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Research Article

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Prediction of Glass Forming Ability of Bulk Metallic Glasses- Machine-Learning

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ABSTRACT

Bulk-Metallic-Glass has been a fascinating class of metallic systems with remarkable corrosion resistance, elastic modulus and wear resistance, while evaluating the glass forming ability has been a very interesting aspect for decades. Machine learning techniques viz., artificial neural networks and random-forest based models have been developed in this work to predict the glass forming ability, given the composition of the bulk metallic glassy alloy. A new criterion of classification of atoms present in a bulk metallic glassy alloy is proposed. Feature importance analysis confirmed that the accuracy of the prediction depends mainly on change in enthalpy of mixing and change in entropy of mixing. However, among the artificial neural network random forest models developed, the former showed a promising accuracy in prediction of the glass formation ability (critical thickness). It has been successfully demonstrated and validated with experimental critical thickness that the glass forming ability can be predicted using an artificial neural network given the elemental composition alone. A computational algorithm was also developed to classify the atoms as big/ small in a given alloy. The outcome of this algorithm was used by models developed by training with experimental data.

Keywords: Bulk Metallic Glasses; Simulation and modelling; Machine-learning; Glass forming ability; Metals and alloys, Amorphous materials;

INTRODUCTION

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Bulk-Metallic-Glasses (BMG) is one of the classes of advanced materials which are known for their superior corrosion resistance, fracture toughness and wear resistance [1-3]. The glass forming ability (GFA), is usually understood as the ease of formation of the vitrified structure. It is measured in terms of critical thickness, i.e., the largest section thickness of the alloy beyond which the alloy starts nucleation of the ordered structure. BMGs with high GFA reveal large critical thickness (or critical diameter, (D_{\max})) [1-9]. Plenty of studies were focused on evaluating the criteria of the GFA. These criteria were mostly based on critical temperatures, thermodynamic parameters, topological parameters etc., [5-9]. While several research works continued to focus on the glass forming ability, few of them performed computational studies on predicting the GFA of the BMGs. Sun et. al. [10] developed a machine-learning model built using a support-vector-machines (SVM) classifier. This method predicts the GFA of BMG given its composition. The model was developed using thermodynamic and physical parameters. However, the predictions of the model [10] were confined to binary alloys alone, and whose output was a classification of binary alloys into ‘good or bad glass-formers’. But, their machine-learning model was capable to predict neither the critical thickness nor the critical cooling rate of a BMG, quantitatively.

Ward et.al.[11] extensively studied the predictions of GFA using random forest approach of machine-learning, which was based on the elemental composition of BMGs as the input parameters. Three models were developed viz., glass forming ability model (which classifies good/ bad glass formers, qualitatively), critical casting thickness model (predicts D_{\max} quantitatively) and the third model was on the prediction of the supercooled liquid range. Interestingly, configurational entropy was not considered in any of their models which turned out to be most important feature in this study. Another independent investigation by Majid et.al. [12] demonstrated few algorithms viz., support vector regression (SVR), artificial neural network (ANN), general regression neural network (GRNN) using the characteristic

temperatures of the BMGs as the input parameters. However, the accuracies of the models developed weren't satisfying. Another limitation of this model was that, the temperatures used as input parameters can be measured only after synthesizing a BMG alloy experimentally. Hence the prediction model proposed by Majid et.al. [12] cannot be used for designing virtual BMG alloys.

Several research works [1-10] proved that the GFA depends on the thermodynamic and physical parameters such as enthalpy of mixing (ΔH_{mix}), difference ratio in electronegativity (Δe), difference ratio in atomic size (Δd) and critical characteristic temperatures of the BMGs. Therefore, in the present work, two different prediction approaches have been developed, which take an alloy composition as input and give D_{max} as output. According to the approach reported by Cai et al. [9] it is required to classify the constituent atoms as big/small to compute the Δe and Δd .

On the other hand, according to the existing classification made by Inoue et al. [2, 13], the atoms (of elements, irrespective of their presence in the alloy) are grouped into small, medium and large. Such classification makes the situation ambiguous in some BMGs, as all the constituent atoms of the alloy fall into only one category (only big/ medium/ small class of atoms). Therefore, in the present work a new method named as 'radius range theory of classification' has been proposed and demonstrated in reference with the classification reported by Inoue et al. [2, 13]. The proposed classification method also uses a computational approach to classify the atoms in to big/ small/ medium, irrespective of the number of elements. The result of this classification has been further used to compute the Δe and Δd values which were used in the prediction models (to predict D_{max}) developed in this work.

Upon providing the alloy composition, an algorithm computes the values of ΔH_{mix} , ΔS_{mix} , Δd and Δe for the alloy. The prediction models (Artificial Neural Network; Random forests) take

these computed values as inputs, process them and give the values of the D_{\max} as output of the alloy. The prediction accuracy of both the methods has been critically validated with experimental values of D_{\max} , of the alloys taken from the literature.

MATERIALS AND METHODS

Radius range theory of classification

It is based on the empirical criterion proposed by Inoue et al. [2, 13] that, in a multicomponent system BMG, the *atomic radii difference should be greater than 12%*. The classification proposed in this work is explained with an arbitrary quaternary alloy containing atoms A, B, C and D with different radii as shown in Fig. 1.

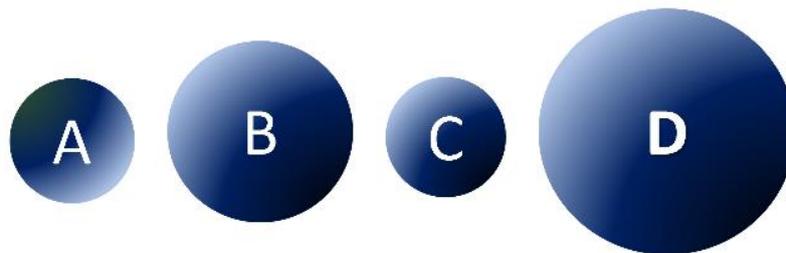


Fig.1 Schematic diagram showing atoms A, B, C and D with different radii

Algorithm of the radius range theory

Step-1: Identify the atom to be compared (eg. “A”)

Step-2: Calculate the radius range ($0.88R_B \sim R_B$; $0.88R_C \sim R_C$ and $0.88R_D \sim R_D$) for elements other than “A”.

Step-3: Compare the radius of A, i.e R_A with the radius range of the respective element

If R_A lies within the radius range of an atom: assign “0”

If R_A is less than the radius range of an atom: assign “-1”

If R_A is greater than the radius range of an atom: assign “+1”

Step-4: Sum up the values assigned in step-3

Step-5: $\text{Sum} > 0$, inferred as big atom. (i.e., atom “A” is bigger than all other atoms)

$\text{Sum} \leq 0$, inferred as small atom (i.e., atom “A” is smaller than all other atoms)

In the above example:

- i. $R_A <$ radius range of atom “B”, therefore assign “-1”
- ii. R_A lies in the radius range of atom “C”, therefore assign “0”
- iii. $R_A <$ radius range of atom “D”, therefore assign “-1”

Sum up the assigned values in (i), (ii) and (iii), i.e., $= (-1) + 0 + (-1) = -2$. Which is < 0 , hence atom “A” is classified as a small atom.

