Machine Learning-Driven Prediction of Fe-(9-12)Cr Steel Properties for Nuclear Structural Applications

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1. Introduction

With the rapid advancement of data science and computational technology, artificial intelligence (AI) has been driving innovation across various industrial sectors. In particular, machine learning (ML) and deep learning (DL) have demonstrated strong capabilities in analyzing large-scale data and learning complex patterns, leading to their increasing applicability in numerous fields. A representative machine learning model is Artificial Neural Networks (ANNs), which can be applied to a variety of problems, such as regression analysis. [1, 2].

Fe-9-12Cr steel exhibits excellent mechanical strength and corrosion resistance, making it widely used as a structural material in nuclear power plants. However, the mechanical properties are influenced by various factors, including manufacturing processes, microstructure, and environmental conditions, leading to significant complexity in property prediction. Traditional experimental approaches alone are insufficient for accurately predicting these characteristics, necessitating the application of machine learning techniques to enhance predictive accuracy. Accordingly, research is required to develop reliable machine learning models that can effectively predict the mechanical properties of Fe-9-12Cr steel and validate their performance through comparison with experimental data [2].

This study aims to develop an optimized machine learning model utilizing a multi-layer neural network to predict the mechanical properties of Fe-9-12Cr steel. To achieve this, data preprocessing, model training and optimization, and performance evaluation will be conducted using experimental datasets.

2. Experimental procedure

2.1 Data Preprocessing and Model Implementation

The performance of machine learning models is highly dependent on the quality and quantity of training data, necessitating careful selection of model structures and hyper-parameters. In this study, both neutron-irradiated and non-irradiated datasets are utilized to train predictive models. A total of 470 data samples were used in this study [3-8]. Table 1 presents the dataset used for machine learning training and model validation. The machine learning approach involves data preprocessing techniques such as normalization and standardization, followed by the application of neural networks incorporating batch normalization, dropout regularization, and adaptive optimization methods [9]. The model architecture consists of multiple hidden layers optimized using the Adam optimizer with weight decay regularization, and the loss function is defined based on Huber loss to improve robustness against outliers. Fig. 1 shows an example of a multi-layer neural network with nodes skipped due to dropouts. The dataset is divided into training, validation, and test sets to evaluate generalization performance, and the model's predictive capability is assessed using statistical metrics such as mean absolute error (MAE), mean squared error (MSE), and the coefficient of determination (R^2). The implemented methodology ensures that the machine learning framework effectively captures the complex relationships governing the mechanical properties of Fe-9-12Cr steel.

Table 1. Dataset used for machine learning training and model validation

(wt%)

	C	Si	Mn	Ni	Cr	Mo	W	Cu	B	N	Ti	V	Nb	Co	Ta
Min	0.05	0.08	0.35	0.01	8.31	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Max	0.23	0.86	0.87	0.94	12.90	2.31	2.01	0.97	0.00	0.07	0.02	0.33	0.09	0.15	0.06
Average	0.13	0.33	0.50	0.31	10.14	0.78	0.61	0.12	0.00	0.03	0.00	0.16	0.03	0.01	0.00

	Normalizing (°C)	Time (min)	Tempering (°C)	Time (min)	Test Temperature (°C)	DPA	Irradiation Temperature (°C)	Tensile Strength (MPa)	0.2% Proof Stress (MPa)	Elongation (%)
Min	900	5	630	30	25	0	25	76	25	0.80
Max	1100	120	800	360	800	67.5	550	1199	1189	105.00
Average	1018.2	38.6	739.9	124.6	364	2.5	80.7	574.3	458.3	24.5

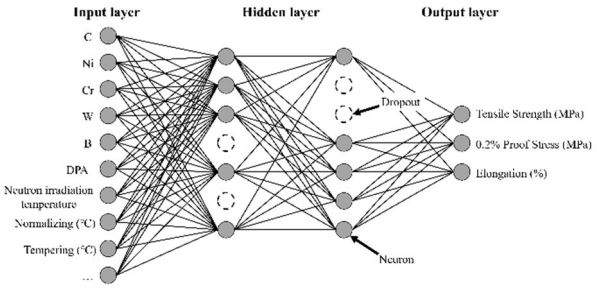

Fig. 1. Neural network architecture with multiple hidden layers and dropout regularization for predicting Fe-9-12Cr steel properties.

