

Effective Heat Conductivity of UO₂

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1. Introduction

The thermal conducting properties of UO₂ pallet degrade over lifetime of a nuclear power plant and it can be a critical limiting factor of the safety and efficiency of the reactor. A commercial UO₂ pallet contains microstructural inhomogeneities, such as grain boundaries, voids and Helium bubbles. Especially, Helium bubbles that nucleate due to the He generation by the fission product have much lower thermal conductivity than that of UO₂. Thus, the formation of bubbles defects might seriously affect thermal properties of the nuclear fuel, and understanding correlation between effective thermal conductivity and temporal distribution of the imperfections is a quite important task. So far, there have been valuable attempts to quantify the correlation between porosity with effective heat conductivity. In this study, we investigated effective heat conductivity of UO₂ with consideration of number of bubbles and its size for a given porosity.

2. Methods and Results

2.1 Modeling approach

In this work, a simple two-dimensional single crystal is considered. Circular-shaped Helium bubbles are placed in the center of crystal, as shown in Fig. 1. To represent the microstructure, simulation parameter, η , is assigned at every grid point. Within crystal and bubbles, the parameter takes on a constant value of 1 and 0 respectively. Within the interfacial regions, its parameter value diffuses smoothly. The thermal conductivity depends on the local microstructure and temperature. The thermal conductivity of He gas is fixed at 0.152 W/m/K, and the conductivity of UO₂ crystal is take from the model suggested by Harding and Martin [1] which has the following temperature dependence:

$$\kappa_0 = \frac{1}{0.0375 + 0.0002165T} + \frac{4.715 \times 10^9}{T^2} \exp\left(-\frac{16361}{T}\right) \quad (1)$$

In the interface region, conductivity values are determined by the microstructure parameters using the following relation:

$$k = k_0 \times \eta^2 \quad (2)$$

A Dirichlet boundary condition of $T=800$ K is applied on the left boundary and a heat flux Neumann boundary condition of $j=50$ MW/m² is applied across

the right boundary. Following boundary conditions are enforced in the y-direction:

$$\begin{cases} T(0, t) = T(1, t) \\ T(nx + 1, t) = T(nx, t) \end{cases} \quad (3)$$

In this simulation, temperature is determined by solving the steady-state heat equation:

$$\frac{\partial T}{\partial t} = \nabla \cdot (K(\eta) \nabla T) \quad (4)$$

Equation is discretized in space with a uniform two-dimensional 1024dx X 1024dy grid and solved using an implicit Crank-Nicolson method. The simulation cell length $L_x=1024$ is 10.24 μm , so the grid spacing dx takes the value of 10 nm. The effective conductivity of the crystal is then found by solving $K = j \times L_x / \Delta T$. The x-directional temperature drop across the simulation cell is determined by averaging the temperature on the right boundary.

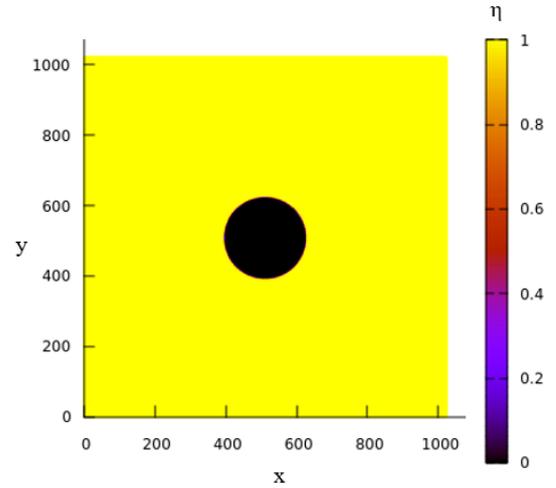


Fig. 1. Plot of microstructure parameter of the simulation cell with a single Helium bubble consistent with porosity 4.0%.

2.2 Result and discussion

The overall temperature at equilibrium is given in Fig. 2, and its one-dimensional temperature profile along a row of $y=512$ is plotted in Fig. 3. The temperature drop is due to the reduction of thermal conductivity in the gas phase, and this lower conductivity result in the difference between the bulk conductivity and effective conductivity.

There are several conductivity models which predict the effect of porosity. One of the general equations, Schulz equation [2] is given as:

$$k_{eff}^{void} = k_{bulk}(1 - v_p)^\beta \cdot \Psi \quad (5)$$

where β is a fitting parameter and $\Psi=1-v_p$ is a correlation factor that relates two-dimensional to three-dimensional heat transport in porous media (for $v_p < 10.0\%$) [3]. Nikolopoulos and Ondracek [4] suggested a lower bound of the parameter, β as 3 for non-interconnected porosity in UO₂.

