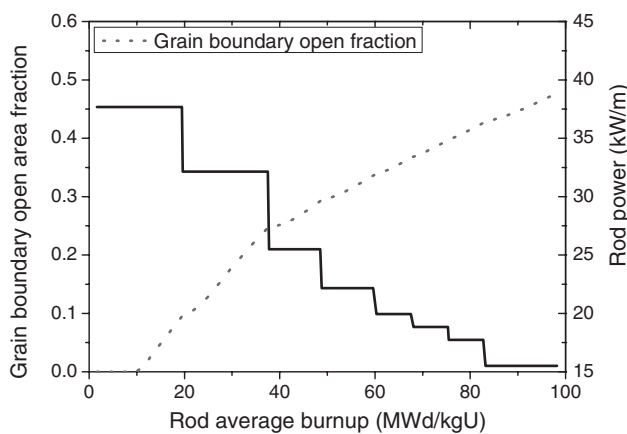


Fig. 21 Variations in grain boundary open area fraction and power with burnup

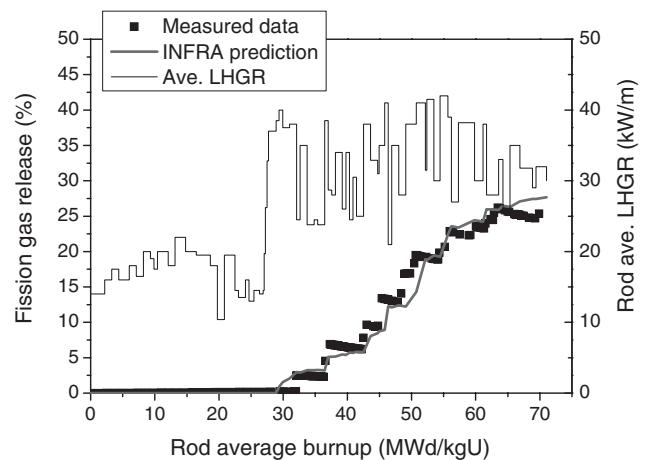


Fig. 24 Comparison of the MEGA fission gas release prediction with the measured data from research reactor²⁷⁾

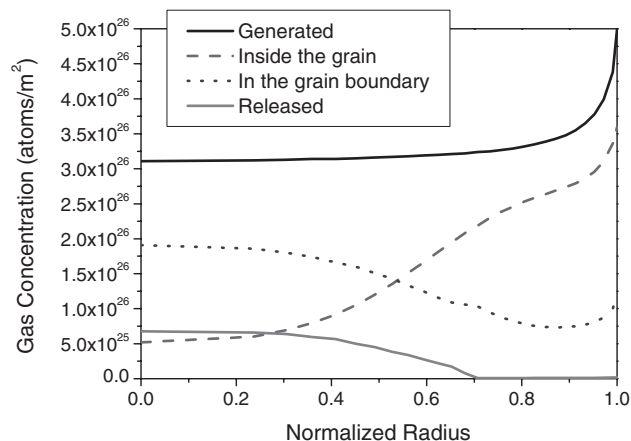


Fig. 22 Radial distribution of the fission gases at 45 MWd/kgU

Figures 22 and 23 show the radial distributions of the fission gases that are generated, remain inside the grain and at the grain boundary, and are released at the burnups of 45 MWd/kgU and 94 MWd/kgU, respectively. In the rim microstructure region, the grain size of the UO_2 fuel is assumed to be transformed to $0.3\mu\text{m}$ in the MEGA model.

Therefore, most of the fission gases are diffused from inside the grain to the grain boundary in the rim microstructure region, as shown in Fig. 23. However, fission gas bubbles in the grain boundary of a finely divided rim microstructure were found to be isolated there with a sphere shape,²⁾ such that the fission gases may not be released by the interconnection of the bubbles, which is the primary fission gas release mechanism in the grain edge bubbles of a normal UO_2 fuel. Therefore, in the MEGA model, fission gases in the grain boundary bubbles in the rim microstructure region are assumed to be not released and remain as bubbles in the grain boundary.

Figure 24 compares the prediction of the MEGA model with the measured fission gas release data from the Halden research reactor, IFA-429.²⁷⁾ It shows that the MEGA model can follow the variation in fission gas release with variations in power and burnup quite well.

Figures 25 and 26 compare the prediction of the MEGA model with the fission gas release data base of UO_2 fuels, which include both the commercial LWR fuels and the irradiation test fuels in the research reactors in the burnup range of 25–98 MWd/kgU and the measured fission gas release range of 1–25%.²⁸⁾ They show that the MEGA model can

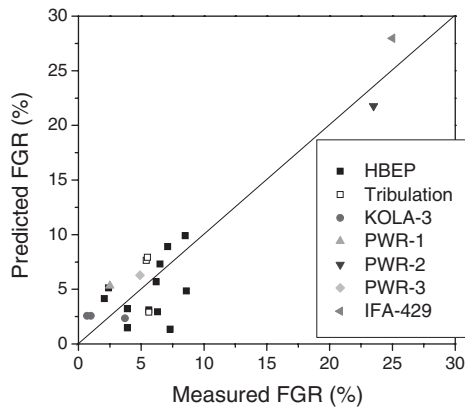


Fig. 25 Comparison of the MEGA prediction with the measured fission gas release

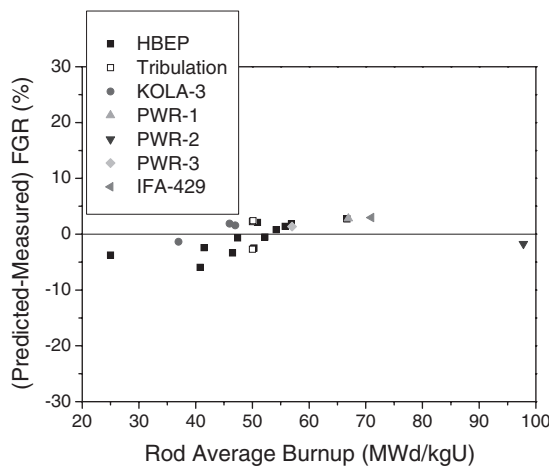


Fig. 26 Differences of the MEGA prediction and the measured fission gas release

predict the fission gas release in the broad ranges of fuel burnups and power histories up to a burnup of 98 MWd/kgU,²¹⁾ even though there are some deviations around the burnup of 40 MWd/kgU in HBEP case data, noting that the MEGA model only considers the diffusional fission gas release and does not consider the direct fission gas release and other empirical fission gas release mechanisms. Especially, at a high burnup at which the fractional fission gas release is higher than several percent at which the diffusional fission gas release mechanism becomes dominant, the MEGA model was found to predict the fission gas release satisfactorily.

IV. Conclusion

A MEGA model for an LWR UO₂ fuel under normal operation conditions was developed. The MEGA model considers only diffusional fission gas release mechanism which is a dominant fission gas release mechanism under normal irradiation conditions, such as the diffusional release of the fission gases from inside the grain to the grain boundary and the release of the fission gases from the grain boundary to the external surface by the interconnection of the fission gas bubbles at the grain boundary. A comparison of the

MEGA prediction with the measured data showed that the MEGA model correctly predicts the fission gas release in the broad ranges of fuel burnups and power histories. The enhancement of the fission gas release in a high-burnup fuel and the reduction of the fission gas release at a high burnup by increasing the grain size of the UO₂ pellet were correctly predicted by the MEGA model without using any artificial factors, such as a burnup enhancement factor.

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