Dataset

A dataset containing 400 BMGs was collected from the work of Long et al [1]. It contains BMG alloys with Cu, La, Ca, Mg, Fe, Zr, Ti, Pd, Co, Pr, Hf, Gd, Au, Y, M as major constituent element. Some of the outliers with very high and low values of D_{\max} are excluded from the dataset. Of the remaining 287 BMGs are used for training purpose (**supplementary data table.1**) and testing/ validation was done on 31 BMGs (**supplementary data table.2**). Figure 1 is the pictorial representation of the number of alloys on Y-axis, with each major constituent element mentioned in the X-axis.

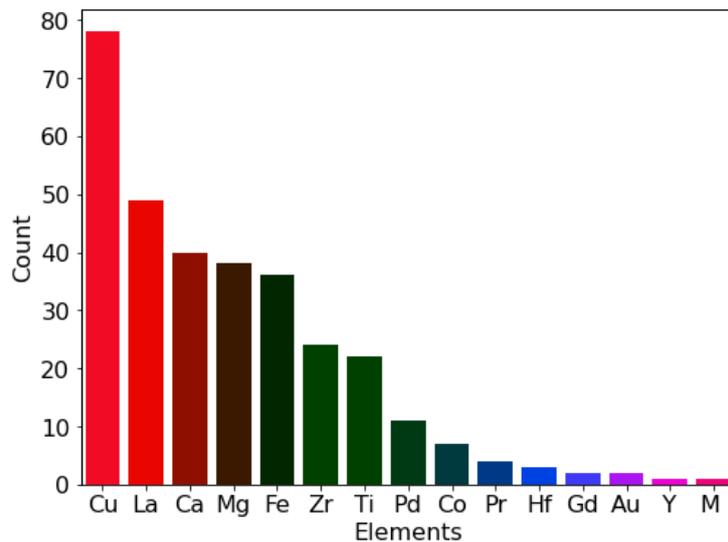


Fig.2 Count of BMGs based on Major constituent element

Feature Engineering

The characteristic temperatures of BMG such as T_x , T_g , T_1 can't be used as input features as they can be known only after synthesizing the BMG. Therefore we need input features that can be calculated without creating the BMG. ΔH_{mix} (Change in enthalpy of mixing), ΔS_{mix} (change in entropy of mixing), Δd (difference in atomic size), Δe are considered as input features of the ANN (deep-learning) and random forests (machine-learning) models. While ΔH_{mix} and ΔS_{mix} were calculated using Eq. (1) and Eq. (2) as adapted from Cai et al. [9]

$$\Delta H_{mix} = \sum \Delta H_i(x_i) \quad (1)$$

$$\Delta S_{mix} = -\sum x_i (\ln x_i) \quad (2)$$

Where, ΔH_i is the enthalpy of the individual element and x_i is the atomic percentage of i^{th} element.

The Δd and Δe are computed based on equations (3) and (4) below, reported by Cai. et al. [9].

$$\Delta d = \frac{\left[\frac{\sum_{i=1}^{n_1} (x_i d_i)}{\sum_{i=1}^{n_1} x_i} \right] - \left[\frac{\sum_{j=1}^{n_2} (x_j d_j)}{\sum_{j=1}^{n_2} x_j} \right]}{\left[\frac{\sum_{i=1}^{n_1} (x_i d_i)}{\sum_{i=1}^{n_1} x_i} \right]} \quad (3)$$

$$\Delta e = \frac{\left[\frac{\sum_{i=1}^{n_1} (x_i e_i)}{\sum_{i=1}^{n_1} x_i} \right] - \left[\frac{\sum_{j=1}^{n_2} (x_j e_j)}{\sum_{j=1}^{n_2} x_j} \right]}{\left[\frac{\sum_{i=1}^{n_1} (x_i e_i)}{\sum_{i=1}^{n_1} x_i} \right]} \quad (4)$$

where x_i is the atomic percent and d_i is the radius of the i^{th} bigger element, whereas j is for the smaller elements.

The input features are normalized using Standard Scaler (sklearn) as having features on same scale helps the ANN to converge faster towards minima while the process of gradient descent.

Demonstration of the radius range theory of classification

Three BMG alloys, $\text{Cu}_{57.5}\text{Zr}_{37.5}\text{Ga}_5$, $\text{Zr}_{50}\text{Cu}_{43}\text{Ag}_7$ and $\text{Pd}_{77}\text{Cu}_6\text{Si}_{17}$ were picked up randomly to demonstrate the proposed classification algorithm described above. The atomic radii of Cu, Zr, Ga, Ag, Pd, Si are 1.28 Å, 1.6 Å, 1.35 Å, 1.44 Å, 1.37 Å and 1.11 Å respectively [2]. If the atoms in $\text{Cu}_{57.5}\text{Zr}_{37.5}\text{Ga}_5$ BMG alloy are classified using proposed classification, the Cu, Zr, and Ga can be classified as small, big and small atoms, respectively but with respect to Inoue's method they come under medium sized atoms. Similar computations were conducted for other two BMG alloys and the elements have been classified basing on the proposed classification and are compared with that reported by Takeuchi and Inoue [13].

Table 1 Demonstration of the radius range theory of classification

BMG alloy	Element atomic radius (Å)	Radius range (Å) (0.88r~r)			Total Score	This work	Inoue's method [8]
		Cu (1.13~1.28)	Zr (1.40~1.6)	Ga (1.18~1.35)			
$\text{Cu}_{57.5}\text{Zr}_{37.5}\text{Ga}_5$	Cu(1.28)	0	-1	1	0	small	medium
	Zr(1.6)	1	0	1	2	big	medium
	Ga(1.35)	1	-1	0	0	small	medium
$\text{Zr}_{50}\text{Cu}_{43}\text{Ag}_7$		Zr (1.4~1.6)	Cu (1.13~1.28)	Ag (1.26~1.44)			
	Zr(1.6)	0	1	1	2	big	medium
	Cu(1.28)	-1	0	0	-1	small	medium
	Ag(1.44)	0	1	0	1	big	medium
$\text{Pd}_{77}\text{Cu}_6\text{Si}_{17}$		Pd(1.2~1.37)	Cu (1.13~1.28)	Si (.976~1.1)			
	Pd(1.37)	0	1	1	2	big	medium
	Cu(1.28)	0	0	1	1	big	medium
	Si(1.11)	-1	-1	0	-2	small	small