We simulate a heat transfer with a single bubble placed in the center of the field. Fig. 4 provides a comparison of effective conductivity between the simulation result and the values based on Schulz equation. The difference increases significantly with increasing porosity. The following is the fitted equation based on the data of single bubble simulation:

$$k_{eff} = -7.32624 \times v_p^{0.875563} + 5.00977 \quad (6)$$

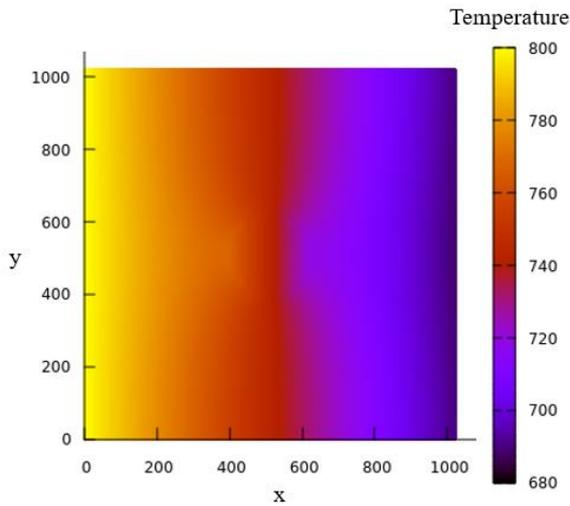


Fig. 2. Equilibrium temperature throughout the field with a single Helium bubble consistent with porosity 4.0%. Temperature gradient in x-direction is shown.

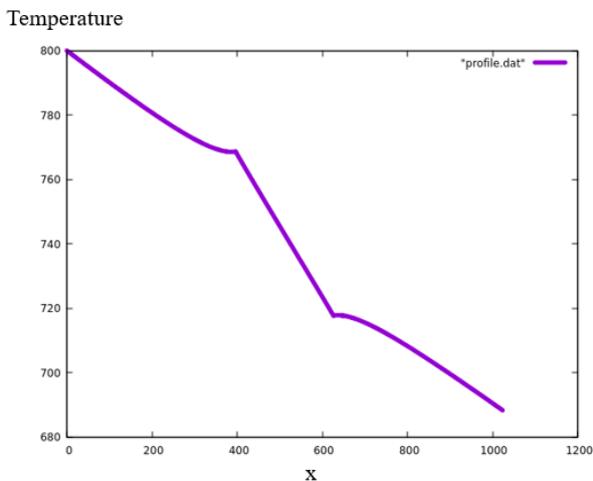


Fig. 3. Equilibrium temperature profile along a row of $y=512$.

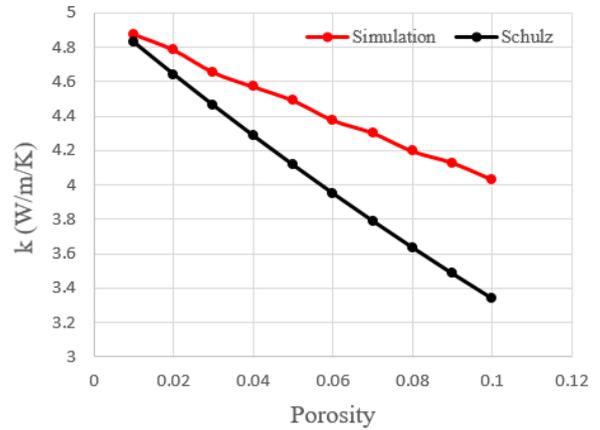


Fig. 4. Plot of effective thermal conductivity versus varying porosity based on the simulation result and the Schulz equation. The bulk conductivity for Schulz equation is calculated using equilibrium temperature data from the simulation.

In order to evaluate the effect of number of bubbles on effective conductivity, we simulate a heat transfer with different number of bubbles. These bubbles are placed in the middle of x-axis and evenly spaced along the y-axis. For a given porosity, bubble radius is varied by changing its numbers. In Fig. 5, effective thermal conductivity is plotted against the number of projected bubbles for varying porosity. The effective conductivity decreases with increasing porosity and also with the increasing number of bubbles. It means, arrangement of bubbles is more important rather than its size under this simulation condition.

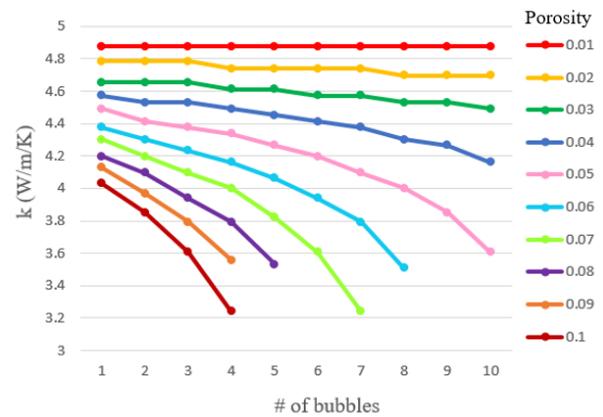


Fig. 5. Effective thermal conductivity versus number of bubbles in simulation field for varying porosity from 1.0% to 10.0%. For lack of the space, bubble numbers are limited at high porosity.

3. Conclusions

In this study, effective thermal conductivity of UO₂ containing He bubbles has been analyzed. The effective conductivity is a strong function of porosity and also related to the position of bubbles. Therefore, the formation of several large bubbles can affect the effective thermal conductivity.

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