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Article

Evaluating Machine Learning Models for Predicting Hardness of AlCoCrCuFeNi High-Entropy Alloys

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Abstract: This study evaluates the predictive capabilities of various machine learning (ML) algorithms for estimating the hardness of AlCoCrCuFeNi high-entropy alloys (HEAs) based on their compositional variables. Among the ML methods explored, a backpropagation neural network (BPNN) model exhibited superior predictive accuracy compared to other algorithms, including Support Vector Machine (SVM), Stochastic Gradient Descent Regressor (SGDR), Bayesian Ridge (BR), Automatic Relevance Determination Regression (ARDR), Passive-Aggressive Regressor (PAR), Theil-Sen Regressor (TSR), Linear Regression (LR), and Random Forest (RF). The BPNN model achieved excellent correlation coefficients (R^2) of 99.54% and 96.39% for training (116 datasets) and testing (39 datasets), respectively. Validation of the BPNN model on an independent dataset (19 alloys) further confirmed its high predictive reliability. Additionally, the developed BPNN model facilitated a comprehensive analysis of the individual effects of alloying elements on hardness, providing valuable metallurgical insights. This comparative evaluation highlights the potential of BPNN as an effective predictive tool for material scientists aiming to understand composition-property relationships in HEAs.

Keywords: machine learning algorithms; backpropagation; artificial neural networks; high entropy alloys; hardness

1. Introduction

High-entropy alloys (HEAs) are a unique class of alloys where multiple principal elements are mixed in relatively high concentrations to maximize the configurational entropy [1]. The HEAs remain a simple solid solution phase, such as face-centered cubic (FCC, using Co, Cr, Fe, and Ni, etc.), body-centered cubic (BCC, using Mo, Nb, Ta, and Zr, etc.), or a mixture of the two instead of forming complex phases and intermetallic compounds [2]. The HEAs possess excellent chemical, and mechanical properties absent in traditional metallic alloys. For instance, the HEAs show high strength, hardness, cryogenic toughness, and thermal stability at elevated temperatures. Further, the alloys resist corrosion and wear [3]. Due to their attractive properties, the alloys have got an immense interest in the scientific community in recent years. Since the HEAs are composed of simple phase constituents (either FCC, BCC, or mixed), the selection of alloying elements has a great influence on mechanical properties.

Due to relatively high amounts of multi-principal elements, the compositions of HEAs are located near or at the center of the composition space [4]. This multi-dimensional compositional space is practically limitless which opens up a vast new realm of alloy design with unprecedented freedom. It comes as no surprise that, even after over a decade only a small fraction of HEAs compositional regions is identified so far within the immense compositional space, and the alloy designing is typically carried out by trial and error methods with low success rate [5]. Hence it is a great challenge to design a search strategy to recognize the desired compositions with some exceptional mechanical properties while minimizing the time and cost-intensive experimentations. In this regard, the progress in computer-aided algorithms with excellent computation capability brings a new opportunity for modelling multicomponent alloy systems [6]. Several novel parameter optimization techniques have been developed to design multivariable complex systems [7]. Especially in the case of HEAs, high throughput CALPHAD [8], high-throughput ab initio method LTVC (for phase identification) [9], DFT, MD (for phase stability, solidification and crystallization kinetics) and genetic algorithms have been developed to accelerate the design of HEAs [10]. However, accurate prediction of the resulting properties for a given combination of constituent elements is crucial to the development and applications of new HEAs. Unlike parametric approaches, machine learning (ML) is a cutting-edge tool that implicit the relations from existing data [11]. The ML method due to its huge success in various fields has become an effective approach and got greater attention in materials science, especially in the HEAs community [12].

