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Machine Learning for degraded Mechanical Properties of Metallic Materials due to the presence of hydrogen.

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ABSTRACT

Machine learning models were introduced to develop a relationship between the elemental composition and degraded mechanical properties in metallic materials due to the presence of hydrogen. Single layer and multilayer feed forward back propagation algorithm was developed as artificial neural network based machine learning models to predict the mechanical properties of hydrogen charged metallic materials. Multilayer feed forward back propagation model was used to predicts the tensile strength, had a network topology of 12-13-3-2. And the single layer feed forward back propagation model was employed to predict the percentage of elongation, has a network topology of 12-11-1. The developed models were validated and tested with unknown inputs and their capability was studied. The models were evaluated using Mean Absolute (MAE) value and represented the scatter diagram to demonstrate the efficiency of the models. The R-value for both the models seems to prove that the models are ready to be used in the practical applications.

Keywords: Machine learning models; Hydrogen; metallic materials; Mechanical properties;

INTRODUCTION

The presence of hydrogen in the metallic material may affects the mechanical properties due to the loss of ductility and leads to delayed failure mechanism called hydrogen embrittlement. Hydrogen may enter in to the metallic materials during manufacturing process or in service condition and degrade the mechanical properties that may leads to catastrophic failure. The rate of degradation of mechanical properties also depends on the elemental composition in metallic materials. So it is important to understand and predict the hydrogen induced degraded mechanical properties of metallic material to avoid catastrophic failures. The present contribution is to employ Machine learning to map the relationship between the elemental compositions and degraded mechanical properties of metallic materials due to the presence of hydrogen. Aluminum alloys, well known for their properties and low density are widely utilized material in aerospace, automobile and military applications. Material used in astronautically applications will be exposed to many environmental conditions such as extreme temperature and pressure variations at the same time as highly reactive and corrosive atmospheres and fluids [1]. Aluminum alloys due to its lightweight, high corrosion resistance and its ability to not absorb hydrogen in normal conditions has made it a suitable material for high-pressure gas canister to store hydrogen storing [2]. Many studies have proved that the aluminum is susceptible to environmentally assisted cracking when exposed to the gaseous environment [3]. Researchers also have reported the concern of environmental degradation of aluminum alloys when exposed to the diffusion of hydrogen. Song et al., described the mechanism of material hydrogen embrittlement in water containing environment as the effect of hydrogen atoms formed which gets absorbed in the crack initiated surface leading to reaction of hydrogen with fracture surface leading to hydrogen embrittlement [4]. Material embrittlement because of hydrogen diffusion has found to be a major issue in industrial applications and has lead to many main failures that thereby attracted the attention of researchers leading to enormous researches [5-7]. Factors such as microstructural interaction between hydrogen atom and materials, microstructural engineering and morphological behavior play a major role in controlling the vulnerability of hydrogen embrittlement in materials [8]. Aluminum alloys, being a candidate material for aerospace applications, and their interaction with this hydrogen must be studied in a detailed manner.

Even though aluminum alloys were believed to be immune to hydrogen embrittlement, studies have proved that the environmentally assisted cracking that takes place in high strength aluminum may be a phenomenon of hydrogen embrittlement [9]. However, studies have also proved that the cathodic charging of hydrogen into aluminum material has enhanced the mechanical properties that include both the hardness and tensile properties to the maximum [10]. A large number of studies have been carried out on the enhancement of the mechanical properties of aluminum alloys by hydrogen charging but a model that predicts the properties based on chemical composition and process parameters has not been developed until now.

Along with aluminum, the effect of hydrogen diffusion into the material and its after effects in bulk properties of the parent metal is studied in a great extent on other metals too these days. Zhu et al studied the effect of retained austenite on hydrogen embrittlement susceptibility in high strength steel under varying heat-treated conditions. Results stated that steel, which underwent quenching and tempering, offered the highest strength, hydrogen diffusion rate and hydrogen embrittlement immunity, when compared with the other heat-treated specimens [11]. Zhu et al proved that providing a nickel- graphene composite coating over the surface of quenching and partitioning steel could protect the substrate from hydrogen embrittlement to an extent. The mechanism behind this was attributed to the hydrogen storing capacity of graphene which reduced the hydrogen permeation into the substrate steel [12]. Yamabe studied the characteristics of two aluminium based coating as hydrogen diffusion barriers under highpressure conditions. A two-layer (alumina/Fe-Al) and three-layer (alumina/aluminum/Fe-Al) coatings was provided onto the surface of austenitic stainless steel of type 304 and was exposed to hydrogen at high-pressure conditions. Results proved that the combined effect of alumina, aluminum, and Fe-Al layers in three-layer coating exhibited excellent hydrogen entry resistance [13]. Brandolt et al provided Niobium coating over the surface of steel substrate and the evaluation of mechanical properties after hydrogen charging states that Niobium acts as a barrier for hydrogen diffusion thereby minimizing the effect of hydrogen in mechanical properties [14]. Dieudonne et al studied the role of copper and aluminum content in Twinning Induced Plasticity steel on hydrogen embrittlement susceptibility and concluded that steel with high copper and aluminum content increases the hydrogen embrittlement resistance [15].Beryllium - copper alloy was hydrogen charged by Ogawa et al and the hydrogen diffusivity, solubility and mechanical properties was evaluated. Results exposed high strength and low high embrittlement along with high thermal conductivity proposing the material to be a suitable material for heat exchangers [16].

