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### The modeling and simulation of the thermal conductivity of irradiated U-Mo dispersion fuel: Estimation of the thermal conductivity of the interaction layer



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#### G R A P H I C A L A B S T R A C T



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#### ABSTRACT

U-Mo dispersion-type fuel is a potential candidate fuel for research and test reactors owing to the relatively stable irradiation performance of U-Mo fuel in comparison with other metallic fuels. However, U-Mo dispersion fuel shows high growth of interaction layers at high burnup irradiation. Although the thermal conductivity of the interaction layer is one of the critical parameters for evaluating U-Mo fuel performance, there have been no studies on the thermal conductivity of the as-irradiated interaction layers based on experimentally measured data. In this study, the thermal conductivities of the as-irradiated interaction layer were estimated using finite element analysis simulation and analytical modeling from the reported thermal conductivities of the fuel meat segments irradiated up to two different fission densities. The thermal conductivities of as-irradiated interaction layer predicted by the analytical modeling and the finite element simulation showed a good agreement when they were estimated by the analytic models considering the interconnected microstructure of the Al matrix.

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#### 1. Introduction

Since the 1970s, research reactor conversion programs such as reduced enrichment for research and test reactors (RERTR) have

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https://doi.org/10.1016/j.jnucmat.2018.08.014 0022-3115/© 2018 Elsevier B.V. All rights reserved. been initiated in order to reduce the proliferation risk and potential threats of the use of highly enriched uranium (HEU) in most research and test reactors. The main objective of these programs was to replace the HEU with low-enriched uranium (LEU) while not sacrificing reactor performance. This objective can be met by increasing the fuel loading or the uranium density of the fuel. The maximum achievable fuel loading is limited, so there is a need to

find a U alloy or compound with a high U density to compensate for the reduction in the U enrichment. Uranium silicide  $(U_3Si_2)$ dispersion fuel, in the form of U<sub>3</sub>Si<sub>2</sub> fuel particles dispersed in an Al matrix (fuel meat) and the fuel meat is clad with an Al alloy, was one of the proposed and used fuels to convert most of the HEU research and test reactors owing to its stable irradiation performance and high U density (4.8 g/cm<sup>3</sup>) [1]. However, some of the high-performance HEU research and test reactors require an estimated U density of 8–9 g/cm<sup>3</sup> in order to be converted from the HEU fueled core to the LEU fueled core [2]. U compounds (i.e. U<sub>6</sub>Mn and U<sub>6</sub>Fe) with a U density higher than that of U<sub>3</sub>Si<sub>2</sub> did not show a stable irradiation performance [3,4]. Therefore, research has focused on the development of U alloys to replace the U<sub>3</sub>Si<sub>2</sub> fuel particles since they have a much higher U density than U compounds and can stabilize the  $\gamma$ -phase of U, which is more stable under irradiation than orthorhombic  $\alpha$ -phase U. Among the proposed high-U-density U alloys,  $\gamma$ -phase U-Mo alloy shows better irradiation behavior [5]. U-Mo alloy dispersion fuel with a Mo content of 6-10 wt.% shows stable irradiation behavior with moderate fuel/matrix interaction and stable fission gas bubble growth when irradiated to a maximum burnup of 70% of the U-235 in LEU at an irradiation temperature of 65 °C [6]. High fission rate irradiation testing showed enhanced fuel meat swelling that is related to high interaction layer (IL) growth and large pore formation at the IL/Al matrix interface [7,8]. This IL is formed during irradiation at the interface between the U-Mo fuel particles and the Al matrix [9]. The formed IL was found to be amorphous whereas the U-Mo fuel particles and the Al matrix remained crystalline during irradiation [9]. The amorphous nature of the IL facilitates the diffusion of fission gases and the formation of debonding at the IL/ Al matrix interface [9]. The formation of the IL adversely affects the thermal properties of the U-Mo/Al dispersion fuel [10]. Though, several methods have been used to prevent the severe formation of IL and large fission gas bubbles including the addition of small amounts (2-5 wt.%) of Si to the Al matrix or coating U-Mo fuel particles with ZrN, UN, and Si [11–13], none of these methods completely prevented the formation of the IL.