Machine learning is a broad computing field where algorithms play a significant role in problem optimization [13]. Several authors reported various ML algorithm types for the optimization of HEAs related issues. For instance, Chang et al. [14] utilized a simulated annealing algorithm (SA) to predict the composition and hardness of HEAs. Menou et al. [15] used a multi-objective optimization genetic algorithm to design the high specific strength HEAs. Therefore, utilizing the best machine learning approach for designing a multi-component system is of great importance. The selection of a proper ML algorithm approach helps to understand the optimum algorithm for designing HEAs with high accuracy as well as high throughput. Several authors used various ML algorithms to design the HEAs, unfortunately, the information regarding the prediction accuracy of train and test datasets, as compared with the other algorithms is often ignored [14]. Finding such information certainly helps the alloy designers to choose a highly accurate ML tool. Comparing the efficiency of various commonly used ML algorithms certainly helps to choose the appropriate ML algorithm for a given problem optimization. However, there is hardly any reported study on this aspect. Considering this, in the present study, we proposed various popular ML algorithms (a total of 9 ML algorithms, namely Support Vector Machine (SVM), Stochastic Gradient Descent Regressor (SGDR), Bayesian Ridge (BR), Automatic Relevance Determination Regression (ARDR), Passive-Aggressive Regressor (PAR), Theil-Sen Regressor (TSR), Linear Regression (LR), Random Forest (RF) and finally the Back Propagation Neural Networks (BPNN)) to predict the hardness of multi-component alloy (Al-Co-Cr-Cu-Fe-Ni) systems. The work mainly concentrated on the AlCoCrCuFeNi alloy system due to its complex phase transitions with alloying as well as limited work availability [16]. In general, the phase formation completely depends on the alloying elements, for example, the CoCrCuFeNi quinary alloying system exhibits only a single solid solution, the FCC phase. On the other hand, the six-elemental alloy, the AlCoCrCuFeNi forms FCC, BCC and a combination of phases according to the alloying content. Thus, the detailed understanding of the alloy behavior with composition is quite complex and challenging, needs significant attention [17]. Therefore, the present study mainly focused on selecting the optimal ML algorithm for understanding the composition-structure-property relationships which helps to design novel multi component AlCoCrCuFeNi alloy systems. The performance of each model was determined with the help of prediction accuracy of both training and testing datasets. Among all ML algorithms, the backpropagation neural networks (BPNN) exhibit a high level of prediction accuracy. Therefore, we utilize the BPNN model to design the new compositions of Al-Co-Cr-Cu-Fe-Ni-based HEAs with excellent mechanical performance.

2. Methods

2.1. *Brief Notes on Various ML Algorithms*

2.1.1. Support Vector Machine

Support Vector Machine is an ML tool that can be used for regression and classification-based tasks (mainly used for classification). By definition, an SVM constructs a hyperplane or set of hyperplanes in a high or infinite-dimensional space, which can be used for classification or regression. For example, for a given set of input data and predicts, for each given input, two possible classes form the output (binary linear classifier). In the case of the non-linear or higher-dimensional features, the SVM uses different kernel functions where the given non-linear problem is reformulated as a linear problem by different kernel functions [18].

2.1.2. SGD Regressor

SGD is one of the descent tools that has been successfully applied to large-scale ML problems. Simply, it is an iterative method and a very efficient approach for optimizing an objective function. Due to its fast computation and easy learning, the SGD regression is interesting in the research perspective [19].

2.1.3. Bayesian Ridge

The Bayesian ridge regression is a kind of linear regression where the predicted value is considered as a linear combination of the input variable. The method is very useful for process regularization [20]. The method has flexibility in the design for any given problem, however the predictions take noticeably more time to be solved and computed.

2.1.4. Automatic Relevance Determination Regression

ARD regression is a hierarchical Bayesian approach widely used for model selection [21]. The main advantage of the ARD is that the model can be able to switch off the irrelevant input variables (which are irrelevant to the prediction of the output variable) by setting the coefficients to zero. Thus, the model is effectively able to infer which variables are relevant and then switch the others off and prevent the model from overfitting. The method is mainly used where a large number of input variables further allows the irrelevant input variables to be left in the model without harm [22]. A detailed description of ARD regression can be found in [21].

2.1.5. (. e) Passive-Aggressive Regressor

Passive-aggressive algorithms are a family of machine learning algorithms mainly used for both classification and regression. These algorithms can be used for large-scale with regulation parameters [23].

2.1.6. Theil-Sen Regressor

Theil-Sen Regression is a method for robustly fitting a line to sample points in the plane by choosing the median of the slopes of all lines through pairs of points. Due to its simplicity in computation, the method can be applicable for various fields to estimate the trends in the given complex system [24].

2.1.7. (. g) Linear Regression

Regression analysis is one of the most widely used techniques for analyzing multi-factor data. The method is simple and easier to implement and interpret the output coefficients [25]. Diversely,

the method over-simplifies real-world problems by assuming a linear relationship among the variables.

2.1.8. Random Forest

Random Forest is a meta estimator that fits several classifying decision trees on various sub-samples of the dataset and uses averaging to improve the predictive accuracy and control over-fitting [23]. Thus, the algorithm builds multiple decision trees and merges them together to get a more accurate and stable prediction. Despite the advantages, the RF has some drawbacks such as much computational power as well as training time.

2.1.9. Backpropagation Neural Networks

Backpropagation is simple, fast and easy to program and is the essence of neural net training. It is a method of fine-tuning the weights of a neural net based on the error rate obtained in the previous epoch. Proper tuning of the weights allows us to reduce error rates and make the model reliable by increasing its generalization. A detailed theory of backpropagation neural networks can be found elsewhere [26].

