Numerical modelling of oxide dispersed strengthened Zircaloy-4 cladding for investigating elastic modulus via finite element method

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1. Introduction

Since a Fukushima nuclear accident in 2011, development of accident tolerant fuel (ATF) cladding has been motivated to meet increased need for safety under the accident conditions. Worldwide, various ATF cladding concepts such as surface modified Zircaloy-4 by coating of Cr and CrAl, and FeCrAl and SiC claddings have been suggested [1-2]. At the Korea Atomic Energy Research Institute (KAERI), as one of the surface modified Zircaloy-4 cladding concepts, oxide dispersed strengthened (ODS) Zircaloy-4 cladding has been developed [3]. The ODS Zircaloy-4 cladding is achieved from laser beam scanning (LBS) treatment as dispersing Y_2O_3 into a Zircaloy-4 substrate to form a ODS layer on an outer surface of a bare Zircaloy-4 cladding. From an experimental tests at a bulk scale, it was confirmed that the ODS Zircaloy-4 cladding has higher strengths and lower creep strain rate when compared with the bare Zircaloy-4 cladding.

But, there is no material data to describe the ODS layer locally, only available for the whole ODS Zircaloy-4 cladding because it is difficult to fabricate bulk size sample of the ODS layer due to thin ODS layer and manufacturing process of the LBS treatment. Each material properties of the Zircaloy-4 substrate and ODS layer can be required in a field of simulation analysis to predict behavior of the ODS Zircaloy-4 cladding. Recently, multi-dimensional fuel codes such as BISON and DRACCAR require high-fidelity material data for an accurate prediction [4-5].

To obtain the local material properties, numerical approach is regarded as a good alternative to the experimental one. Finite element method (FEM) is one of the efficient numerical solutions to calculate highly accurate material properties because the FEM can reflect detailed features of the material. Various studies have been conducted to predict the local mechanical properties of a particle reinforced material (PRM) such as the ODS Zircaloy-4 using the FEM as follows. Elastic modulus of the PRM with respect to the particle geometry was successfully obtained [6]. Effect of interface damage, particle size and morphology on tensile properties of the PRM was investigated by constructing three-dimensional representative volume element (3D RVE) model [7].

Therefore, in this study, numerical modeling was conducted via the FEM to investigate elastic modulus of the ODS Zircaloy-4 as focusing on the ODS layer because the elastic modulus is a fundamental material property for a structural analysis. The 3D RVE model of the ODS layer was established by considering randomly distributed Y_2O_3 particles. Then, the elastic modulus of the ODS layer with respect to a volume fraction (VF) of the Y_2O_3 particles was calculated and compared with an analytical model.

2. Numerical model

2.1 Generation of random position for the Y_2O_3 particles

Fig. 1 shows cross-sectional SEM images of the ODS Zircaloy-4 cladding. It was observed that the ODS layer was formed on the outer surface of the Zircaloy-4 cladding. Within the ODS layer, spherical Y_2O_3 particles were randomly distributed. The average radius of the Y_2O_3 particles was measured as about 100 nm.

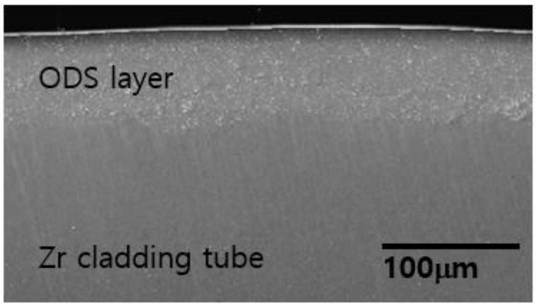

Fig. 1. Cross-sectional SEM images of the ODS Zircaloy-4 [3]

To model these randomly distributed Y_2O_3 particles, generation algorithm of random position for the Y_2O_3 particles was designed as shown in Fig. 2. Based on the SEM measurement results, the particles were assumed as spherical shape with radius of 100 nm. In the algorithm, the random positions are generated while checking collisions between the particles. The generation continues until the VF of Y_2O_3 particles reaches targeted VF.