Table.1 suggests that the proposed classification (**this work**) differs with that of the contemporary method [13], as the former is based on relative atomic sizes present in a BMG. Further, a python language program was developed in this work, which is based on the proposed classification (code enclosed as a supplementary document). This program takes the

elements and concentration as inputs and result in the classified elements in any multi-component BMG alloy, as shown in Fig.2. The outputs i.e., big/ small atom classification obtained from this program can be used to calculate Δe and Δd , which further influence assessment of the glass forming ability of the alloy studied.

```

Enter the BMG : Cu47Ti33Zr11Si1Ni6Sn2
Elements in BMG are : ['Cu' 'Ti' 'Zr' 'Si' 'Ni' 'Sn']

Scoring Matrix :
   Cu Ti Zr Si Ni Sn
Cu  0  1  1 -1  1  1
Ti  0  0  1 -1  1  1
Zr -1 -1  0 -1 -1  0
Si  1  1  1  0  1  1
Ni -1  0  1 -1  0  1
Sn -1 -1  1 -1 -1  0

Big Atoms : ['Zr', 'Ni', 'Sn']
Small Atoms : ['Cu', 'Ti', 'Si']

Enter the BMG : Mg65Cu7.5Ni7.5Ag5Zn5Gd7.5Y2.5
Elements in BMG are : ['Mg' 'Cu' 'Ni' 'Ag' 'Zn' 'Gd' 'Y']

Scoring Matrix :
   Mg Cu Ni Ag Zn Gd Y
Mg  0 -1  0  0 -1  1  1
Cu  1  0  1  1  0  1  1
Ni  1 -1  0  1 -1  1  1
Ag  1 -1  0  0 -1  1  1
Zn  1  1  1  1  0  1  1
Gd  0 -1  0  0 -1  0  1
Y  -1 -1 -1 -1 -1 -1  0

Big Atoms : ['Mg', 'Ni', 'Ag', 'Gd', 'Y']
Small Atoms : ['Cu', 'Zn']

Enter the BMG : Fe68.3C6.9Si2.5B6.7P8.8Cr2.2Mo2.5Al2.1
Elements in BMG are : ['Fe' 'C' 'Si' 'B' 'P' 'Cr' 'Mo' 'Al']

Scoring Matrix :
   Fe C Si B P Cr Mo Al
Fe  0 -1  0 -1  1  1  1  1
C   1  0  1  1  1  1  1  1
Si  1 -1  0 -1  1  1  1  1
B   1 -1  1  0  1  1  1  1
P  -1 -1 -1 -1  0 -1  0 -1
Cr  0 -1 -1 -1  1  0  1  1
Mo -1 -1 -1 -1  1 -1  0 -1
Al  0 -1 -1 -1  1  0  1  0

Big Atoms : ['Fe', 'P', 'Cr', 'Mo', 'Al']
Small Atoms : ['C', 'Si', 'B']

Enter the BMG : Cu 57.5 Zr 37.5 Ga5
Elements in BMG are : ['Cu' 'Zr' 'Ga']

Scoring Matrix :
   Cu Zr Ga
Cu  0  1  1
Zr -1  0 -1
Ga -1  1  0

Big Atoms : ['Zr']
Small Atoms : ['Cu', 'Ga']

```

Fig.3 Screenshots of the python program which classify the atoms based on the radius range classification in multi-component BMG alloys

Multi-Collinearity Check

An important aspect which has to be considered during modelling is to check the multicollinearity between the input parameters chosen. A high multicollinearity would result in interdependency between the input parameters and this violates the assumption that all parameters are independent of each other. The collinearity was assessed by using the following equation, Eq. (5). Where 'r' represents the collinearity factor between the where parameters 'x' and 'y' can be any two of the input parameters ΔH_{mix} , ΔS_{mix} , Δe , Δd .

$$r = \frac{n(\sum(xy)) - (\sum x)(\sum y)}{\sqrt{[n \sum x^2 - (\sum x)^2][n \sum y^2 - (\sum y)^2]}} \quad (5)$$

Figure. 4 represents the collinearity matrix constructed between ΔH_{mix} , ΔS_{mix} , Δe , Δd . It can be seen that the multicollinearity between any of the two parameters is not high, i.e. $r < 0.7$. This means there is no significant interdependency between any two parameters among ΔH_{mix} , ΔS_{mix} , Δe , Δd ; and therefore none of them was excluded in the prediction of D_{max} .

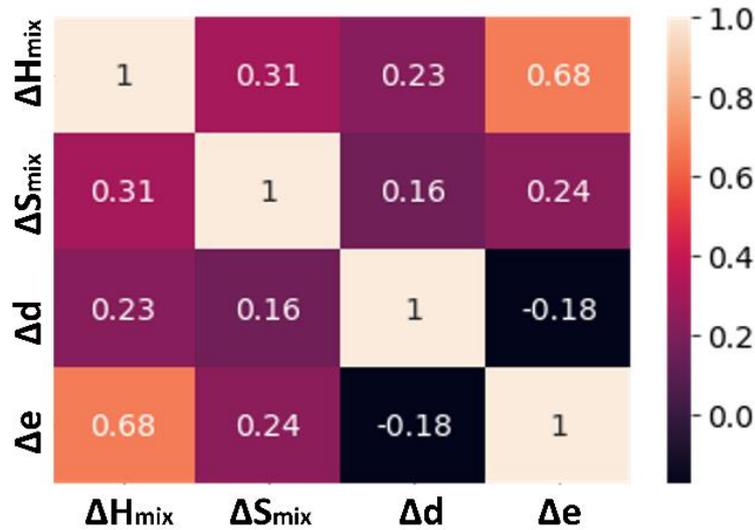


Fig 4 Collinearity matrix of input parameters

Modelling

The next step is creating machine learning models to predict the D_{max} of the BMGs. We evaluated the performance by R-squared score and MSE (mean squared error) over several models like ANN, Random Forest Regressor, Support Vector Regressor, Decision Tree Regressor, Linear Regression. Out of them the ANN (Artificial Neural Network) was selected and Random Forest Regressor models as they gave better and reasonable R-squared score and MSE. The description of ANN and Random Forest Regressor models developed is shown below.

Random Forest Regression method

Random Forest Regressor is an ensemble learning algorithm that trains a number of decision trees. Each decision tree is trained over several different random sub samples of dataset and uses mean or averaging to improve the predicting accuracy and also increases the robustness against over-fitting. The optimization of MSE and reducing over-fitting is performed by

Hyper-Parameter tuning. We used a python package Hypopt for the purpose of Hyper parameter training, which performs grid search hyper-parameter optimization using validation set, the major advantage is it uses all threads available on CPU for fast results. The model is trained over 7938 parameter configuration fits, the optimal configuration is as below:

```
{'bootstrap': True,
  'criterion': 'mse',
  'max_depth': 11,
  'max_features': 'sqrt',
  'max_leaf_nodes': None,
  'max_samples': None,
  'min_impurity_decrease': 0.0,
  'min_impurity_split': None,
  'min_samples_leaf': 1,
  'min_samples_split': 2,
  'min_weight_fraction_leaf': 0.0,
  'n_estimators': 16
}
```

The `n_estimators` is set to 10 and increased at a step of 2 till 50 and `max_depth` is set to 5 and increased at step of 1 till 25. The hyper-parameters `n_estimators` and `max_depth` ranges are set between 10-50 and 5-25 , which are low, to reduce the problem of overfitting.

The R-squared score is found to 0.868 over training set, 0.71 over testing set and MSE is found to be 5.12 over test set using optimized Random Forest Regressor model. Random Forest Regressor gave better results than classical machine learning models comparatively.

