

## Thermal conductivity modeling of the interaction layer of the irradiated U-Mo dispersion fuel

Qusai Mistarihi<sup>1</sup>, Junteak Hwang<sup>2</sup>, and Ho Jin Ryu<sup>1\*</sup>

<sup>1</sup>Korea Advanced Institute of Science and Technology, Nuclear & Quantum Engineering Dept. 291 Daehakro, Yuseong, 34141, Republic of Korea

<sup>2</sup>Seoul National University, Nuclear Engineering Department, Gwanak-gu, Seoul, 08826, Republic of Korea

\*Corresponding author: [hojinryu@kaist.ac.kr](mailto:hojinryu@kaist.ac.kr)

### 1. Introduction

U-Mo dispersion fuel is proposed to be used as a fuel for the conversion of high performance research reactors due its relatively stable irradiation performance in comparison with other high U density U alloys or U compounds [1]. The U-Mo dispersion fuel is composed of a fuel meat cladded with Al alloy. The fuel meat is composed of U-Mo fuel particles dispersed in an Al matrix. One of the limitations of the U-Mo dispersion type fuel is the formation of an interaction layer (IL) due to the interaction between the U-Mo fuel particles and the Al matrix. The formation of the IL results in the degradation of the properties of the U-Mo dispersion type fuel due to the consumption of the high thermal conductivity Al matrix and the amorphous nature of the IL [2]. However, due to the small thickness of IL, the direct measurement of the IL thermal conductivity is difficult. Therefore, the objective of this study is the determination of the IL thermal conductivity from the experimentally measured fuel meat thermal conductivity using the analytical modeling and the finite element method (FEM) simulation.

### 2. Methodology

#### 2.1 A review of the experimentally measured fuel meat thermal conductivity

The experimentally measured thermal conductivities of two U-Mo dispersion type fuel meat as function of temperature were reported by Burkes et al. [3]. They measured the thermal conductivity of the fuel meat as function of temperature using the laser flash method. The first fuel meat segment was irradiated at a fission density of  $5.19 \times 10^{21}$  f/cm<sup>3</sup> and was composed of U-7Mo fuel particles, IL, and Al-2Si matrix (TL segment). In the second fuel meat segment (TK segment), irradiated at higher fission density of  $6.49 \times 10^{21}$  f/cm<sup>3</sup>, the Al-2Si matrix was totally consumed by the matrix due to the higher irradiation fission density. A schematic diagram of the low and high irradiation density fuel meat segments is shown in Fig 1.

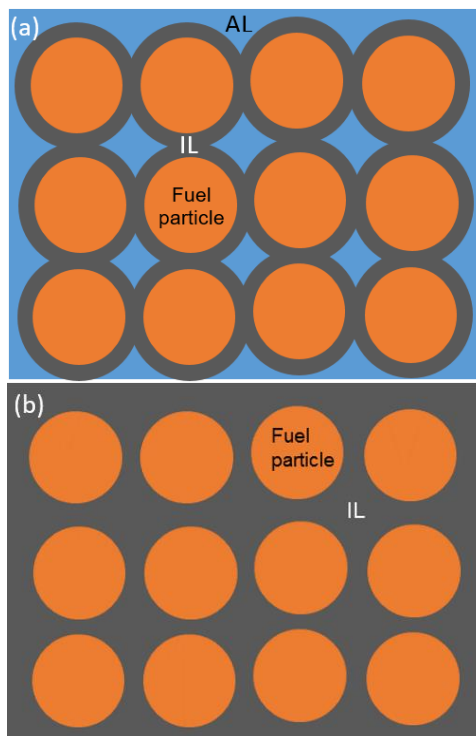
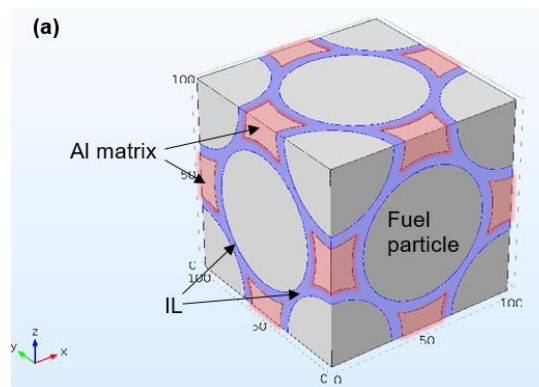


Fig. 1. A schematic diagram for the microstructure of the (a) TL, and (b) TK fuel segments.

