Modeling of the Thermal Conductivity of Mo-ZrO_2 Composites for Inert Matrix Fuel

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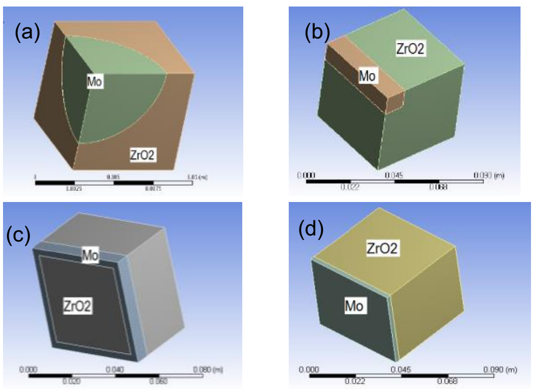
1. Introduction

Inert matrix fuel (IMF), in which the TRUs including Pu and minor actinides (MAs) are dispersed in a neutron transparent matrix, is one of the concepts developed for the management of radioactive spent fuel [1]. ZrO_2 is one of the candidate materials for the matrix of IMF owing to high melting point, low neutron absorption cross section, and good chemical and irradiation stability [2]. However, it has a low thermal conductivity that reduces its performance. The fabrication of Mo reinforced ZrO_2 composites with a low volume fraction of the reinforcement has been recently demonstrated and the effect of the reinforcement microstructure on the thermal conductivity of ZrO_2 has been measured [3]. The objective of this paper to investigate the effect of reinforcement microstructure on the thermal conductivity of ZrO_2 matrix using finite element method (FEM) and analytical modeling and to benchmark the theoretically predicted results with the experimentally measured ones.

2. Thermal conductivity modeling

2.1 Finite element method

Solid models of Mo-ZrO_2 composites with different structures were developed as shown in Fig. 1.



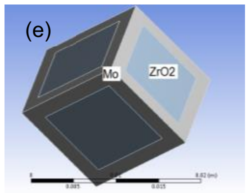


Fig. 1. Solid models of (a) Mo particle- (b) Mo fiber- (c) Mo mesh- (d) Mo sheet-, and (e) 3D interconnected Mo-ZrO_2 composites.

The thermal conductivities of Mo-ZrO_2 composites as function of temperature were calculated using the following equation:

$$K_{eff} = \frac{Q \times L}{A \times \Delta T} \quad (1)$$

where Q is the applied heat flux, L is the length along which the heat flows, A is the cross-sectional area, and ΔT is the temperature difference between the two surfaces. The thermal conductivity was calculated by applying a constant heat flux at one surface and a constant temperature at the opposite surface.

2.2 Analytical modeling

Maxwell model [4] is one of the earliest models that have been developed based on the effective medium theory. The Maxwell model was developed for composites with dilute concentration of uniformly distributed spherical particles (Eq. 2):

$$K_{eff} = K_m \frac{(2 - 2V_r)K_m + (1 + 2V_r)K_r}{(2 + V_r)K_m + (1 - V_r)K_r} \quad (2)$$

where K_r, K_m, and K_{eff} are the thermal conductivities of the reinforcement, matrix, and composite, respectively, and V_r is the volume fraction of the reinforcement.

3. Results and discussions

FEM modeling of the thermal conductivity of Mo fiber, mesh, sheet-ZrO_2 composites when the heat flux was applied parallel and perpendicular to the direction of the reinforcement is shown in Fig. 2 together with the Maxwell model predictions. When the heat flux was applied parallel to the direction of the reinforcement, the thermal conductivity increased from fiber, mesh, to sheet microstructure due to the increased degree of high thermal conductivity reinforcement. When the heat flux was perpendicular to the direction of the reinforcement, the thermal conductivity of the reinforced ZrO_2 composites from mesh, fiber, to sheet due to the increased density of the reinforcement matrix interfaces.

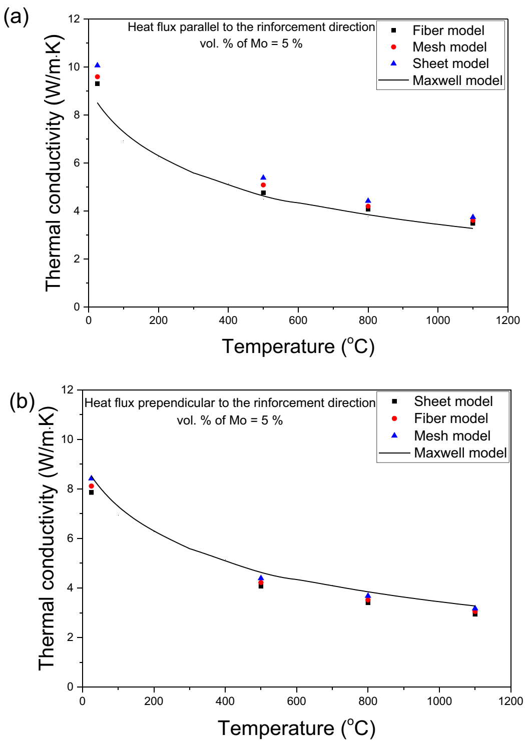


Fig. 2. FEM predicted thermal conductivity of Mo-ZrO_2 composites with different reinforcement structures and Maxwell model predictions.

Fig. 3 Shows a comparison between the experimentally measured thermal conductivity of Mo-ZrO_2 composited with dispersed particle and randomly distributed Mo wire mesh structures with the FEM and Maxwell model predictions. The thermal conductivity of Mo powder-ZrO_2 composites were corrected for the experimentally measured porosity of 99.0% using the modified Maxwell-Eucken correlation [5]. In general, the theoretically predicted thermal conductivity values are in good agreement with the experimentally measured ones.

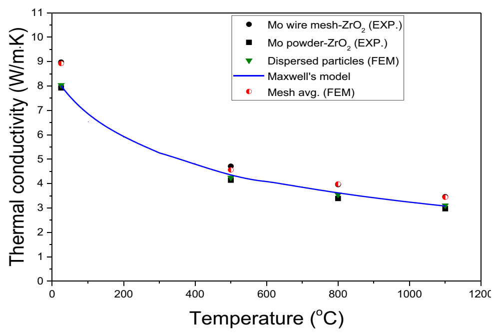


Fig. 3. Comparison between the theoretical predictions and the experimental measurements of Mo-ZrO_2 composites.

4. Conclusion

The FEM modeling of the thermal conductivity of Mo-ZrO_2 composites showed that with increasing the interconnectivity of the reinforcement structure, the thermal conductivity significantly improved due to the higher degree of interconnectivity of high thermal conductivity pathways and the reduced intensity of reinforcement/matrix interfaces. The theoretically predicted thermal conductivities of Mo-ZrO_2 composites were compared with the experimentally results and a good agreement was found.

Acknowledgments

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