Artificial Neural Network method

An Artificial Neural Network developed in this work contains 8 layers of which 5 are dense hidden layers and 2 drop out layers are used to control the over-fitting and the other one is an output layer.

$$\text{Sigmoidal function, } f(x) = \frac{1}{1+e^{-x}} \quad (6)$$

$$\text{ReLu function, } R(x) = \max(0, x) \quad (7)$$

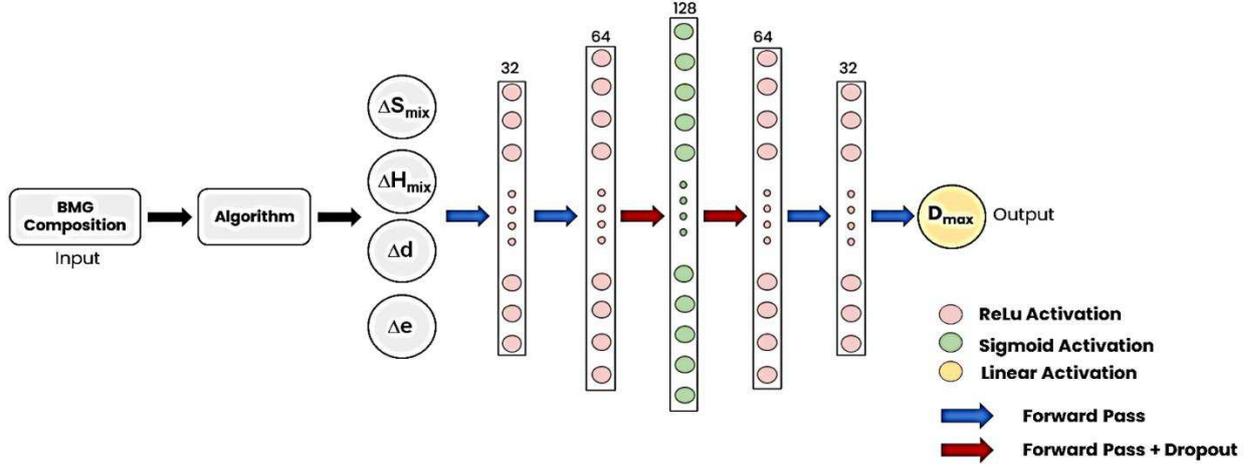


Fig.5. Architecture of the ANN model used for prediction of D_{\max}

The ANN used in this work is a dense layer neural network with five hidden Dense layers. The first, second, fourth, sixth and seventh hidden layers consist of 32, 64, 128, 64 and 32 nodes, respectively, from left to right in the Fig.4. Two dropout layers with drop probability of 0.2 are used in the model to control the model from overfitting. The output layer, provided with linear regression activation function consists of a single output node which gives out the value of predicted D_{\max} , which is continuous. The activation function used in the fourth dense layer is sigmoid, while Rectified Linear Unit (ReLu) was used as activation function for other layers of the model. The model was compiled with Adam optimizer with a learning rate of 0.01 and the loss function used was mean squared error. The model was trained for 2000 epochs.

Table.2 Details of the deep-learning model architecture

Layer (type)	Output Shape	Param #
dense_0 (Dense)	(None, 32)	160
dense_1 (Dense)	(None, 64)	2112
dropout_0 (Dropout 0.2)	(None, 64)	0

dense_2 (Dense)	(None, 128)	8320
dropout_1 (Dropout 0.2)	(None, 128)	0
dense_3 (Dense)	(None, 64)	8256
dense_4 (Dense)	(None, 32)	2080
dense_5 (Dense)	(None, 1)	33
Total params: 20,961 ; Trainable params: 20,961 ; Non-trainable params: 0		

RESULTS AND DISCUSSION

Independent influence of each of the parameters on the accuracy of the model was investigated. In this process, one of the parameters was excluded from the model at a time and the model was reconstructed with the remaining parameters. The drop in the performance of each such model was considered to calculate the feature influence on the model. Figure.6 represents the % importance of each of the parameters in decreasing order, obtained from such a method. In this approach, it has been observed that ΔS_{mix} is more vital in determining the accuracy of the model, followed by ΔH_{mix} and others. This observation is well in agreement with the thermodynamics of BMGs reported in the literature.

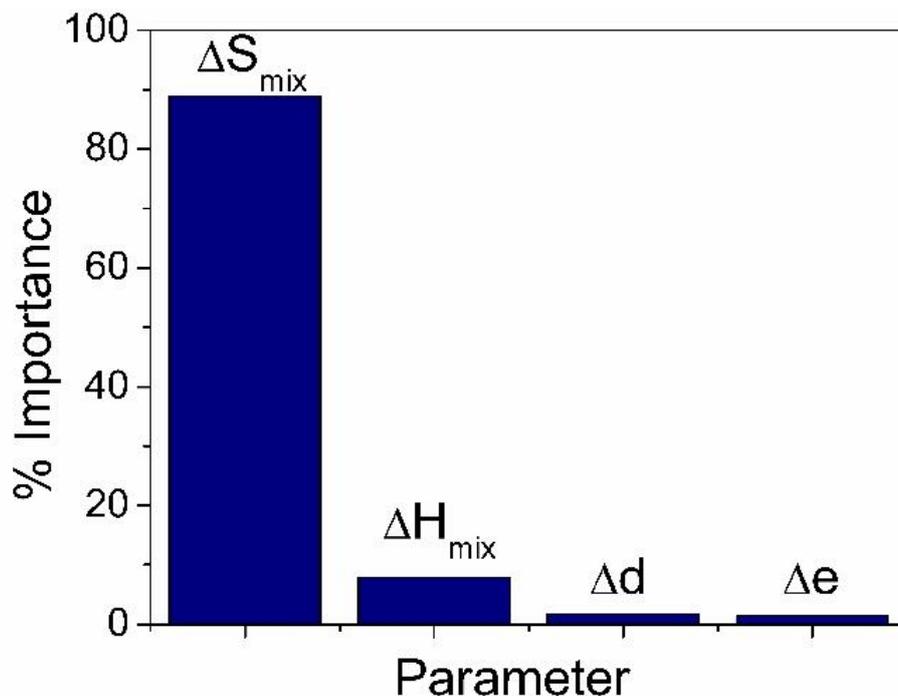


Fig. 6. Importance of individual parameter on the efficiency of the model

Figure 7(a-b) demonstrate the comparison between the performance of ANN and Random Forest models developed in this work. The Optimized Random Forest Regressor model developed in the present work, showed an R-squared score of 0.71 on the prediction of D_{\max} on the validation dataset with a mean squared error of 5.12. As it is evident from the Fig.7a and Fig. 7b, the ANN model resulted in a R-squared score of 0.87 and a mean squared error of 2.32 on the *testing dataset*. While the same has shown a R-squared score of 0.91 and a mean squared error of 1.02 on the training dataset. Hence it is clear that the ANN model is more accurate than the Random Forest Regressor model in predicting the D_{\max} .

The predicted D_{\max} values obtained from both the models developed in this work have been compared with the actual experimental values of D_{\max} , shown in Fig. 8. From the figure, predicted D_{\max} values of ANN model do not deviate much from the experimental D_{\max} of the respective BMG alloys. Hence, it can be inferred that the present work is capable of predicting the GFA of BMGs.

