Application of Deep-Neural-Network Model for Predicting Mechanical Properties of ZIRLO™ Cladding under Embrittlement Conditions

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1. Introduction

Spent Nuclear Fuel (SNF) requires regardful management in preparation for high temperature and radioactivity causing material embrittlement factors such as hydrogen charging and irradiation. etc. Integrity of practical cladding could be estimated against embrittlement effect combined with comprehensive damage conditions before permanent disposal.

In previous studies, embrittlement effects of typical cladding materials such as Zircaloy-2 and Zircaloy-4 mainly have been evaluated using experimental approach. Furthermore, evaluation of an advanced zirconium alloy (ZIRLO™) is in the early stage using some of the practical cladding extracted from the SNF pool [1]. Recently, experimental studies of mechanical behavior under limitations have been supplemented applying machine learning model to find complex correlations [2].

In this study, mechanical properties of ZIRLO™ cladding under embrittlement conditions were predicted based on a machine learning technique. In order to construct Data Base (DB), axial tensile test data [3, 4] and virtual data derived using empirical correlations were organized and preprocessed [5]. Predicted properties were compared with empirical test results and analyzed using coefficient of determination.

2. DB Construction

2.1 Data organization

The axial tensile test data of 79 Zircaloy-4 and 68 ZIRLO™ specimens under different temperatures (T), hydrogen concentrations ([H]), and hoop stress (σ_h) were collected. The test conditions are summarized in Table I and specimens are described in Figure 1 [3].

Table I: Tensile test conditions

Material	T (°C)	σ_h (MPa)	[H] (wppm)
Zircaloy-4	25, 100,	0, 90,	0~845.8
ZIRLO™	200	120,150	0~907.9

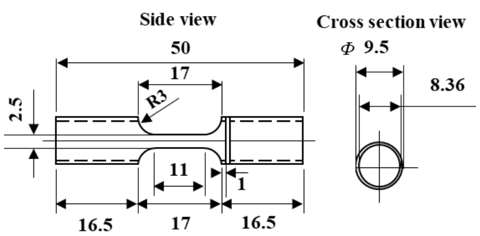

Fig. 1. Schematic of the tensile specimen

Experimental data are insufficient to learn the correlation of the parameters with irradiation environment information. Therefore, virtual specimen data were produced through the PNNL-17700 model [4].

The model describes the stress-strain constitutive relation of irradiated Zircaloy-4 cladding using Hook's law and power law. These are defined as:

$$\sigma = E(T,\Phi)\cdot\varepsilon \tag{1}$$

$$\sigma = K(T,\Phi)\cdot\varepsilon^{n(T,\Phi)}\cdot\left(\frac{\dot{\varepsilon}}{10^{-3}}\right)^{m(T)} \tag{2}$$

$$YS = \left[\frac{K(T,\Phi)}{E(T,\Phi)}\left(\frac{\dot{\varepsilon}}{10^{-3}}\right)^{m(T)}\right]^{\left(\frac{1}{1-n(T,\Phi)}\right)} \tag{3}$$

Here, σ is stress (Pa), ε is strain (mm/mm), *YS* is Yield Strength (Pa), *E* is Elastic modulus (Pa), *K* is Strength coefficient (Pa) and $\dot{\varepsilon}$ is strain rate(s^{-1}). *E*, *K*, Strain hardening component (*n*), and strain rate exponent (*m*) are functions of T and neutron fluence (Φ).

Based on the above function, 210 virtual specimen data were generated under different T in the range of 25-200°C, [H] in the range of 0-1000wppm, and Φ in the range of 0-15× 10^{-25}n/m^2. Values of Φ were considered in the relationship with [H] and burnup rate [4, 6]. Figure 2 shows the stress-strain curve generated by the PNNL-17700 model. *UE* is Uniform Elongation, UE_p is Uniform plastic Elongation, and *UTS* is Ultimate Tensile Strength.

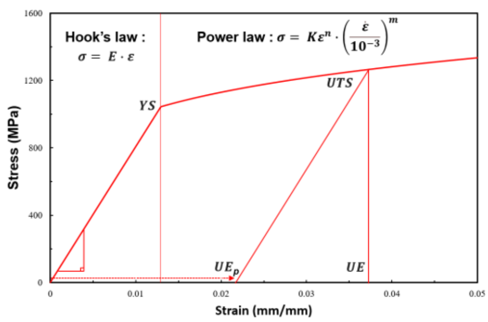

Fig. 2. Stress-strain curve used in this study

Furthermore, four axial tensile test data of irradiated ZIRLO™ specimens [5] were added to the DB. The number of data is relatively small compared to the experimental and virtual ones. Although, it will improve the ability to identify tensors in the model.