2.2. Data Processing

The database used in the present study was taken from published literature. A total of 155 combinations of alloy compositions (in at. %) and their respective hardness values [27] were reported in [14]. Overall, the composition of each element varies in vast range and is multi-dimensional.

The minimum, maximum, mean and standard deviation values of each element and hardness values were tabulated in Table. 1. The pair plot (or scatter plot matrix) shown in Fig. 1 describes the distribution of a single variable and its relationship with all the other variables present in the multi-dimensional variable system [28]. Briefly, the pair plot provides a matrix of the pairwise scatter plots of all variables in the data frame. The principal diagonal of the matrix running from the top left to its bottom right contains the distribution plots or histograms of each variable. Thus, from the pair plot, one can get an idea about the distribution of each variable and the corresponding relation with the other variables present in the database. The data points are randomly distributed and the correlation value (Pearson’s r) between any two given variables is weak and complex. On the other hand, the histogram and the fitted normal distribution curve summarize the distribution of the variable in the database.

Table 1. The minimum, maximum, average and standard deviation values of variables.

Variable	Variables	Minimum	Maximum	Average	Std. Dev.
Inputs	Al	0	46.2	16.89	11.26
	Co	0	42.9	14.56	10.23
	Cr	0	55.6	18.52	8.52
	Cu	0	29	10.65	9.2
	Fe	0	46.9	18.07	7.44
	Ni	0	50	21.31	9.2
Output	Hardness	110	775	422.07	187.66

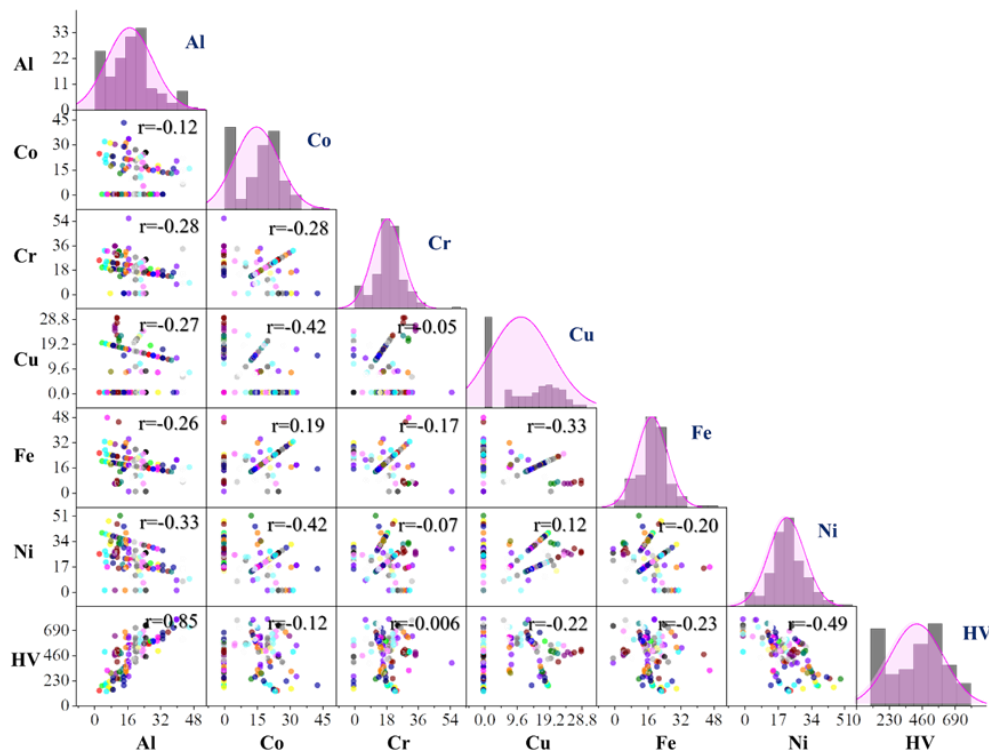


Figure 1. Data distribution plots and pairwise relationships among chemical components and hardness. Respective Pearson correlation coefficient r between each pair of variables is mentioned in each plot.

3. Results

4.1. Model Development

The composition of the alloy consists of Al, Co, Cr, Cu, Fe, and Ni (in at. %) are considered as the input variables and the hardness [27] is the output variable for constructing the model. The predictive models have been developed with various ML algorithms. Among 155 datasets, 116 datasets were used for training whereas the remaining 39 datasets were used to test the optimal performance of the various ML algorithms. The optimum model for each ML algorithm was determined based on the cross-validation error calculated using Equation 1.

$$E_{cve}(y) = \frac{1}{N} \sum_{i=1}^N |(T_i(y) - O_i(y))| \quad (1)$$

Where $E_{cve}(y)$ = cross-validation error in prediction of training and testing data set for output parameter y . N = Number of datasets, $T_i(y)$ = Targeted output and $O_i(y)$ = Output calculated.