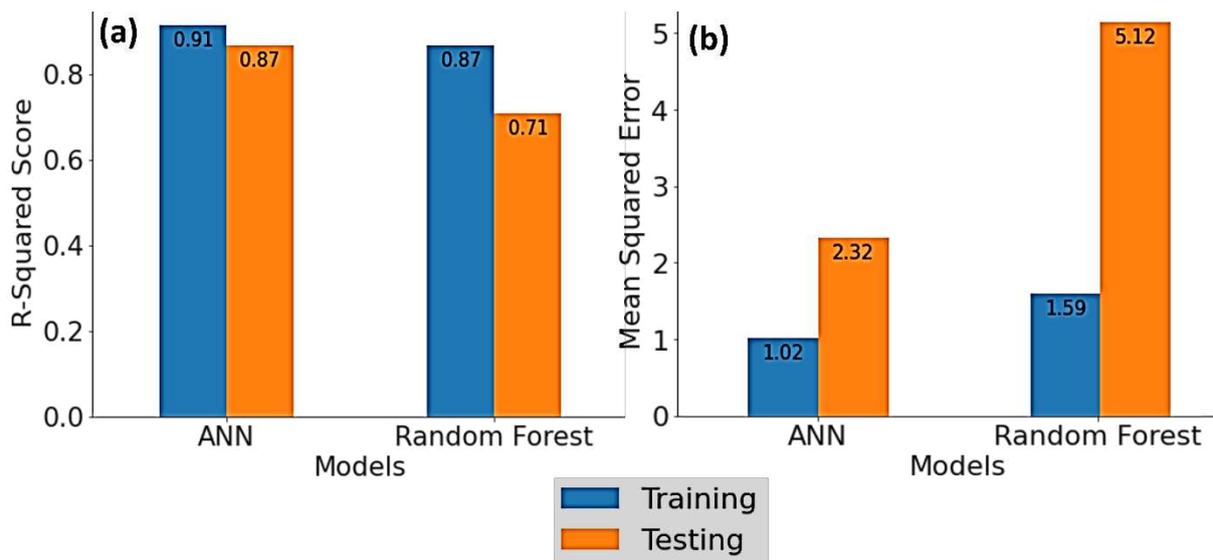


Fig 7. Comparison of (a) R-squared score (b) Mean squared error in ANN and Random forest regressor model

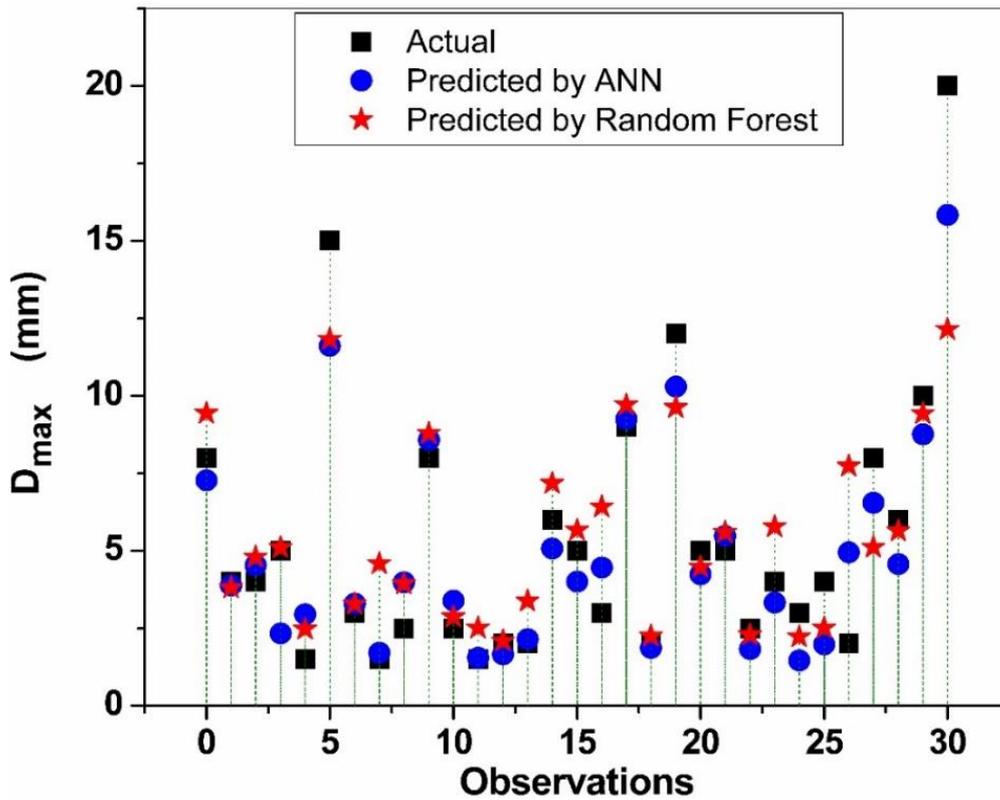


Fig. 8 A comparison of the predictions with actual D_{\max} values

Although, Ward et. al. [11] demonstrated machine learning model with R-squared score of 0.89 on testing set which is slightly higher than that of the current model, no systematic analysis of feature importance or multicollinearity was reported. Another work by Majid et. al.'s [12] cannot be applied without conducting experiments, as the characteristic temperatures (glass transition temperature, undercooling range etc.), the inputs for such a model are to be measured for a synthesized a BMG, hence cannot be used for designing virtual BMGs. In contrast, the model demonstrated in this work successfully predicts the GFA, i.e., the D_{\max} for virtual alloys, just by considering their chemical composition as input, with an accuracy above 85%.

Further, earlier studies neither analysed multicollinearity nor conducted feature importance, which are crucial to identify the parameters which are highly influential on the GFA or D_{\max} of a BMG. Present model was successfully tested on various BMG alloys which were not

used for training. Present work has shown promising results irrespective of the alloy's chemistry, i.e, whether it is Pd-based, Fe-based, Mg-based, Cu-based or Zr-based.

CONCLUSIONS

The radius range classification demonstrated in this work based on the relative sizes of the constituent elements in a BMG alloy, successfully overcomes the ambiguity in the contemporary theories. The algorithm helps in the classification, which is independent of the alloy systems.

Multi-collinearity study revealed that there is no significant interdependency between any two parameters among ΔH_{mix} , ΔS_{mix} , Δe , Δd ; and therefore, none of them was excluded in the prediction of D_{max} .

Feature importance analysis confirmed that the accuracy of the prediction models depends mainly on ΔH_{mix} and ΔS_{mix} . However, among the ANN and random forest models developed, ANN, a deep-learning model shows a promising accuracy in prediction of the D_{max} than the random-forest, a machine-learning model as evident from the validation with the experimental values.

It has been successfully demonstrated that the glass forming ability of a BMG can be predicted using machine-learning, given the elemental composition alone. Hence can be used for developing virtual BMGs.

DATA AVAILABILITY

The processed data required to reproduce these findings are available to download from [<https://github.com/jaideep99/Atom-Classification>].