In order to predict the performance of the U-Mo dispersion-type fuel, several analytical models [14–17] and numerical methods [18,19] have been developed to simulate its properties such as its thermal conductivity and temperature distribution in irradiated and non-irradiated environments. Kim et al. [14] modeled the thermal conductivity of non-irradiated U-Mo/Al with different Mo alloying content (6, 8, and 10 wt.%) by modifying a model developed by Hsu et al. [20] for dispersed fuel particles with a high volume fraction to consider the IL formation as an interfacial thermal resistance between the U-Mo fuel particles and the Al matrix. Burkes et al. [15] modeled the thermal conductivity of nonirradiated U-10Mo/Al dispersion-type fuel using the model developed by Hsu et al. [20] and a model developed by Badrinarayan et al. [21] for coated fuel particles to study the effect of the IL volume fraction, IL thermal conductivity, and U-Mo fuel particle size on the thermal conductivity of U-10Mo/Al fuel. Burkes et al. [16] extended the use of the same model to predict the thermal conductivity of irradiated U-7Mo/Al-2Si dispersion type fuel. Cho et al. [19] estimated the thermal conductivity of non-irradiated U-10Mo/ Al dispersion fuel by the finite element analysis (FEA) method, considering the particle size distribution of U-Mo fuel particles, IL formation, and heat generation, and they studied the effects of particle sphericity and IL formation by implementing an anisotropy correction factor (which is the ratio of the Fricke equation [22] developed for composites with ellipsoidal particle fillers-to the Maxwell equation [23]) and an interfacial thermal resistance correction factor (which is the ratio of the Hasselman and Johnson equation [24] when the interfacial thermal resistance is not equal to zero to the Hasselman and Johnson [24] equation when the interfacial thermal resistance is equal to zero). The value of the interfacial thermal resistance correction factor was estimated to provide the best fitting between the FEA predictions and the experimental results. Marelle et al. [17] studied the temperature distribution in U-7Mo/Al dispersion-type fuel and modeled the thermal conductivity of the fuel meat by first using the inverse rule of mixtures to find the thermal conductivity of the dispersed particles (assuming they were composites of U-Mo fuel particles and the IL) and then using effective medium theory (EMT) model to find the thermal conductivity of U-Mo/Al dispersion-type fuel meat. Williams et al. [18] developed a finite element model for the microstructure of U-10Mo/Al fuel by considering the particle size distribution and the IL formation. The microstructural models were developed for a range of fuel compositions and loadings with a uniform IL thickness and fission gas bubbles to simulate the microstructure of U-10Mo/Al dispersion fuel, which may develop during irradiation.

The material properties of the IL are important variables for the evaluation of U-Mo dispersion fuel performance. An empirical model was recently developed to predict the IL growth between the U-Mo fuel particles and the Al matrix during irradiation [25,26]. The IL density has been estimated based on the value that provided the best fitting for the fuel meat swelling of U-7Mo/Al dispersiontype fuel [27]. For IL thermal conductivity, studies about the performance of the U-Mo/Al dispersion-type fuel in irradiated and non-irradiated environments used different strategies to estimate the thermal conductivity of the IL. For the non-irradiated IL thermal conductivity, the theoretically predicted thermal conductivities for the U-10Mo/Al dispersion-type fuel meat by combining models developed by Badrinarayan et al. [21] for coated fuel particles and Hsu et al. [20] for a high volume fraction of dispersed fuel particles were fitted to the experimentally measured ones, using the experimentally measured IL thickness with the assumption that the IL only consumed the Al matrix and that the U-10Mo fuel particles have a uniform particle size of  $60 \,\mu m$  [15]. The IL thermal conductivity values that provided the best fitting were 0.5 times the thermal conductivity of the non-irradiated U-10Mo fuel particles (~6–12 W/m·K in the temperature range 25–300 °C) [15]. Williams et al. obtained thermal conductivities of the IL by fitting the experimentally measured thermal conductivities for the nonirradiated U-10Mo/Al dispersion-type fuel for different volume fractions of the IL with those predicted by the FEA considering the U-Mo fuel particle size distribution and found that the IL thermal conductivity value that provided the best fitting was 5.5 W/m·K [18]. Cho et al. [19] followed the same procedures and found that the IL thermal conductivity that provided the best fitting was 3 W/ m·K. Cho et al. [28] compared the experimentally measured thermal conductivity of the un-irradiated U-7Mo/Al dispersion by those predicted by combining the EMT model with the inverse rule of mixtures model using the estimated IL thermal conductivity from Cho et al. [19] and found that the analytical modeling overestimated the experimentally measured data. Cho et al. [28], assuming that the IL is composed of UAl<sub>3.7</sub>, have estimated the thermal conductivity of the IL to be 4.6 W/m K by interpolating the thermal conductivities of the UAl<sub>3</sub> and UAl<sub>4</sub> [29]. For the thermal conductivities of the irradiated IL, Ryu et al. [30] assumed the IL thermal conductivity to be equal to  $10 \text{ W/m} \cdot \text{K}$ . Burkes et al. [16] fitted the experimentally measured thermal conductivities of irradiated U-7Mo/Al-2Si with those predicted by combining models developed by Badrinarayan et al. [21] and Hsu et al. [20] and found that the IL thermal conductivity value that provided the best fitting was 1.13 times the thermal conductivity of the non-irradiated U-10Mo fuel particles (~13-27 W/m·K). Table 1 summarizes the data of the un-irradiated IL thermal conductivities.

The IL composition changes with burnup [31], and therefore, its

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