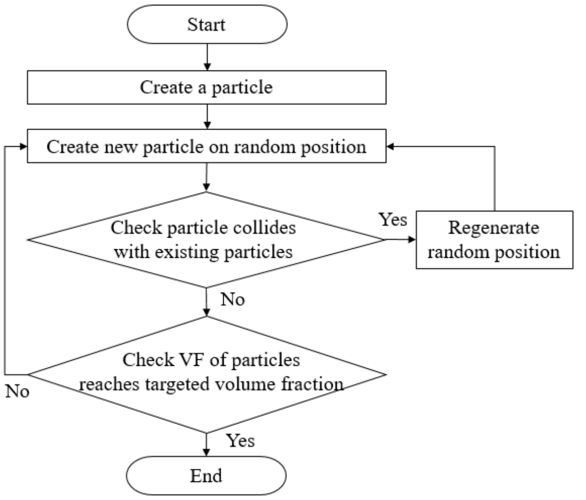

Fig. 2. Generation algorithm for random position of the Y_2O_3 particles

2.2 3D RVE model of the ODS layer

A 3D RVE model of the ODS layer was developed using a commercial finite element software ABAQUS. The Y_2O_3 particles were modeled based on the generated random position from the above algorithm. The Zircaloy-4 substrate was modeled as cubic. Based on the assumption that the Zircaloy-4 and Y_2O_3 particles are perfectly bonded, the Zircaloy-4 substrate and particles are merged to construct the 3D RVE model. Fig. 3 (a) shows the 3D RVE model with different VF of the Y_2O_3 particles such as 10 % and 15 %. As shown in Fig. 3 (b), the 3D RVE model was meshed using a linear 3D solid elements C3D4 (4-node) to apply periodic boundary conditions (PBCs) devised by Xia et al [8]. The PBCs are expressed as follow:

$$u_i^{j+} - u_i^{j-} = c_i^j \quad (i, j = x, y, z) \tag{1}$$

Where $u_i^{\,j+}$ and $u_j^{\,j-}$ are displacements of one pair of nodes at opposite boundary faces, i is normal direction to three pairs of boundary surfaces and three directions of nodal displacement, j is three direction of nodal displacement, and c_i^j is constant defined by displacement difference.

Finally, for a tensile simulation within an elastic region, only elastic properties for the Zircaloy-4 substrate and Y_2O_3 particles were considered as follows: the elastic modulus of the Zircaloy-4 and Y_2O_3 particle are assumed as 80 and 160 GPa, respectively. Poisson's ratio of the Zircaloy-4 and oxide particle are assumed as 0.3. The tensile loading was applied to the 3D RVE model along the X direction.

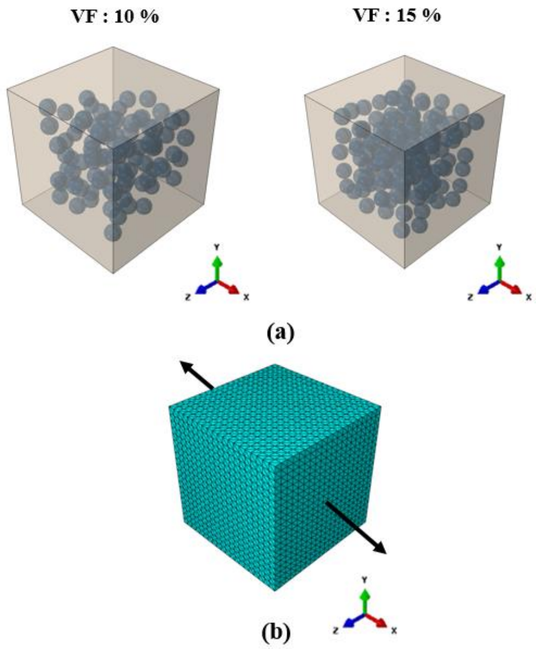

Fig. 3. (a) 3D RVE model of the ODS layer with different VF of the Y_2O_3 particles and (b) loading for the elastic simulation

3. Halphin-Tsai analytical model

A Halpin-Tsai (HT) model is one of the analytical models to calculate elastic modulus of the PRM [9]. According to the HT model, the elastic modulus of the PRM can be obtained by

$$E_c = \frac{E_m(1+2sqV_p)}{1-qV_p} \tag{2}$$

$$q = \frac{((E_p/E_m)-1)}{((E_p/E_m)+2s)} \tag{3}$$

Where, E_c, E_m and E_p are an elastic modulus of the PRM, matrix, and particle, respectively. S is an aspect ratio of the particles, and V_p is a VF of the particles.

