# Hardness Prediction of Refractory High Entropy Alloy by Neural Network

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**Abstract:** The hardness of refractory high entropy alloys (RHEAs) is an essential property but its prediction remains challenging. In this study, we propose a neural network mode (NN) that is capable of predicting the hardness of RHEAs. With this NN model, we predict the hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$ and found a good agreement with the experiment. This study provides an alternative path to calculate hardness before the alloys are synthesized and allows the researcher to design RHEAs until the desired hardness is reached.

**Keywords:** High entropy alloy, neural network, hardness, $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$.

## 1. Introduction

High entropy alloys (HEAs) are new concepts used to design metallic alloys by mixing five or more metallic elements. Almost all HEAs are strong, superconductive, high yield strength and are resistant to crack, fatigue, and corrosion [1]. Recently, machine learning (ML) approaches have been utilized to predict the crystal structures and properties of materials [2,3]. Islam *et al.* [4] developed neural network (NN) models that can analyze the phase of multi-principal element alloys with 118 data sets. The NN model is a machine learning prediction method that is highly inspired by the functionalities of the human brain system. Wen *et al.* developed a material design strategy using ML for predicting the desired properties of HEAs [5]. George *et al.* [6] also utilized the machine learning model which can predict the elasticity of HEAs with experimental validation. These studies have shown that ML methods are capable and reliable in discovering new HEAs and predicting their phases. However, many studies focus on phase formation predictions and a few on predicting the mechanical or functional properties of complex RHEAs.

In this study, the Vickers hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$ was predicted by utilizing the NN model. The measured Vickers hardness was found to be consistent with the NN model prediction.

## 2. Computational method

The hardness data used in this study were summarized from the previous publications [7,8,9,10]. The other 5 features of data set i.e. entropy ($\Delta S_{mix}$) [11], bulk modulus ($B$), Shear modulus ($G$), valence electron concentration ($VEC$) [12], and melting temperature ($T_m$) were calculated using the rule of mixture as follows.

$$\Delta S_{\text{mix}} = -R \sum_{i=1}^{n} C_i \ln C_i \tag{1}$$

$$B = \sum_{i}^{n} (C_i B_i) \tag{2}$$

$$G = \sum_{i}^{n} (C_i G_i) \tag{3}$$

$$T_m = C_i \, (T_m)_i \tag{4}$$

$$VEC = \sum_{i=1}^{n} C_i \, (VEC)_i \tag{5}$$

where $C_i$ is the atomic percentages of the $i^{th}$ element, $(B_i)$ is the bulk modulus of the $i^{th}$ element, $(G_i)$ is the Shear modulus of the $i^{th}$ element, $(T_m)_i$ is the melting point of the $i^{th}$ element and $(VEC)_i$ is the valence electron concentration of $i^{th}$ element.

There were total 128 samples out of which 90% were used for training and 10% were used for testing after random shuffling. At first, Pandas library [13] is used to normalize the value of the features so that they range from 0 to 1. This normalization of data helps in formatting the features in such a way that it can be easily analyzed. The open-source library PyTorch was employed to train the NN model for predicting the hardness of RHEAs.

The NN model consists of three layers namely the input layer, hidden layer, and output layer. The main function of the input layer is to pass initial data or information into the NN model. The hidden layer lies in between the input and output layers in a NN where all computational jobs are done. It is capable of extracting the hidden patterns of the input data. The output layer is the last layer of the NN model which simply produces the outputs of the previous neurons. The following relation can be used to calculate the output of each neuron ($a_j$):

$$a_j = \sum_{i=1}^{n} x_i \, W_{ij} + b_j \tag{6}$$

where $x_i$ and $b_j$ are the bias terms and $W_{ij}$ are the weights provided with each input features. The value of $a_j$ proceeds through an activation function. Then, the activation function will define the output of given neurons by learning the complex pattern of input data. Each layer consists of different numbers of neurons and are connected with each other by channels. These channels are connected and provided with a specific weight value. Each neuron computes the $a_j$ value from Eq. (6). The computed value of $a_j$ is passed to the activation function. The type of activation function used in this NN model is leaky ReLU [14]. Both training and testing data were standardized using the mean and variance obtained from the training data only to avoid data leakage. The training was done for 200 epochs on a machine with NVIDIA GTX 1050 Ti Max Q graphics card. The optimization criterion to optimize was a loss. The batch size was set to 1 since the time complexity was not an issue for a small training data size. The gradient decent methods of learning rate of 0.01 was set up. The weights and bias are randomly initialized at the start of the training process and were updated at each epoch by minimizing the cost function.

## 3. Results and discussion

The training data was shuffled before each epoch to avoid the NN model from hardcoding the true values of training data. The working process of the NN model is very simple, if the user provides RHEA with its molar composition of elements as inputs, then the model will predict the hardness. The screenshot of the predicted Vickers hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$ is shown in **Fig. 1**. The predicted Vickers hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$ was 552.49 $H_v$.

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Found a model with a decreased testing loss in epoch  32 . Saving the model as: target_Hardness_features

Predicted hardness of the Mo15Nb20Re15Ta30W20 is:  tensor([552.4902], grad_fn=<AddBackward0>) .
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**Fig. 1.** Snapshot of hardness prediction for $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$.

The average loss as a function of the epoch shown in **Fig. 2**. The graph seems to be a good fit, since the training loss and testing loss graph decreases with each number of epochs until it reaches a point of stability. The stability is reached after the 75 epochs.

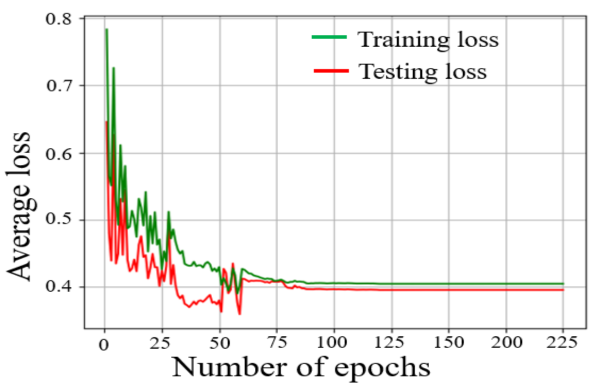


**Fig. 2.** The average loss as a function of number of epochs.

**Table 1.** The predicted and experimental Vickers hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$.

| Our work | Predicted value ($H_v$) | Measured value ($H_v$) | Error (%) |
|---|---|---|---|
| $Mo_{11.9}Nb_{20}Re_{15}Ta_{30}W_{20}$ | 552.49 | 600 [1] | 6.6% |

The predicted and experimental Vickers hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$ is presented in **Table 1.** The experimentally measured Vickers hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$ agrees with the NN prediction. The hardness prediction from the current model seems very promising because they were studied with small training data sets. The close agreements between predictions and experiments validate the reliability of current NN model. The prediction accuracy can be further improved with sufficiently larger data sets. A similar neural NN model could be used in predicting novel RHEAs properties such as yield strength, ductility, and tensile strength, etc.

## 4. Conclusion

In this study, a neural network model was introduced and the hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$ was predicted. This model was created based on 128 data samples. The predicted hardness of $Mo_{15}Nb_{20}Re_{15}Ta_{30}W_{20}$ was 552.49 *S* that agreed with the experiment. The current NN method will allow researchers to synthesize virtual RHEAs until the expected hardness is reached. Therefore, it finds a promising scope in accelerating RHEAs designs with desired hardness.

## 5. Acknowledgments

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