2.2 Model Optimization

To enhance predictive performance, this study employs a systematic hyper-parameter optimization process for neural network training. The optimization involves tuning the number of hidden layers, neurons per layer, learning rate, and the number of training epochs. The hyper-parameter optimization is performed in four stages: (1) determining the optimal number of hidden layers by varying from one to four layers, (2) optimizing the number of neurons per layer within a range of 1 to 20, (3) selecting the best learning rate from values between 0.001 and 0.01, and (4) fine-tuning the number of epochs from 1000 to 5000 in increments of 500. Each configuration is evaluated using root mean squared error (RMSE) on the test set, and the best-performing model parameters are selected. Fig. 2 shows the neural network structure optimized for predicting the mechanical properties of Fe-9-12Cr steel, visualized through RMSE trend analysis.

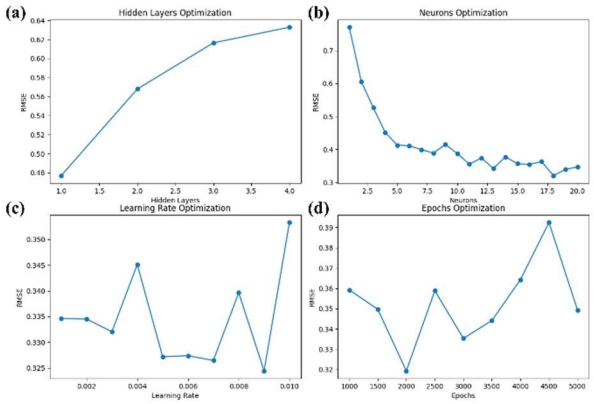

Fig. 2. Hyper-parameter optimization results: (a) hidden layers, (b) neurons per layer, (c) learning rate, and (d) training epochs, evaluated based on RMSE trends

3. Results and Discussion

The performance of the optimized neural network model was evaluated by comparing the predicted mechanical properties of Fe-9-12Cr steel with experimental values. Fig. 3 illustrates the actual versus predicted values for (a) tensile strength, (b) 0.2% proof stress, and (c) elongation, demonstrating the model's ability to capture complex material behaviors. The results indicate that the model effectively predicts mechanical properties with a reasonable level of accuracy, though some deviations are observed due to inherent material variability and data limitations. The RMSE values across different properties suggest that while the model performs well in generalization, further improvements, such as incorporating additional features or refining the network architecture, could enhance predictive accuracy. These findings highlight the potential of machine learning in material property prediction, supporting its application in nuclear structural materials research.

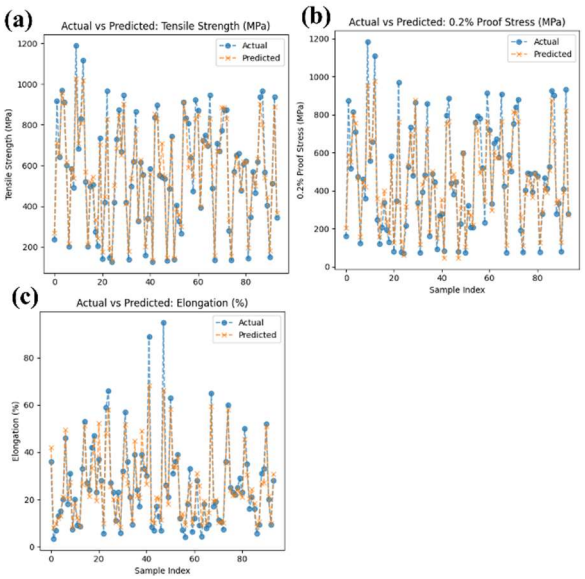

Fig. 3. Comparison of actual and predicted mechanical properties: (a) tensile strength, (b) 0.2% proof stress, and (c) elongation, demonstrating model accuracy and deviations.

4. Conclusion

This study developed and optimized a machine learning model for predicting the mechanical properties of Fe-9-12Cr steel used in nuclear reactors. Through systematic hyper-parameter tuning, including adjustments to hidden layers, neuron counts, learning rates, and training epochs, the model demonstrated strong predictive performance. The comparison between actual and predicted values confirms that the neural network effectively captures complex material behaviors, though minor discrepancies highlight areas for further refinement. These findings underscore the potential of machine learning in material property prediction, reducing reliance on extensive experimental testing and supporting the design of nuclear structural materials. Future work should focus on expanding the dataset with

additional experimental data and refining model architectures to enhance predictive accuracy and generalizability.

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