The cross-validation error during the development of neural networks with the backpropagation ML algorithm is shown in Fig. 2. The cross-validation error of training datasets (116) tends to decrease with increasing iterations hence it is quite difficult to find the optimum model with only the training datasets. On the other hand, the cross-validation error of test datasets decreased with increasing iterations at the initial stage and attained a minimum value at 20000 iterations (as indicated in Fig. 2). Afterward, the error significantly increased with increasing iterations. Hence, the optimum model was determined based on the minimum test data error.

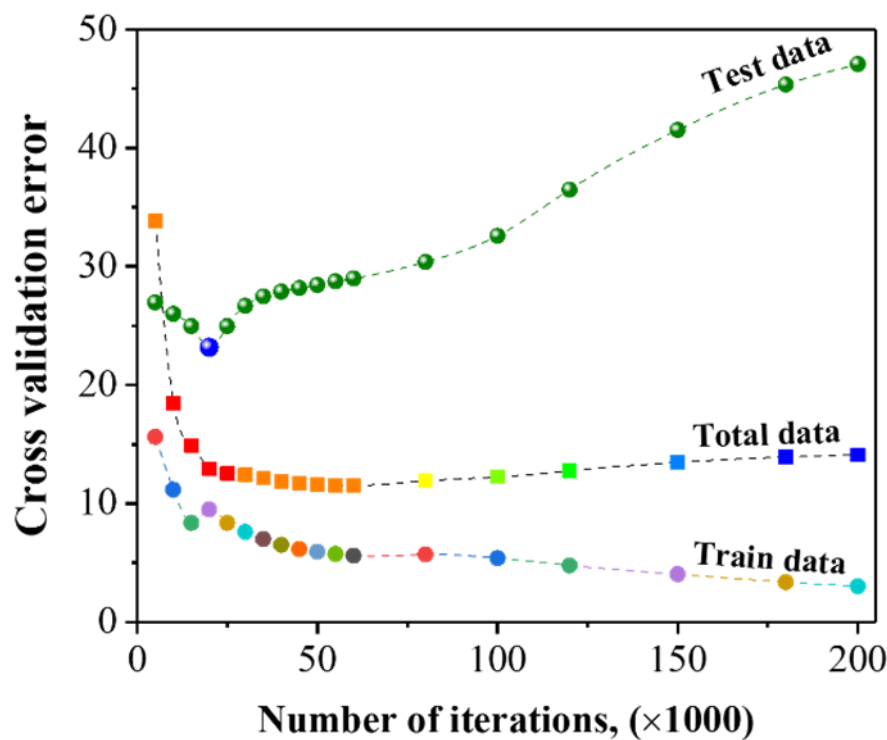


Figure 2. Change in cross-validation error as a function of iterations in the BPNN model.

4.2. Comparing Prediction Accuracy of Various ML Algorithms

The predictive performances of different machine learning (ML) algorithms were compared by examining correlation plots of experimental versus predicted hardness values, as depicted in Figure 3. These plots illustrate the correlation between experimental and predicted hardness values and provide the corresponding correlation coefficient (R^2) values for the 39 test datasets. The Passive-Aggressive Regressor (PAR) demonstrated the lowest prediction accuracy, achieving an R^2 value of only 52.93%. Conversely, both the Support Vector Machine (SVM) and Backpropagation Neural Network (BPNN) models showed excellent predictive performance, each yielding R^2 values exceeding 90%. Among all the algorithms, the BPNN exhibited the highest accuracy, achieving an R^2 of 96.39%. For a clearer comparative evaluation, Figure 4 summarizes the R^2 values of the various ML algorithms for both training (116 datasets) and testing (39 datasets) phases. Based on the correlation coefficients obtained from both datasets, the BPNN model exhibited minimal prediction error and demonstrated outstanding reliability for predicting the hardness of high-entropy alloys (HEAs).