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Figures

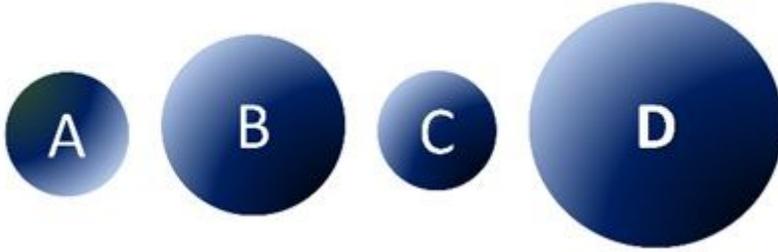


Figure 1

Schematic diagram showing atoms A, B, C and D with different radii

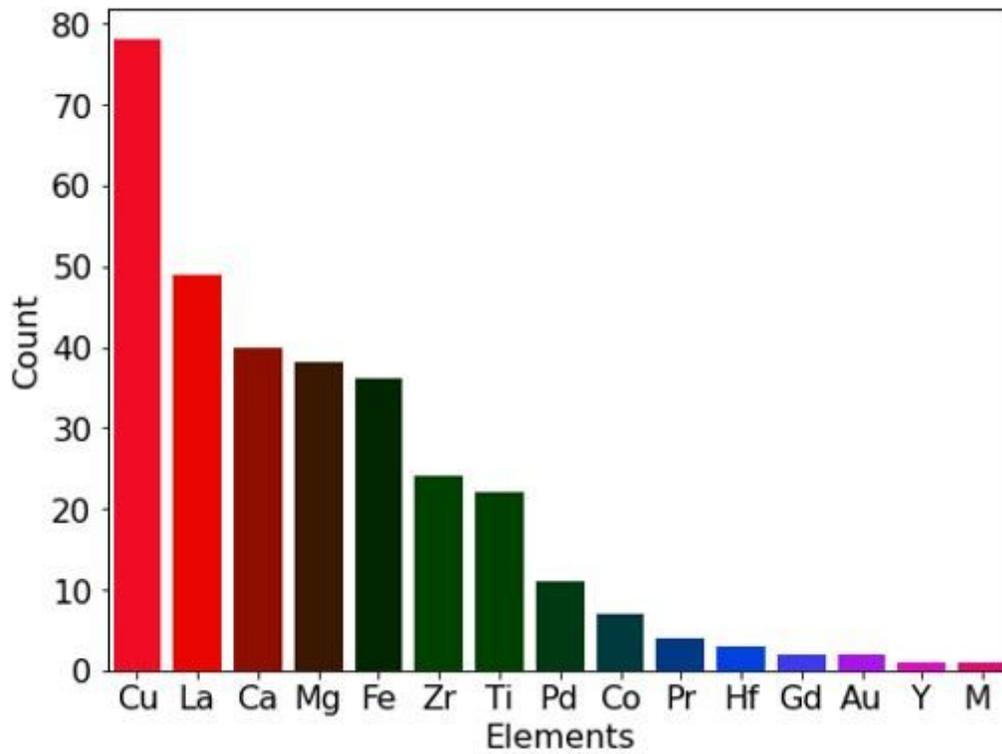


Figure 2

Count of BMGs based on Major constituent element

```

Enter the BMG : Cu47Ti33Zr11Si1Ni6Sn2
Elements in BMG are : ['Cu' 'Ti' 'Zr' 'Si' 'Ni' 'Sn']

Scoring Matrix :
   Cu Ti Zr Si Ni Sn
Cu  0  1  1 -1  1  1
Ti  0  0  1 -1  1  1
Zr -1 -1  0 -1 -1  0
Si  1  1  1  0  1  1
Ni -1  0  1 -1  0  1
Sn -1 -1  1 -1 -1  0

Big Atoms : ['Zr', 'Ni', 'Sn']
Small Atoms : ['Cu', 'Ti', 'Si']

```

```

Enter the BMG : Mg65Cu7.5Ni7.5Ag5Zn5Gd7.5Y2.5
Elements in BMG are : ['Mg' 'Cu' 'Ni' 'Ag' 'Zn' 'Gd' 'Y']

Scoring Matrix :
   Mg Cu Ni Ag Zn Gd Y
Mg  0 -1  0  0 -1  1  1
Cu  1  0  1  1  0  1  1
Ni  1 -1  0  1 -1  1  1
Ag  1 -1  0  0 -1  1  1
Zn  1  1  1  1  0  1  1
Gd  0 -1  0  0 -1  0  1
Y  -1 -1 -1 -1 -1 -1  0

Big Atoms : ['Mg', 'Ni', 'Ag', 'Gd', 'Y']
Small Atoms : ['Cu', 'Zn']

```

```

Enter the BMG : Fe68.3C6.9Si2.5B6.7P8.8Cr2.2Mo2.5Al2.1
Elements in BMG are : ['Fe' 'C' 'Si' 'B' 'P' 'Cr' 'Mo' 'Al']

Scoring Matrix :
   Fe C Si B P Cr Mo Al
Fe  0 -1  0 -1  1  1  1  1
C   1  0  1  1  1  1  1  1
Si  1 -1  0 -1  1  1  1  1
B   1 -1  1  0  1  1  1  1
P  -1 -1 -1 -1  0 -1  0 -1
Cr  0 -1 -1 -1  1  0  1  1
Mo -1 -1 -1 -1  1 -1  0 -1
Al  0 -1 -1 -1  1  0  1  0

Big Atoms : ['Fe', 'P', 'Cr', 'Mo', 'Al']
Small Atoms : ['C', 'Si', 'B']

```

```

Enter the BMG : Cu 57.5 Zr 37.5 Ga5
Elements in BMG are : ['Cu' 'Zr' 'Ga']

Scoring Matrix :
   Cu Zr Ga
Cu  0  1  1
Zr -1  0 -1
Ga -1  1  0

Big Atoms : ['Zr']
Small Atoms : ['Cu', 'Ga']

```

Figure 3

Screenshots of the python program which classify the atoms based on the radius range classification in multi-component BMG alloys