#### 2.2 Finite element method (FEM) modeling

The thermal conductivity simulation was performed using COMSOL code version 5.2. Two model geometries were developed in order to simulate the microstructure of the low (TL) and high (TK) fission density fuel segments as shown in Fig. 2.



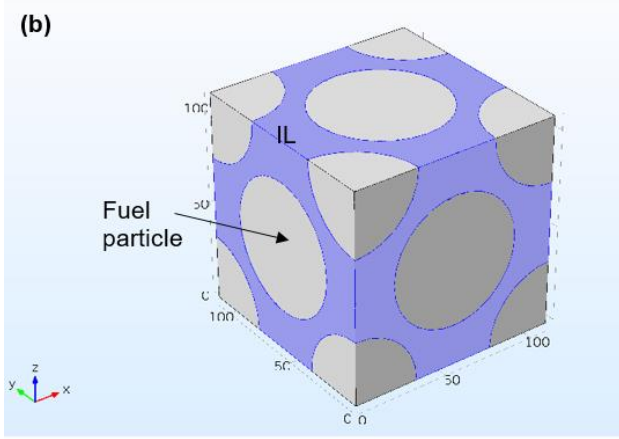


Fig. 2. Simulation model geometries for (a) TL, and (b) TK fuel meat segments

The thermal conductivity of each fuel segment was found by solving the steady state heat transfer equation (Eqn. 1) with the boundary conditions of a constant heat flux at one surface, a constant temperature at the opposite surface, and insulated side surfaces. Then, the IL thermal conductivity was calculated by matching the FEM calculated thermal conductivity of the fuel meat with the experimental measured ones by Burkes et al. [3]. The IL thermal conductivity values that provided the best fitting with an error of less than 1.5 % were used.

$$k_{\text{eff}} = \frac{q'' \times L}{\Delta T} \quad (1)$$

Where where  $q''$  is the applied heat flux,  $L$  is the height of the model geometry, and  $\Delta T$  is the difference between the average top and bottom surface temperatures.

### 2.3 Analytical modeling:

Several models have been developed to study the thermal conductivity of composites and Maxwell model is the basis for most of them. The Maxwell model was developed for composites with a low volume fraction of randomly distributed spherical particles reinforcement [4]. Bruggeman [5] developed another model to consider a higher volume fraction of the reinforcement [5]. Lewis and Nielsen [6] considered the shape, orientation, and the maximum packing of the dispersed particles. Hsu et al. [7] considered the high concentration of freely overlapped dispersed particles in a continuous matrix and developed a model by combining the effective medium theory with the percolation theory. Sevostianov and Kachanov et al. [8] modeled the thermal conductivity of coated fuel particles by finding the thermal conductivity of the equivalent homogenous inclusion.

Since the microstructure of the low fission density (TL) fuel segment was composed of U-Mo fuel particles coated with the IL and dispersed in the Al matrix, Sevostianov and Kachanov et al. [8] was combined with Maxwell [4], Bruggeman [5], Lewis and Nielsen [6], or Hsu et al. [7] models to study its thermal conductivity. The thermal conductivity of the high fission density (TK) segment which was composed of the U-Mo fuel particles embedded in the IL was modeled using Maxwell [4], Bruggeman [5], Lewis and Nielsen [6], and Hsu et al. [7] models.

The thermal conductivity values of the IL as predicted with theoretical models were benchmarked with FEM predicted values.

### 2.4 Materials thermal conductivities

The non-irradiated thermal conductivity data of the U-Mo fuel particles was calculated using a model developed by fitting the experimentally measured thermal conductivity data of U-Mo alloy with different concentration of Mo [9]. Here, we modified the model by considering the swelling correlation for the U-7Mo alloy provided in [10-11] (Eqs. 14 and 15) as the volume fractions of the fission products including the solid fission products and the fission gases. The modified model calculates the thermal conductivity according to the following equations:

$$k_{\text{U-Mo}} = 1/4 \left( A + \sqrt{A^2 + 8k_{\text{U-Mo}}^0 k_{\text{FP}}} \right) \quad (2)$$

