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Comparison of Theoretical Models and Finite Element Simulation of ZrO_2-based Composites for Inert Matrix Fuel

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1. Introduction

The improvement of thermal properties of ZrO_2 has been investigated in many ways to enhance the performance of inert matrix fuel (IMF). Inert matrix fuel is a useful concept to burn transuranic elements (TRU) without increasing extra plutonium [1]. The addition of reinforcements with a high thermal conductivity has been proposed in the previous studies [2-4]. Molybdenum and silicon carbide are good candidate materials for the reinforcement because of their high thermal conductivities and low neutron absorption cross sections. Recently, ZrO_2-based composites reinforced with Mo-wire mesh or carbon foam were fabricated by spark plasma sintering [5, 6]. When the effects of the structures of reinforcements were compared, interconnected structures provided more enhanced thermal conductivity than discrete structures. The effective thermal conductivity of composite materials with various reinforcement structures can be calculated by using the finite element analyses. Raj et al calculated the effective thermal conductivities of ZrO_2-based composites with various structured Mo reinforcements as schematically shown in Fig. 1 [7].

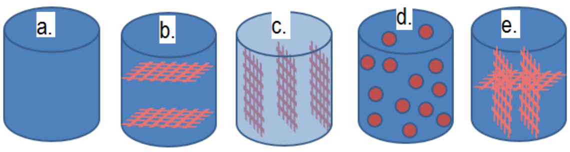

Fig. 1. a) ZrO_2 b) ZrO_2-Perpendicular Mo Mesh Plane c) ZrO_2-Parallel Mo Mesh Plane d) ZrO_2- Mo Powder reinforcement e) ZrO_2- Mo 3D Network

The objective of this study is to compare the results of finite element analyses and the analytical models in predicting the thermal conductivity of ZrO_2 composites reinforced with discrete phase Mo particles and interconnected Mo structure.

2. Finite Element Simulation

In this study, various structures of Mo reinforcements have been used as shown in Fig. 2. They are three dimensional interconnected Mo wire, particulate discrete Mo powder, Mo wire mesh, Mo fiber and Mo sheet. 3D model of ZrO_2-Mo unit cells has been constructed using Solidworks^{TM} and finite element analyses have been performed by using ANSYS^{TM}. The effective thermal conductivities of the ZrO_2-Mo composites can be calculated using the thermal conductivity equation:

$$K = \frac{Q * L}{A * \Delta T} \qquad (1)$$

Where Q is the heat flux applied, L is the length along which heat flows, A is the cross sectional area, ΔT is the temperature difference between the two surfaces where constant temperature and heat flux conditions are applied.

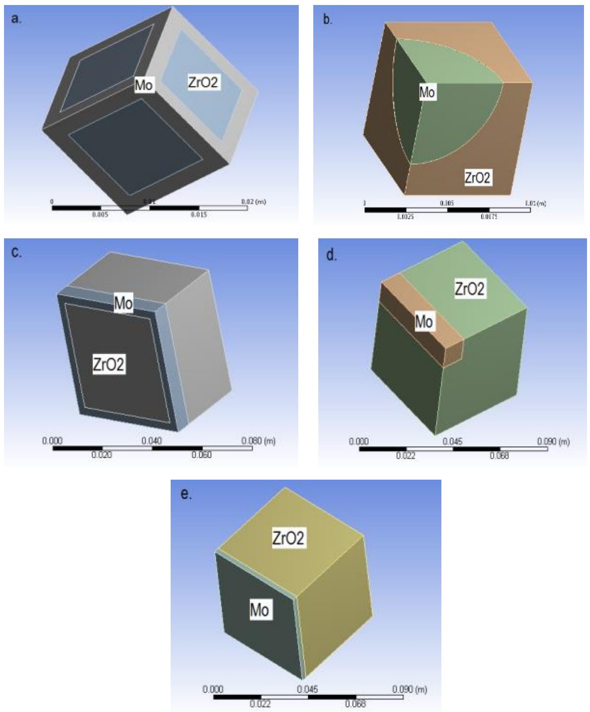

Fig. 2. Solid models of various structured Mo reinforced ZrO_2 composites; a) 3D Mo, b) Mo particle, c) Mo mesh, d) Mo fiber, e) Mo sheet.