2.2 Data preprocessing

For accuracy of prediction, data preprocessing is necessary. The stress-strain curves were refined using linear interpolation with increasing strain by 0.001mm/mm. The input variable ε^n were added for the tendency of pow law on the model. The range of n was created in 0.025 units from 0.14 to 0.19. By substitute 0 and 1 to ZIRLO™ and Zircaloy-4, the model can learn the difference between the two.

3. Machine Learning

3.1 Model construction and training

Deep-Neural-Network (DNN) is mainly used for classification or numerical prediction by learning nonlinear relationships of parameters. The DNN model was constructed based on open source [7], 26 nodes in the first hidden layer, 52 nodes in the second hidden layer, 0.3 in the dropout ratio layer, and 1 node in the output layer. The number of nodes was determined through trial and error. Activation function determining the output of each node was set to a ‘Relu’ function in the hidden layers and a ‘linear’ function in the output layer. The loss function presents difference between real value and predicted output value using mean squared error. ‘Adam’ was adopted as the optimizer updating the weights of each layer. Input variables were composed of T, [H], Φ, type of material, ε and ε^n {n:0.14~0.19}, the output variable was σ. Hoop stress was excluded from the DB because of insensitivity under the tensile test conditions [3]. Figure 3 shows the training algorithm of the model.

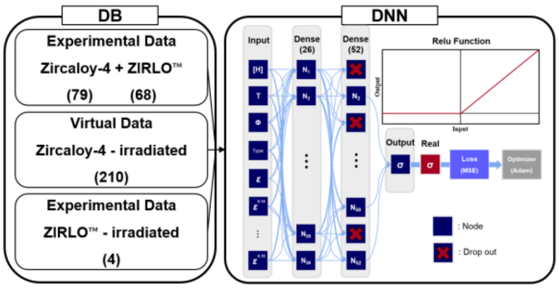

Fig. 3. Training algorithm of the DNN model

3.2 Assessment

Stress values under the conditions summarized in Table II were predicted up to *UE* by DNN model. The results were compared with two irradiated ZIRLO™ specimens not included in learned data, as shown in Figure 4. R-squared (R^2) of ZIRLO-1 is 0.9919 and ZIRLO-2 is 0.9884. Additionally, *YS* and *UTS* were compared. *YS* was calculated by 0.2% offset method, and *UTS* was set to stress value at *UE*, and the detailed results are presented in Table III.

Table II: Information of ZIRLO™ tensile test

Specimen	T (°C)	[H] (wppm)	Φ ($\times 10^{-25}$n/m^2)	*UE* (%)
ZIRLO-1	25	279	7.79	4.4
ZIRLO-2	200	47	5.47	3.9

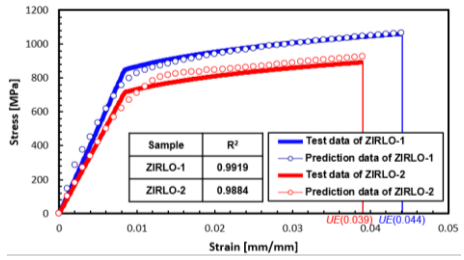

Fig. 4. Comparison of test and prediction data

Table III: Summary of empirical and estimated values

Specimen	Property	Test	DNN	Difference (%)
		(MPa)		
ZIRLO-1	*YS*	847	831	1.89
	UTS	1,038	1,040	0.17
ZIRLO-2	*YS*	721	711	1.39
	UTS	873	915	4.59

4. Conclusions

In this study, DNN, one of the machine learning methods, was applied to predict the mechanical properties of the ZIRLO™ cladding in an embrittlement environment. In the subsequent, stress-strain curves were predicted and compared to validation data.

(1) As a result of predicting two specimens, values of R^2 were about 0.9919 and 0.9884, which can provide a reasonable estimation.

(2) Both of the maximum difference of *YS* and *UTS* values between experiments and predictions were less than 5% for ZIRLO™.

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