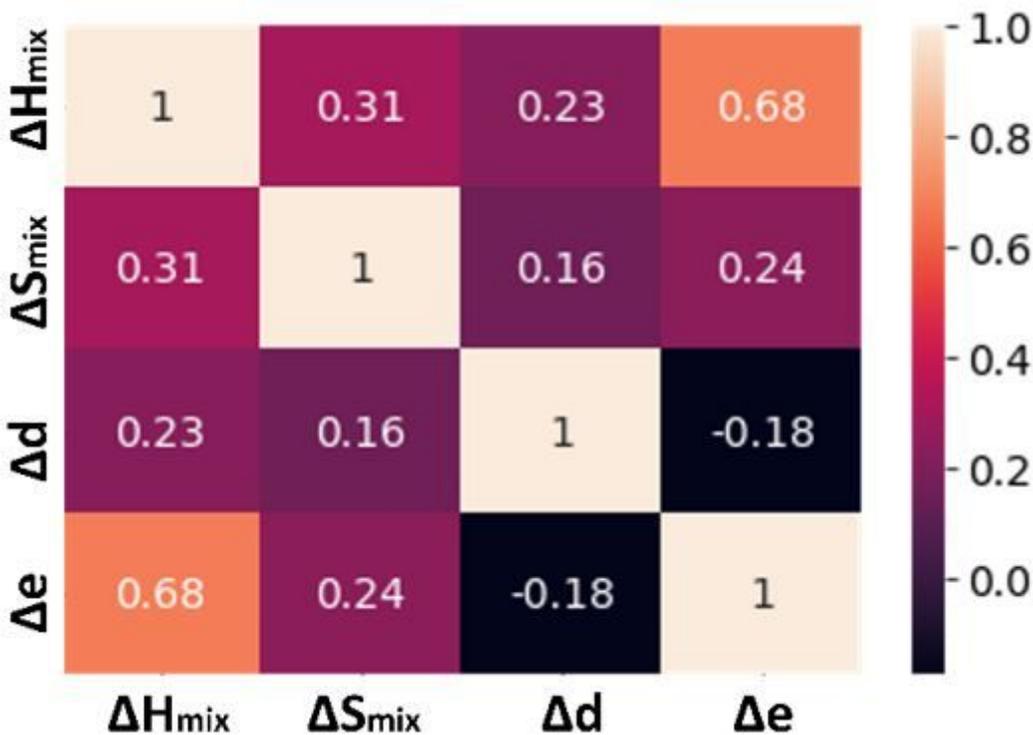


Figure 4

Collinearity matrix of input parameters

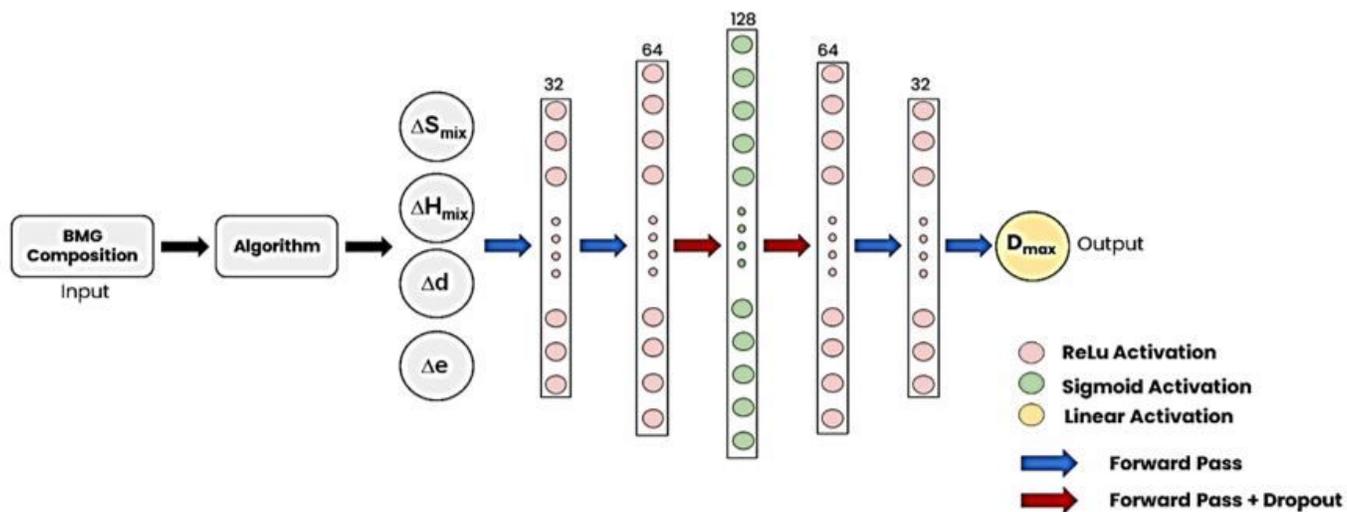


Figure 5

Architecture of the ANN model used for prediction of D_{max}

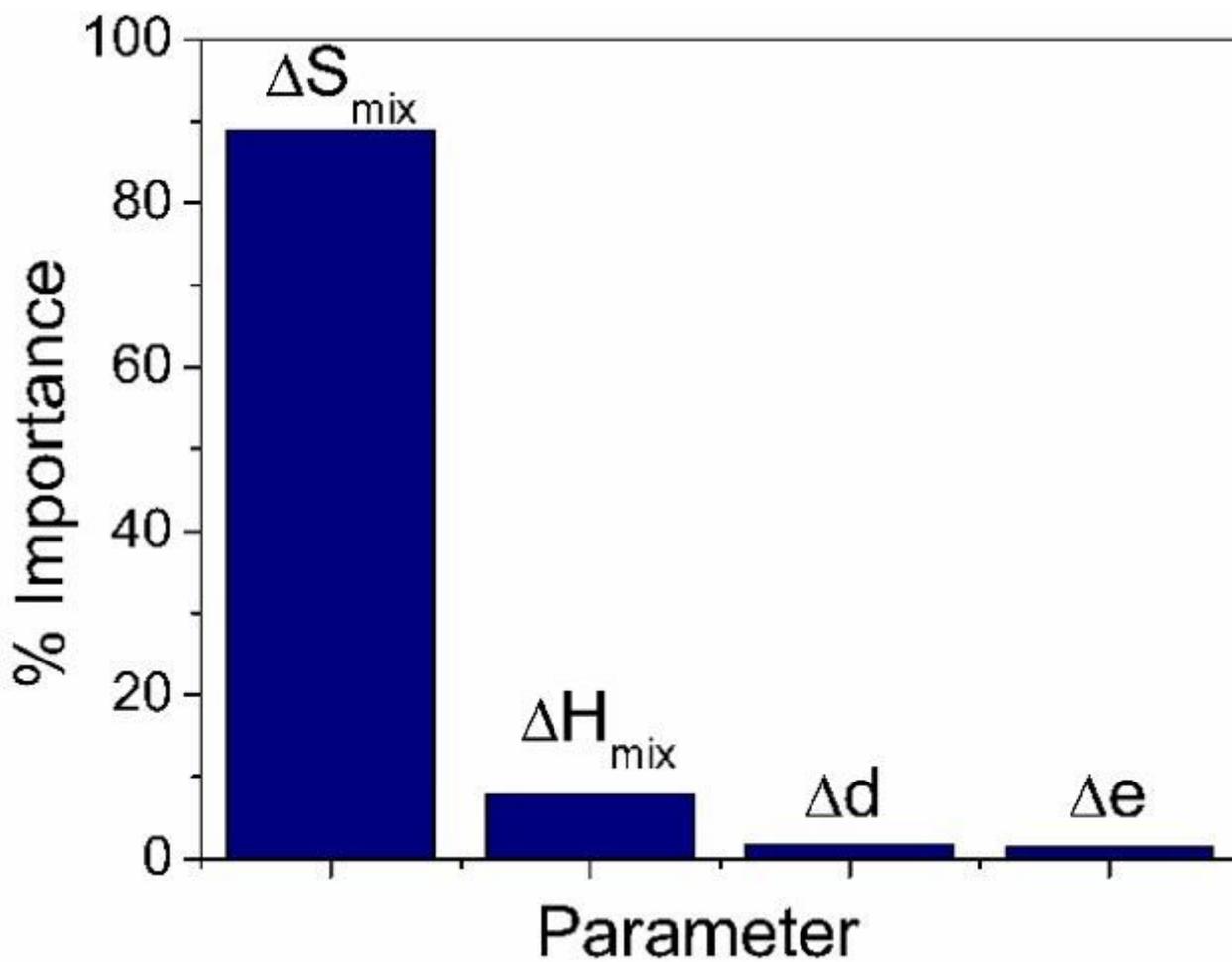


Figure 6

Importance of individual parameter on the efficiency of the model