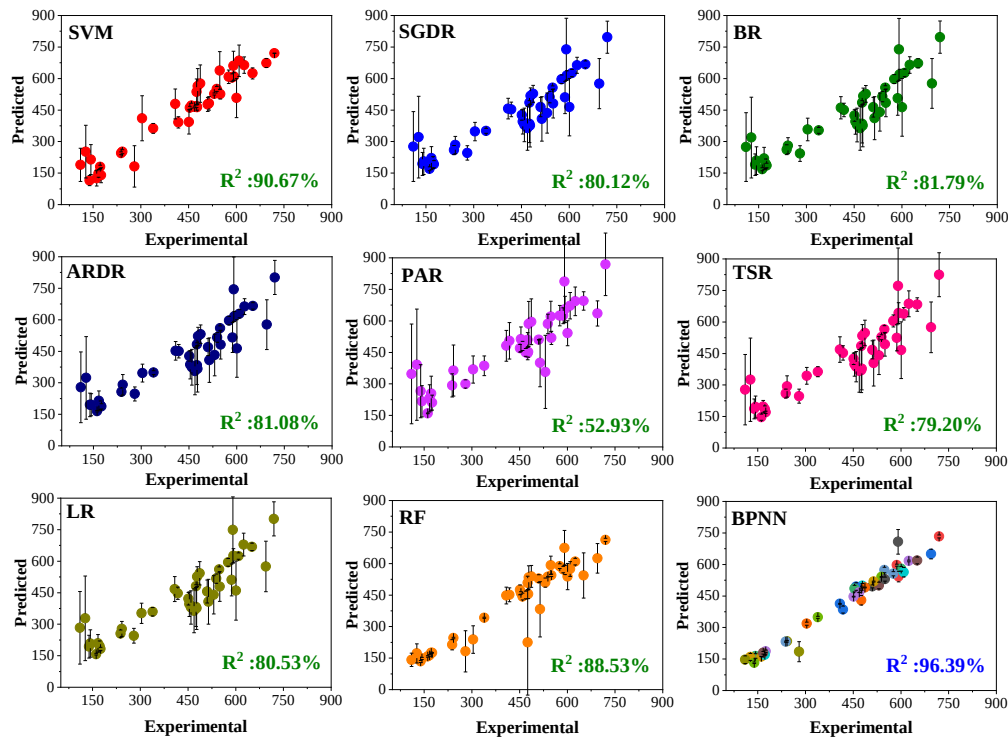


Figure 3. Performance of various ML algorithms for 39 test datasets.

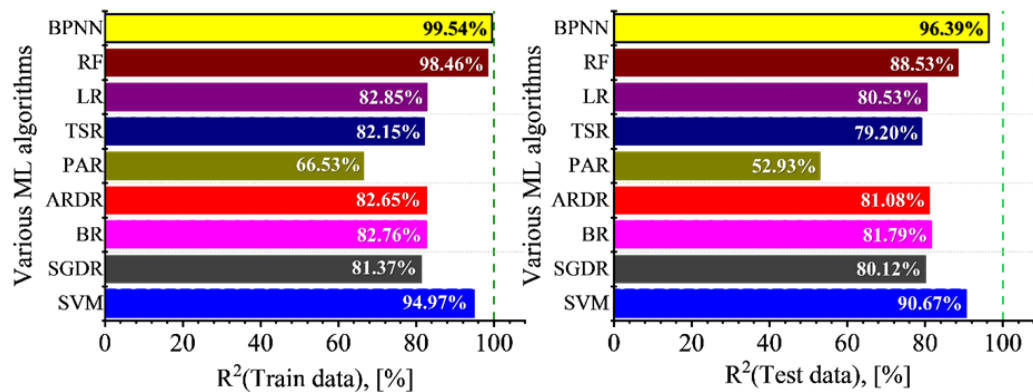


Figure 4. Correlation coefficient (R^2) values of various ML algorithms: (a) train datasets and (b) test datasets.

4.3. Validation of BPNN Model

To validate the developed BPNN model we further considered the various HEAs (total of 14 as shown in Table 2) compositions from the literature [7, 20]. The alloy hardness was predicted using the finalized optimal BPNN model. The predicted hardness and respective error values were tabulated in Table 2. The model was able to estimate the hardness values of the validation set of HEAs with considerable accuracy. The average error in the predictions was noted as 18.19. Hence, the developed neural networks model with the backpropagation algorithm could correlate the complex relations among the composition and hardness of HEAs compared with other well-known ML algorithms. Moreover, the BPNN model was able to provide significant prediction accuracy even for validation (unknown) datasets.

Table 2. The list of datasets used for validation of the BPNN machine learning model.

S No	Composition (at. %)						Hardness (Exp.)	Hardness (BPNN)	Error	Ref.
	Al	Co	Cr	Cu	Fe	Ni				
1	0	22.2	22.2	11.1	22.2	22.2	174	160.63	13.37	[7]

