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# Fission gas bubble percolation on crystallographically consistent grain boundary networks

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## HIGHLIGHTS

- Fission gas release in nuclear fuels was studied in the framework of percolation theory.
- The nuclear fuel cross-section microstructure was modeled through grain boundary networks.
- The grain boundaries were classified randomly or according to its crystallography.
- Differences in topology and percolation behavior for both kinds networks were determined.

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## ABSTRACT

Fission gas release in nuclear fuels can be modeled in the framework of percolation theory, where each grain boundary is classified as open or closed to the release of the fission gas. In the present work, two-dimensional grain boundary networks were assembled both at random and in a crystallographically consistent manner resembling a general textured microstructure. In the crystallographically consistent networks, grain boundaries were classified according to its misorientation. The percolation behavior of the grain boundary networks was evaluated as a function of radial cracks and radial thermal gradients in the fuel pellet. Percolation thresholds tend to shift to the left with increasing length and number of cracks, especially in the presence of thermal gradients. In general, the topology and percolation behavior of the crystallographically consistent networks differs from those of the random network.

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## 1. Introduction

During the fission process in nuclear reactors, a broad spectrum of fission products is formed and can be released from the fuel pellets. Particularly, fission gas release (FGR) can reduce the thermal conductivity of the gas in the fuel-cladding gap and increase the pressure in the plenum, which eventually can lead to cladding failure. These deleterious phenomena are among the main concerns that must be considered in the development of next generation reactors [1,2]. Hence, it is essential understand the mechanisms that determine FGR.

FGR is generally considered to be controlled by the diffusion of fission gas atoms from the grain interior to the grain boundaries, followed by the nucleation, growth and interconnection of fission gas bubbles, which eventually percolate across the grain boundary network (GBN) to free surface and leads to venting of the fission gas [3].

Because of observations [4,5] that intergranular bubble morphology can vary significantly from grain boundary to grain boundary and that traditional FGR models do not take this variability into account, Millett [6] developed a simple model to study the percolation behavior of fission gas bubbles by considering the distribution and connectivity of the grain boundaries that have a percolated path of fission gas bubbles. Millett model uses random grain boundary networks (RGBNs); however, real GBNs are known to be nonrandom, and their topology is severely restricted by crystallographic constraints, which are known to impact the connectivity and percolation behavior of the GBNs [7,8].

In order to classify a grain boundary in a crystallographically consistent grain boundary network (CCGBN), it is necessary to understand how the grain boundary crystallography can affect the grain boundary properties. Computer simulations have evaluated diffusion [9,10] and fracture behaviors [11] for grain boundaries in $UO_2$, and have shown that, in general, the grain boundary energy,

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diffusion and fracture behavior are influenced by the structure and misorientation of the grain boundary. Nerikar et al. [12] developed atomistic simulations using experimental data of grain boundary distribution in $UO_2$ and calculated higher boundary energy for highly disordered boundaries. Also, they indicated that boundaries with low energy can be expected to have low segregation energy, which is the driving force for fission gases to migrate to the grain boundary.

In the present work, we implemented Millett model to study the fission gas bubble percolation behavior in two-dimensional GBNs by considering crystallographic constraints throughout the microstructure. The model evaluates the effect of radial cracks and radial gradients in the percolation threshold of the fraction of grain boundaries vented to the free surface.

## 2. Model description

GBNs were simulated in two-dimensional honeycomb lattices with circular macroscale shape that correspond to the cross-section microstructure of an $UO_2$ pellet with a diameter of 1000 grains. Fission gas bubble percolation considers a binary classification that identifies each grain boundary as ‘open’ or ‘closed’, which indicates if the grain boundary has a percolated path of fission gas bubbles or not. In a RGBN, as implemented in Millett model, each grain boundary is randomly classified as open or closed; however, this procedure generates GNBs whose topologies differ qualitatively and quantitatively from those of real GBNs, as mentioned earlier. Fig. 1 shows the spatial distribution of open (thicker lines) and closed (thin lines) grain boundaries on a RGBN and a CCGBN for a fraction of open grain boundaries equal to $p = 0.55$. For ease of visualization, the size of the GBNs shown in the figures is smaller than that of the simulated GBNs.