$$A = (1 - 3P)k_{\text{U-Mo}}^0 + (3P - 1)k_{\text{FP}} \quad (3)$$

$$P = \left( \frac{\Delta V}{V_0} \right)_T \quad (4)$$

$$\left( \frac{\Delta V}{V_0} \right)_T = \frac{\left( \frac{\Delta V}{V_0} \right)_G}{1 + \left( \frac{\Delta V}{V_0} \right)_G} + \frac{\left( \frac{\Delta V}{V_0} \right)_s}{1 + \left( \frac{\Delta V}{V_0} \right)_s} \quad (5)$$

$$\left( \frac{\Delta V}{V_0} \right)_G = 0.02 + 0.027(f_d - 2) + 0.0058(f_d - 2)^2, \quad (6)$$

$$\text{For } f_d < 2 \times 10^{21} \frac{\text{fissions}}{\text{cm}^3} \quad \left( \frac{\Delta V}{V_0} \right)_s = 0.04f_d \quad (7)$$

where  $k_{\text{FP}}$  is the thermal conductivity of the fission products including the fission gases and the solid fission products, and  $P$  is the percentage of the change in volume

induced by fission product swelling.  $\left( \frac{\Delta V}{V_0} \right)_G$  and  $\left( \frac{\Delta V}{V_0} \right)_s$  are the percentages of the U-7Mo fuel swelling induced by the fission gases and the solid fission products, respectively, and  $f_d$  is the fuel particle fission density in  $10^{21}$  fissions/cm<sup>3</sup>. The thermal conductivities of the fission products ( $k_{\text{FP}}$ ) were calculated from the experimentally measured thermal conductivities of the U-10Mo alloy with a fission density of  $4.52 \times 10^{21}$  f/cm<sup>3</sup> [12] (Eqs. 10-15) by Hsu model, using the thermal conductivity of the non-irradiated U-10Mo alloy and the swelling data of the U-10Mo as provided in [11]. The data was then validated against the experimentally measured thermal conductivity of another U-10Mo alloy segment with a fission density of  $3.63 \times 10^{21}$  f/cm<sup>3</sup> [12], and the results are shown in Fig. 4.

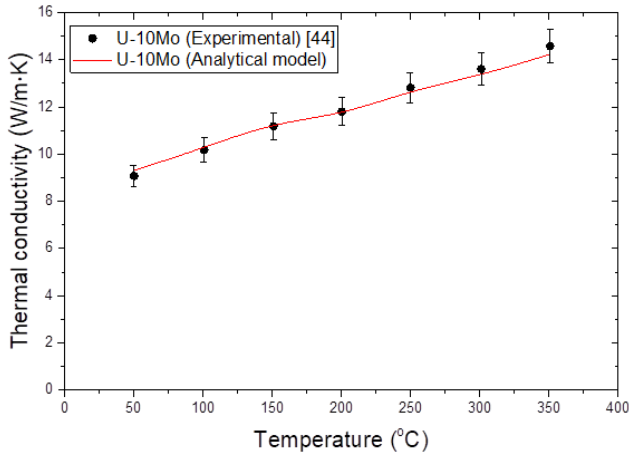


Fig. 4: Validation of the thermal conductivity data for the calculated fission products with the experimentally measured thermal conductivity data of the U-10Mo alloy [12].

The thermal conductivity of the Al-2 wt.% Si matrix was measured by Cho et al [13]. The thermal conductivities measured at room temperature and 200°C were 191.4 and 197.6 W/m·K, respectively. For the simulation, the model used 191.4 W/m·K for the matrix thermal conductivity within the range 50–150°C and 197.6 W/m·K for the operating temperatures above 150°C [13].

### 3. Results and discussions

The comparison between the FEM predicted thermal conductivity values of the IL and the theoretically predicted values are shown in Fig. 5 together with thermal conductivities assumed by Burkes et al. [3]. Burkes et al. [19] estimated the thermal conductivity of the IL during irradiation by finding the IL thermal conductivity that best fit the experimentally measured thermal conductivity data of the TL and TK fuel meat segments and by combining the model of Hsu et al. with another for coated fuel particles.