2	7	23.3	23.3	0	23.3	23.3	125	113.68	11.32	[7]
3	22.2	22.2	22.2	11.1	0	22.2	564	552.28	11.72	[7]
4	25	0	25	0	25	25	558	517.52	40.48	[7]
5	27.3	18.2	18.2	0	18.2	18.2	482	462.23	19.77	[7]
6	10	20	20	10	20	20	204	197.94	6.06	[7]
7	33.3	16.7	16.7	0	16.7	16.7	510	542.74	32.74	[7]
8	18.2	18.2	18.2	9.1	18.2	18.2	563	560.96	2.04	[7]
9	11.1	22.2	22.2	0	22.2	22.2	160	172.77	12.77	[7]
10	16.7	16.7	16.7	16.7	16.7	16.7	410	409.6	0.4	[7]
11	0.5	19.9	19.9	19.9	19.9	19.9	208	161.84	46.16	[37]
12	19.9	0.5	19.9	19.9	19.9	19.9	473	469.61	3.39	[37]
13	19.9	19.9	19.9	19.9	0.5	19.9	418	407.25	10.75	[37]
14	19.9	19.9	19.9	19.9	19.9	0.5	423	466.72	43.72	[37]

4.4. Effect of Element Concentration on the Hardness

The mechanical properties of HEAs strongly depend on the composition and microstructure. D.B. Miracle et al. [30] reported that the alloy composition determines the existing phases and their volume fractions, atomic interactions that influence the properties through the intrinsic properties of the phases. However, the individual elemental effect on hardness values of HEAs is rather limited and only a few studies focused on the variation of individual element amount effect on the mechanical properties of HEAs [31-33]. Therefore, herein with the help of the developed BPNN model, we tried to estimate the effect of alloying elements on the hardness of HEAs. The metallurgical reasoning of predicted hardness results was given, and the results were ensured with the published data. As illustrated in Fig. 5a, Al tends to increase the hardness with concentration. As reported in [30,34] the concentration of Al increases, the single-phase FCC (low hardness phase ~ HV 100-200) transforms to BCC+FCC and then to the single-phase BCC/B2 phase which has the higher hardness ranging from HV 500-600. The BPNN predicted trend regarding the variation in hardness as a function of Al content shows close agreement with the experimental trend [39, 42]. As shown in Fig. 5b, the effect of Co on hardness is quite negligible yet it tends to minimize the hardness slightly. Qin et al. [35] reported that increase in Co content leads to the formation of the FCC phase which tends to decrease the hardness, and the other possible reason is due to the low solubility of Co in the BCC solid solution the element gets rejected from the high hardness phases and causes a reduction in hardness [36]. In contrast to the Co, the Cr gradually increases the hardness as depicted in Fig. 5c. Shun et al. [33] observed that at low concentrations Cr forms the FCC phase and with increasing the Cr content the phase fraction of FCC was decreased, and the element stabilizes the BCC phase. Accordingly, we observed the lowest hardness value at the low content Cr and with increasing Cr, the hardness increased gradually (Fig. 5c). The Cu doesn't show considerable influence on the hardness and the value is almost constant throughout the given range of Cu concentration (0 to 30 at. %) as illustrated in Fig. 5d. The estimated behavior of hardness as a function of Fe content is plotted in Fig. 5e. From the figure, it is clear that an increase in Fe content leads to a continuous decrement in the hardness and similar results have been reported in the literature [37]. According to Chen et al. [37], the lattice distortion and absence of the Cr₃Ni₂ phase are the main possible reasons caused by Fe content which results in deterioration of hardness. Finally, the effect of Ni content on hardness is shown in Fig. 5f. The Ni tends to increase the hardness in low content levels (< 8 at. %) however, with increasing Ni content leads to decrease the hardness up to 20 at. % and the hardness remained constant with further increase in Ni content. The similar trend of Ni effect has been reported by Suresh et al. [32]. They investigated the effect of Ni content on hardness and found that the higher Ni content (> 10 at. %) significantly decrease the hardness due to the stabilization of single FCC phase. At lower concentrations the increase in hardness is due to the presence of a mixture of both FCC and hard tetragonal phases. Hence, from the estimated results it can be concluded that the develop BPNN

model was able to correlate the concentration and hardness of HEAs and provides detailed knowledge regarding the qualitative influence of alloying elements on hardness.

