*Transactions of the Korean Nuclear Society Autumn Meeting*
*Changwon, Korea, October 24-25, 2024*

# Simulation of Microstructure-dependent Mechanical Properties of Zircaloy-4 by Crystal-plasticity Finite Element Method (CPFEM)

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## 1. Introduction

Zircaloy-4, an alloy extensively used in nuclear reactors, is a crucial material for cladding fuel rods due to its favorable properties, such as low neutron absorbing cross section. The microstructure, grain size, grain orientation (texture), and phase distribution, play a pivotal role in determining the mechanical behavior of Zircaloy-4 (Zr-4). Moreover, the Zirconium hydride ($ZrH_2$) formation, influenced by hydrogen concentration, temperature, and stress state, critically affects the alloy's ductility and fracture toughness.

Traditional continuum-based models have been employed to predict the behavior of Zircaloy-4; however, these models often fall short of capturing the complex microstructural effects accurately because Zr-4 exhibits anisotropic mechanical properties due to its hexagonal close-packed (HCP) crystal structure. The Crystal-Plasticity Finite Element Method (CPFEM) is a powerful tool to address these challenges. CPFEM explicitly considers the crystallographic slip systems, dislocation interactions, and heterogeneity within the microstructure, providing a more accurate and comprehensive understanding of material behavior under various loading conditions.

In this study, the previously developed CPFEM framework was utilized to generate a virtual microstructure of Zr-4. The impact of rolling texture with various rolling directions and δ - $ZrH_2$ formation on the mechanical properties of Zr-4 was analyzed.

## 2. Methods and Results

### *2.1 CPFEM system setup*

In the present work, numerical implementation of CPFEM is conducted by the UMAT subroutine in ABAQUS which is developed by OXFORD [1–3]. This approach takes into account slip and Geometrically Necessary Dislocations (GND), making it a method capable of capturing the effects of the microstructure. Detailed elastic and plastic properties considering anisotropy of HCP Zr-4 and FCC δ - $ZrH_2$ are mentioned in previous studies [4,5].

### *2.2 Microstructure and ABAQUS input generation*

The virtual microstructure of Zr-4 was created using the DREAM-3D software, with the grain size distribution employed shown in Fig. 1. (a). The grain size was represented using the Equivalent Sphere Diameter (ESD), with the average grain size set to 13 μm. Fig. 1. (b) and (c) show the equiaxed grain and rolled grain morphologies, respectively, which were created using this method and converted into ABAQUS input files. The dimensions for both morphologies were set to 50 × 50 × 50 μm. In Fig. 1. (c), the blue arrow indicates the tensile direction labeled as TD (Transverse Direction), and the red arrow indicates the tensile direction labeled as RD (Rolling Direction).

An identical size CPFEM input for Zr-4, including δ-$ZrH_2$, was also created. The fraction of δ at the grain boundary was set to 0.9, and the precipitation shape of δ was equiaxed as shown in Fig. 2.

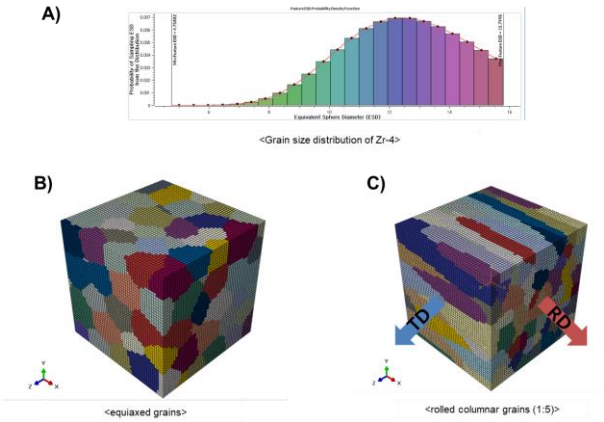


Fig. 1. Schematic of the (a) grain size distribution profile, generated (b) equiaxed grain and (c) rolled columnar grain morphology

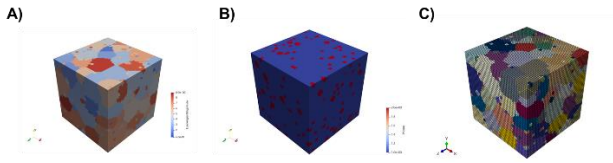


Fig. 2. Schematic of the Zr-$ZrH_2$ (a) generated microstructure, (b) phase distribution (Blue: matrix (Zr), Red: precipitate($ZrH_2$), and (c) ABAQUS input

### *2.3 Calculation results*

Fig. 3 shows the tensile test results of the virtual microstructures obtained through CPFEM. The black, red, and blue lines represent unrolled Zr-4, rolled Zr-4 in the RD (Rolling Direction), and rolled Zr-4 in the TD (Transverse Direction), respectively. The uniform elongation (~12%) in the equiaxed case is significantly higher than that in the rolled columnar Zr-4 for both the RD and TD cases (~9.5% and ~10.5%, respectively). For the TD sample, the calculated yield stress and ultimate tensile strength are similar to those of the equiaxed

texture. However, the RD rolled sample exhibits higher yield stress and higher ultimate tensile strength. The strain hardening rate in the RD is higher after yielding, indicating that dislocation multiplication and plastic deformation occur more rapidly in the RD direction. This phenomenon is attributed to the anisotropic deformation behavior of the rolling-textured Zr-4. In HCP crystals, there are three primary slip systems: pyramidal, basal, and prismatic. The initial Critical Resolved Shear Stress (CRSS, $\tau$) is known to follow the order $\tau_{pyramidal} > \tau_{basal} > \tau_{prsmatic}$. In the RD, prismatic slip is dominant, while in the TD, both prismatic and basal slips are simultaneously dominant [6]. After yielding, more prismatic slip systems are activated in the RD, and since the prismatic slip system has the lowest CRSS, the dislocation density becomes much larger compared to the TD, leading to increased strain hardening. In the case of the two-phase particle/matrix, indicated by the green line, it is observed that the hard phase $ZrH_2$ transfers a higher load, leading to greater plastic deformation in the matrix.

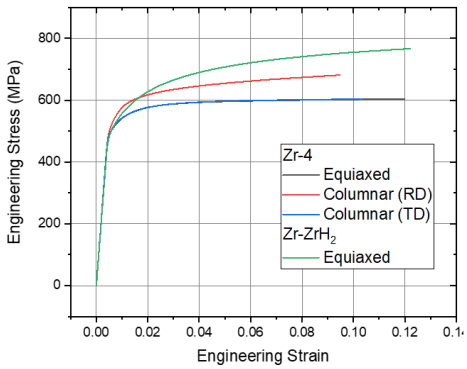


Fig. 3. CPFEM tensile test result

## 3. Conclusion

In this study, the effect of microstructure and hydride precipitation on the mechanical properties of Zr-4 was investigated. Through dislocation density-based CPFEM, the impact of Zr-4's anisotropic deformation behavior on its mechanical properties during tensile in different directions was effectively analyzed. Additionally, it was demonstrated that CPFEM can be applied to calculate the anisotropy in particle/matrix two-phase systems with different crystal structures.

## ACKNOWLEDGMENT

This work was supported by the National Research Foundation of Korea (NRF, No. 2022M2E9A304619011) grant funded by the Korea government (MSIT)

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