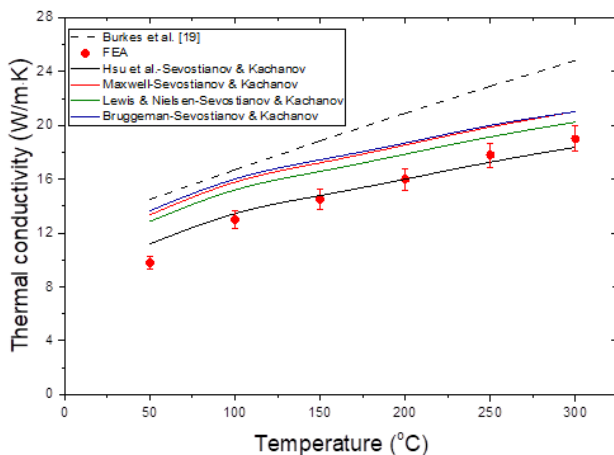


Fig. 5. Calculated thermal conductivity values of the IL for TL segment.

The FEM-predicted IL thermal conductivities are much lower than those predicted by Burkes et al. [3] (Fig. 5)

because Burkes et al. [3] assumed the IL thermal conductivity was independent of the fuel particle fission density. Clearly, the IL thermal conductivities predicted by combining the models of Hsu et al. and Sevostianov and Kachanov were close to those predicted by the FEM simulation; the difference was less than 5% in almost all the temperature ranges. However, the IL thermal conductivities predicted by combining either the models of Maxwell, Bruggeman, or Lewis and Nielsen with the model of Sevostianov and Kachanov were much higher than FEM-predicted IL thermal conductivities. The discrepancy could be attributed to the overlapped dispersed particles.

The experimentally measured and FEM-simulated thermal conductivities of the IL are provided in Fig. 6 together with the thermal conductivities assumed by Burkes et al. [3] and those predicted using the analytical models (Maxwell, Lewis & Nielsen, and Bruggeman).

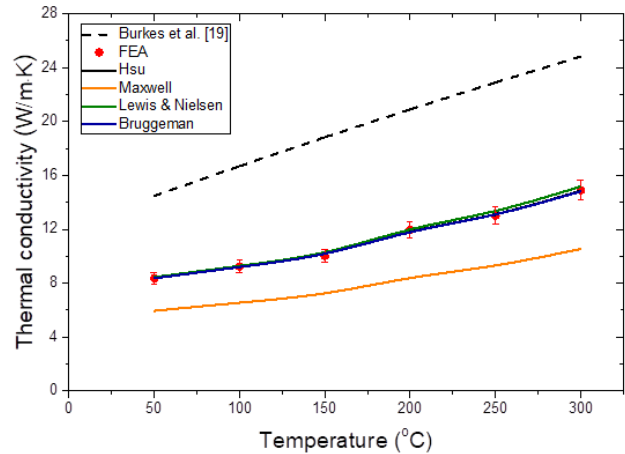


Fig. 6. Calculated thermal conductivity of the IL for the TK fuel meat segment.

The thermal conductivities of the IL assumed by Burkes et al. [3] were much higher than those predicted by the FEM simulation and the analytical modeling because Burkes et al. assumed the thermal conductivity of the IL was independent of the fission density. The thermal conductivities of the IL predicted by the FEM simulation and the models of Lewis and Nielsen, Bruggeman, and Hsu et al. because the U-Mo fuel particles were not overlapping. The thermal conductivity of the IL for the TK fuel meat segment as predicted by the Maxwell model were lower than the FEM predicted values because Maxwell model under-estimated the degree of reduction in the fuel meat thermal conductivity by the U-Mo dispersed fuel particles.

### 4. Conclusions

The irradiated thermal conductivity of the IL were calculated from the experimentally measured thermal conductivity of two fuel meat segments with different irradiation fission density and different microstructure using FEM simulation and analytical models.

For the case of the fuel meat segment with a low fission density which was composed of overlapped U-Mo fuel particles coated with IL and dispersed in the Al matrix, the FEM predicted IL thermal conductivity values were close to those predicted by combining the Hsu et al. model with the Sevostianov and Kachanov model where other combined models over-estimated the values since Hsu et al. model considered the overlapping between the dispersed particles. For the case of the high fission density fuel meat segment which was composed of U-Mo fuel particles dispersed in the IL without overlapping between the dispersed particles, most of the analytical models prediction of the IL thermal conductivity values were close to the FEM prediction except the Maxwell model because Maxwell model was developed for a low volume fraction of the dispersed particles whereas the U-Mo fuel particles volume fraction for the TK segment was around 50 %.

Future work will focus about developing a correlation for the IL thermal conductivity as function of the fission density.

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