In order to construct a CCGBN, the crystal structure of each grain is first rotated about a randomly selected axis within a prescribed tolerance. This procedure resemble a ‘general’ textured microstructure that ranges from an ideal single-component texture to ideally random, which is a good approximation to describe the texture of a $UO_2$ pellet that has either a random or fairly weak crystallographic texture according to the experimental results of Nerikar et al. [12]. Then, grain boundary misorientations are calculated from the orientations of neighboring grains and grain boundaries are classified as either low or high angle grain boundaries, as described by Frary and Shuh [7]. As mentioned previously, different works showed that the structure and misorientation of $UO_2$ grain boundaries can affect the properties of the boundary in such way that is favorable for the nucleation and growth of fission gas bubbles. Therefore, the high and low angle grain boundaries are classified as open and closed grain boundaries, respectively.

Following Millett's GBN model, we evaluated the effect of radial cracks and radial gradients in the percolation behavior of ‘vented’ grain boundaries, which correspond to the connected network of open grain boundaries that extents from the free surface and represent the possible pathways for venting and release of fission gas from the fuel pellet.

Radial cracks are formed early in the life of the fuel pellet because of the thermal stress in the outer region, however in the inner core the thermal stresses are compressive and no cracking occurs [1,2]. Because radial cracks contribute to the release of fission products from the fuel pellet, the open boundaries connected to the crack are also considered vented grain boundaries as shown in Fig. 2.

Since $UO_2$ is a poor heat conductor, the heat transfer between the fuel pellet and the coolant is slow and strong radial thermal gradient between the pellet center and pellet rim develops under steady state conditions [13]. Because of the presence of this radial thermal gradient in the fuel pellet, the bubble growth and coalescence is accelerated in central region because of high temperatures. Therefore, Millett model adopts a radial profile for $p$, similar to a radial thermal profile, which is given by:

$$p = p_{max} - (p_{max} - p_{min})\left(\frac{r}{r_p}\right)^2 \quad (1)$$

where $r_p$ is the fuel pellet radius, and $p_{max}$ and $p_{min}$ are constants that correspond to the maximum $p$ at the centerline and the minimum $p$ at the rim of the fuel pellets, respectively. Although Millett model use an exponent of 2.5 arguing the decrease in $UO_2$ conductivity with increasing temperature, we kept the quadratic relation as in the temperature profile assumed in Ref. [14].

## 3. Results and discussion

Fig. 1 shows how the topology of a RGBN differs from that of a CCGBN. While the spatial distribution of open and closed grain boundaries is the same for the RGBN, it is different for the CCGBN. It is important to note that the open grain boundaries tend to cluster together in the CCGBN, while in the RGBN tend to distribute uniformly. As we will see later, this has implications in the fraction of the vented grain boundaries. Quantification of this clustering tendency by considering triple-junction distributions can be found in

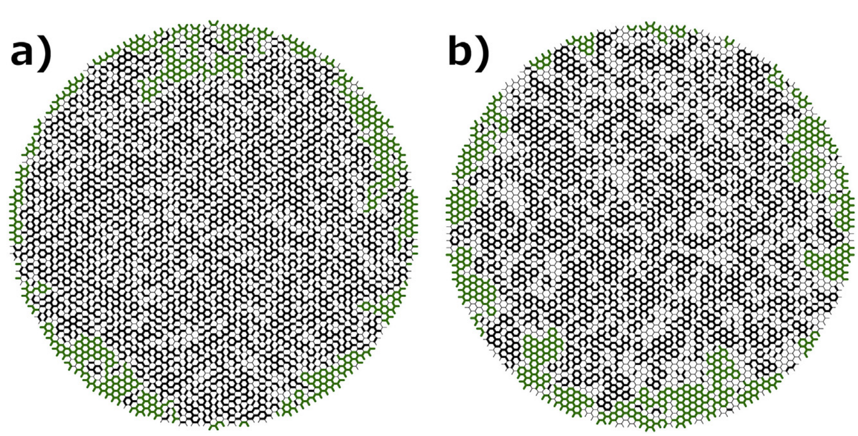


**Fig. 1.** Spatial distribution of open (thicker lines) and closed (thin lines) grain boundaries on (a) a small RGBN and (b) a CCGBN. Green thicker lines represent the vented grain boundaries. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

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