In this study, E_c, E_m and E_p represent elastic modulus for the ODS layer, Zircaloy-4 substrate, and Y_2O_3 particles, respectively.

3. Results and discussion

Fig. 4 (a) shows simulation results of displacement along the X direction for the 3D RVE model with the VF of 10 %. It was observed that the tensile loading was well applied along the X direction. Fig. 4 (b) shows von Mises stress distribution of the Y_2O_3 particles and Zircaloy-4 substrate. It was confirmed that the Y_2O_3 particles have a higher stress than adjacent Zircaloy-4 substrate because the Y_2O_3 particles have a higher elastic modulus than one of the Zircaloy-4 substrate. This load transfer can be one of factors on strengthening mechanisms of the ODS Zircaloy-4.

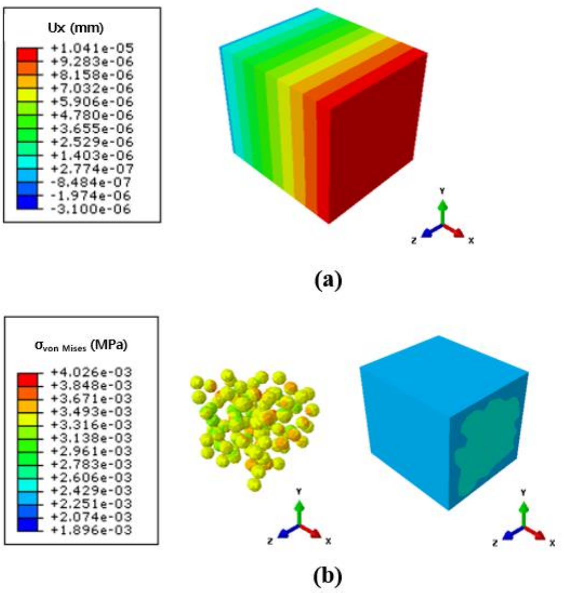

Fig. 4. Simulation results of (a) displacement along the X direction and (b) von Mises stress distribution of the Y_2O_3 particles and Zircaloy-4 substrate for the 3D RVE model with VF of 10 %.

Table I shows comparison results of calculated elastic modulus for the ODS layer with the VF of 10 % and 15% by the 3D RVE and HT models. It was confirmed that two models predicted that the elastic modulus of the ODS layer increases as the VF of Y_2O_3 particles increases while the two models have a slight difference. This difference can be caused by the facts that the H-T model assumes a perfectly oriented discontinuous particles in the PRM, parallel to an applied loading, and features of the particles such as the random distribution could not be considered in the H-T Model.

Therefore, it can be concluded that established 3D RVE model can effectively predict local mechanical properties of the ODS Zircaloy-4 while reflecting the features of Y_2O_3 particles including the shape, size and distribution.

Table I: Comparison results of calculated elastic modulus for the ODS layer by the 3D RVE and HT models

	3D RVE model (GPa)	HT model (GPa)
VF 10%	85.11	86.15
VF 15%	87.81	89.35

4. Conclusions

Numerical modelling of the ODS layer was conducted via the finite element method to investigate the elastic modulus for the ODS Zircaloy-4. The randomly dispersed Y_2O_3 particles were modeled while considering the collision between the particles. The 3D RVE models with different VF of the particles were established by applying the PBCs. From the tensile simulation, the elastic modulus of 3D RVE model was effectively obtained. The calculated results were compared with the H-T analytical model. The two results of the H-T and 3D RVE models showed similar results with an acceptable difference.

For the future work, other mechanical properties such as thermal expansion coefficient and creep constants will be obtained from the developed 3D RVE models. Further, the obtained properties can be employed for a simulation to investigate behavior of the ODS Zircaloy-4 cladding.

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