3. Theoretical Models

The Maxell's model of composite materials predicts the effective thermal conductivity with a good accuracy for spherical, non-interacting reinforcement particles with a low volume fraction (less than 10%) [8].

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

Dul'nev et al. proposed a 3D model with a cubic unit cell structure to predict the thermal conductivity of interconnected reinforcement materials [9]. The effective thermal conductivity is expressed by equation 3.

$$K = K_r\, t^2 + K_m(1-t)^2 + \frac{2t(1-t)K_r\, K_m}{K_m t + K_r(1-t)} \quad (3)$$

$$t = \frac{1}{2} + cos\left(\frac{1}{3}cos^{-1}(2p-1) + \frac{4\pi}{3}\right)$$

where K_r, K_m and K is the thermal conductivity of the reinforcement, the matrix and the composite, respectively, V_r is the volume fraction of the reinforcement, P is the porosity, t is dimensionless thickness of the foam skeleton.

Fig. 3 shows the thermal conductivity of ZrO_2-Mo (5 vol. %) composites at different temperature as predicted by FEM method and analytical models (Maxwell and Dul'ven) for discrete particles and interconnected phase and Fig. 4 shows the effect of the volume fraction of Mo phase. As can be seen from Fig. 3 and Fig. 4, a good agreement was found between the analytical models and FEM method.

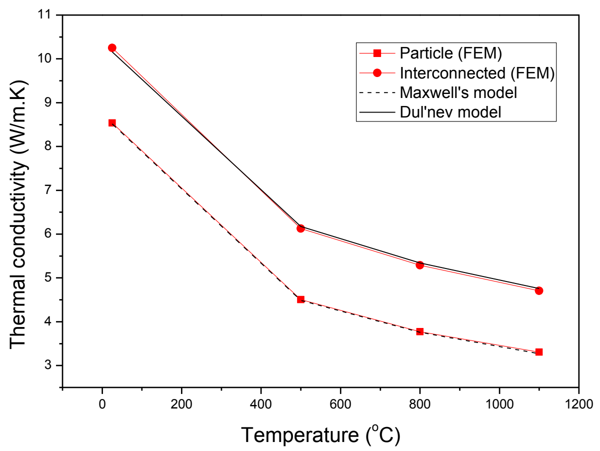

Fig. 3. Calculated thermal Conductivities of 5 vol.%Mo reinforced ZrO_2 composites as function of temperature.

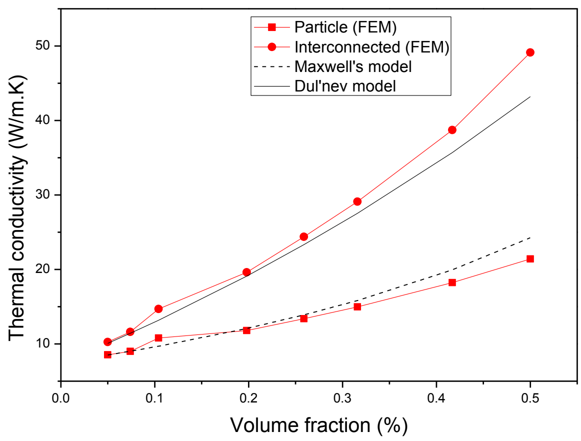

Fig. 4. Calculated thermal Conductivities of Mo reinforced ZrO_2 composites as function of volume fraction.

4. Conclusions

The finite element analyses presented a good agreement with theoretical models in estimating the effects of the reinforcement on the thermal conductivities of discrete Mo reinforced ZrO_2 nanocomposites. It is found that the effects of interconnected thermal reinforcements on the effective thermal conductivity can be estimated by using the percolation model.

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