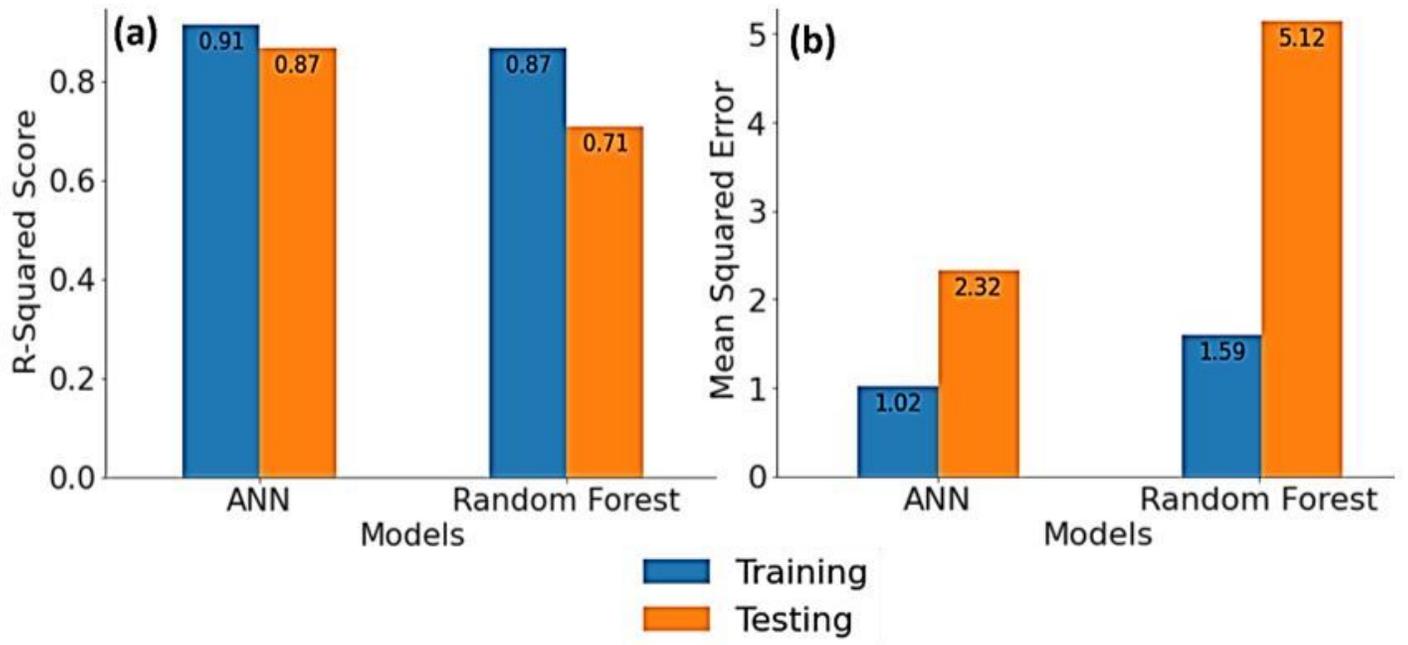


Figure 7

Comparison of (a) R-squared score (b) Mean squared error in ANN and Random forest regressor model

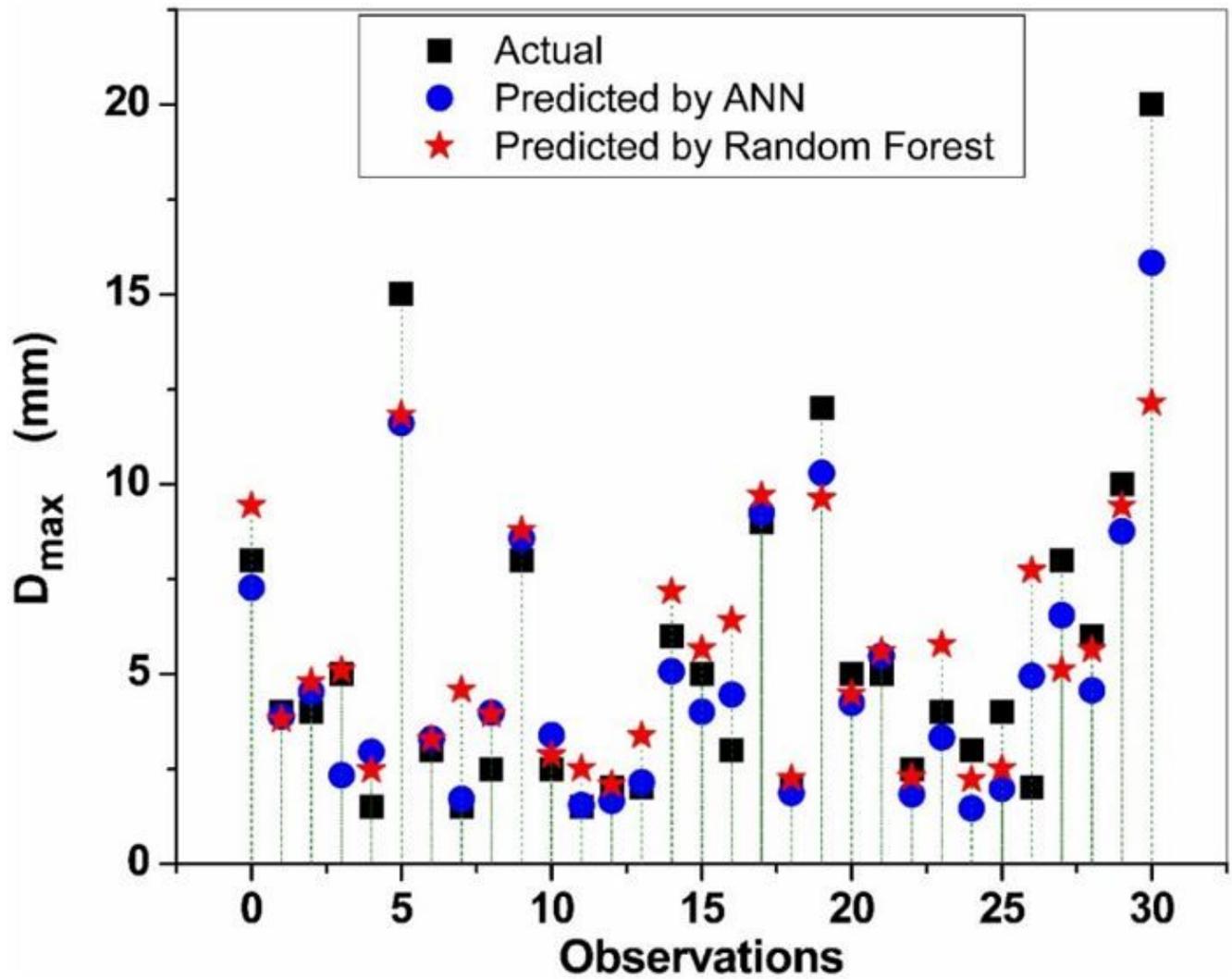


Figure 8

A comparison of the predictions with actual Dmax values

Supplementary Files

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- [SupplementaryMaterial.docx](#)