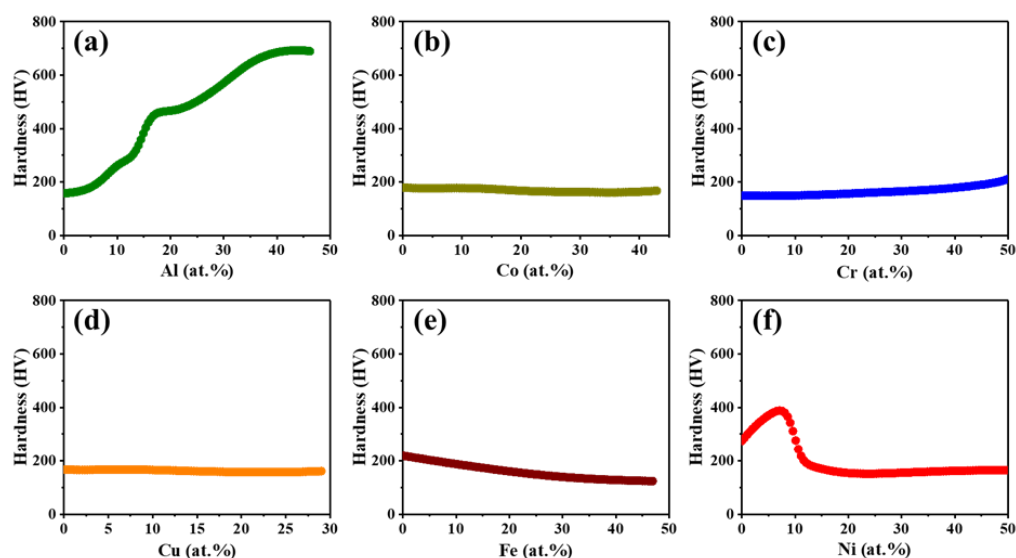


Figure 5. The BPNN model estimated the results of the element concentration effect on hardness behavior: (a) Al, (b) Co, (c) Cr, (d) Cu, (e) Fe and (f) Ni.

4.5. Validation of the Model Predictions with Experimental Results

The composition-property correlations predicted by the BPNN model were validated with the experimental results. Such validation ensures a great degree of confidence in the accuracy of predictions made by the present study. To verify the predicted behavior of hardness, we compared the experimental hardness values of various $\text{Al}_x\text{CoCrCuFeNi}$ alloys. Fig. 6 shows the experimentally measured effect of Al content on hardness (shown with a solid red line connecting the triangles) of $\text{Al}_x\text{CoCrCuFeNi}$ where x is varying from 0 to ~40 at.%. It is evident that increasing Al content significantly increases the hardness value (from 130 to 650 HV). On the other hand, the BPNN model predicted hardness values as a function of Al content were denoted with the green-colored circles (Fig. 6), and the predicted hardness values were well-matched with the experimental results. The overall experimental and model-predicted hardness values as a function of Al content obey a similar trend. It has been well reported that the properties of HEAs certainly depend on the alloy composition. In particular, the addition of Al can harden the HEAs. This is mainly because of the formation of a hard BCC phase. Initially, the AlCoCrCuFeNi alloy with a lower concentration of Al usually consists of the FCC phase. With increasing the Al content (>10-12 at. %), the formation of the BCC phase can be noticed thus the alloy with a mixture of FCC+BCC reveals higher hardness which further increases with Al content. Finally, the higher Al content (>35 at. %) completely stabilizes the hard BCC phase and raises the hardness values > 700 HV. The variations in the microstructural constituents with increasing Al content in the $\text{Al}_x\text{CoCrCuFeNi}$ HEAs system have been systematically reported in [38,39]. Besides the microstructural variations, the stronger cohesive bonding between Al and other elements and larger atomic size can partly harden the alloy and this phenomenon is generally named as a Cocktail effect [34]. Therefore, the present BPNN model was able to correlate the complex relations that are present among the composition properties of HEAs. More importantly, the predicted behavior follows the experimental trend which certainly helps us to understand the metallurgical phenomenon of other alloying elements that exist in the HEAs. Such clear knowledge about the system helps to design the HEAs with desired properties.

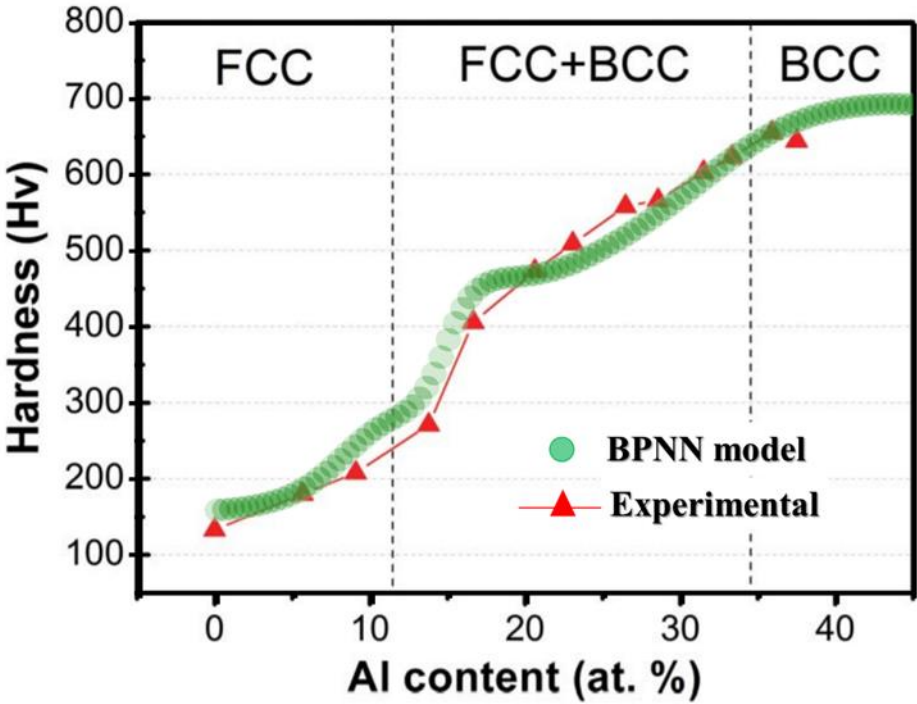


Figure 6. Comparing the experimental [42] and BPNN model predicted hardness variation trend as a function of Al content in cast $Al_xCoCrCuFeNi$ alloys.

4.6. Significance of Alloy Components on the Hardness

The overall influence of each input variable on the output can be explained with the help of the index of relative importance (I_{RI}). A detailed explanation of this method has been reported in previous studies [40]. The significance of each chemical component on the hardness was represented with the help of a pie chart as shown in Fig. 7. According to Fig. 7, among all chemical components, the Al shows a positive I_{RI} value (+0.0775) which indicates the element can lead to an increase in hardness value. On the other hand, the Ni exhibits a strong negative impact (with an I_{RI} value of -0.0412) and leads to decline in the hardness value. The order of relative importance of the chemical components on the hardness value of HEAs can be summarized as “Al > Cr > Co > Cu > Fe > Ni”. Therefore, with the help of this method, one can clearly understand the influence of individual components on the hardness.

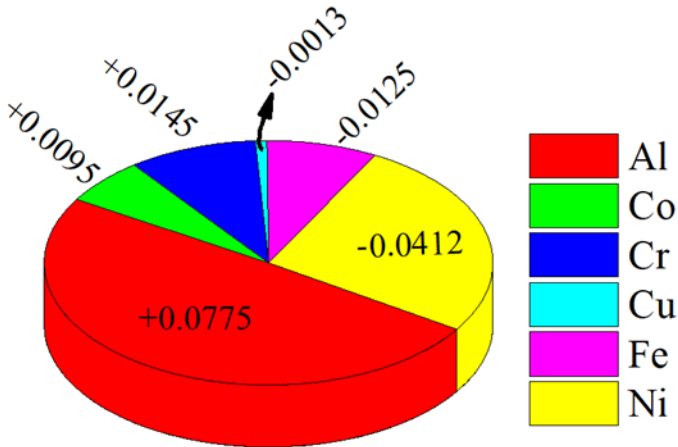


Figure 7. The significance of chemical components on the hardness of HEAs was estimated using the BPNN model.

4. Conclusions

The results of the present work demonstrate that compared to the other ML models, the BPNN method is in good agreement with the predictions for both train and test datasets (99.54% and 96.39%, respectively). According to correlating index values of train and test datasets, the backpropagation ML model can be used as a standalone unit for optimizing the multi-component concentration to achieve better mechanical properties. Furthermore, the model corroborated the hardness values of unknown datasets with considerable accuracy. The graphical user interface was developed to understand the influence of multi-component concentration on hardness which can help to reduce the level of effort required for the experimentation. The model can also be able to provide a huge number of virtual alloy systems within the given range of input variables. Finally, the relative importance index of the components one can utilize to understand the hierarchical order of input variables on the output

Supplementary Materials: The following supporting information can be downloaded at: www.mdpi.com/xxx/s1, Figure S1: title; Table S1: title; Video S1: title.

Author Contributions: N.S.R. and P.L.N. conceptualized the study. The methodology was developed by P.L.N. and M.I. ANN model Software was developed by N.S.R and P.L.N., while validation was performed by A.K.M. and M.I. Formal analysis was conducted by P.L.N. and M.I., with investigation carried out by A.K.M. and U.M.R. Resources were provided by S.W.C. and N.S.R., and data curation was handled by P.L.N. The original draft was written by U.M.R., A.K.M., and P.L.N., and reviewed and edited by N.S.R. and S.W.C. Visualization was prepared by U.M.R and M.I. The research was supervised by S.W.C. and N.S.R. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

BPNN	Back propagation neural network
I _{RI}	Index of relative importance
HEA	High entropy alloy
FCC	Face centered cubic
BCC	Body centered cubic

Appendix A

All appendix sections must be cited in the main text. In the appendices, Figures, Tables, etc. should be labeled starting with “A” —e.g., Figure A1, Figure A2, etc.

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