Even though numerous works has been carried over in hydrogen embrittlement related to various metal, study over aluminum is minimal. Alexopoulos investigated the interaction of hydrogen embrittlement on structural integrity of aluminum 2024 alloy and it was concluded that 27% of the ductility decrease occurred is attributed for hydrogen embrittlement while the rest for micro crack mechanism [17]. Barnoush and Vehoff investigated the effect of hydrogen on the mechanical properties of aluminum with the aid of classical dislocation theory. The mechanisms was studied and stated that the mechanical properties of the material was influenced by hydrogen to an extent [18]. Qi et al proposed that hydrogen charging reduced the mechanical properties of aluminum 7075 alloy while susceptibility of hydrogen in Al-Cr alloys and the mechanisms behind the trapping of hydrogen element by aluminum oxide at highest temperatures were explained [20].

Artificial neural networks (ANN) mimics the functioning of human brain and are influencing the research field nowadays due to their significant ability to learn from the available data and predict results from new unknown inputs. A mathematical or computational model capable of imitating the formation and biological functioning of a human nervous system can be defined as an ANN. Neuron being the basic function of a human nervous system, an ANN has a similar computational system called nodes. Nodes are interconnected to each other in layers forming an interconnected network to provide an output. This interconnected network acts as a non-linear statistical modeling tool capable of studying and imitating according to the patterns provided to it in form of inputs and target data. The ability of the same computational method to study from the available experiments and provide an output from an unknown input makes it an efficient and commonly used methodology in the field of materials engineering [21]. Comparing with its ancestral technique, the regression method; ANN performs much better based on both

accuracy and precision and at the same time its ability to be trained from the available factors which impact the output avoiding the factors that are not available or can't be obtained.

This has greatly influenced materials engineering both in industry and research allowing them to develop new alloys as well as study the processing parameters that produce the required material properties for specific applications. Haghdadi et al developed an artificial neural network model with single hidden layer comprising of 20 hidden nodes to predict the high temperature flow behaviour of A356 aluminum alloy based on the temperature, strain and strain rate. Results proposed ANN as a statistically efficient and robust tool for property design [22]. Han et al developed a back propagation ANN model to predict the high temperature flow stress of 904L austenitic stainless steel in as cast condition. Model developed considered strain, strain rate and temperature as the input data; the developed model was found to be precise and reliable in predicting the output based on the above said input characteristics [23]. Krajewski and Nowacki developed an ANN model based on the experimentally validated data of dual steel to correlate the alloying element, transition temperature and microstructural features along with its tensile strength. The same model was reliable enough to investigate the effect of these inputs on the tensile and yield strength of dual phase steel [24]. Palavar et al studied the wear behavior of Inconel 706 prepared through powder metallurgy with the aid of ANN models. Computational models for weight loss predictions were prepared with aging time, load and sliding distance as inputs. Developed model expressed higher reliability and predictability [25]. ANN have been used by researchers and found to be effective for studying the varying properties of different aluminum alloys in a range of applications [26-28].

Even though many studies on the effective use of ANN in different processes, including wear resistance, machining, dendrite spacing, aging processes etc., are carried out for aluminum alloys, their application in the field of hydrogen charging is minimal. In this research, the effective utilization of ANN in modeling the tensile properties of aluminum alloys of varying chemical composition after hydrogen charging with differing processing parameters is carried out.

MATERIALS AND METHODOLOGY

Experimental methods:

In this research, tensile properties of the various aluminum alloy before and after the hydrogen charging for varying temperature, strain rate and current density were collected from journals [1,10, 29-33]. From the journals the percentage weights of the major alloying elements were recorded which included aluminum (Al), copper (Cu), magnesium (Mg), manganese (Mn), iron (Fe), lithium (Li), zirconium (Zr) and zinc (Zn). Elements like silicon were not considered as in most of the alloys considered in this study the composition remained more or less constant. The process parameters such as temperature, time, strain rate and current density for the charging process at varying levels were considered as the inputs along with the chemical compositions for training the artificial neural network model. The tensile properties of the aluminum alloys before

and after charging were considered as the target outputs to the ANN model which constitutes UTS, YS and percentage elongation.

Artificial Neural Network Modelling:

ANN, is considered by researchers as one of the most robust predictive methods among the different computational methods available. A human neuron mainly consists of dendrites which accept the signals from the other neurons, a cell body which performs the biological summation and the axons which provide the signals to the next neuron. An artificial neuron or node, the basic element in ANN, has three governing components which are weight, bias and activation functions. The node receives the signals from an input which is multiplied and summed up in the node. A connection weight, a non- zero value called bias will be added up with the input summations. An activation function or transfer function is responsible for the conversion based on the signal received. The working of an ANN node can be explained from Figure 1 which was studied and developed by McCulloch in 1940's. In this figure 'w' denotes the connection weights, 'b', bias and 'a', inputs of the node.





The ANN model consists of an input layer which accepts the input signals as independent variables. The total number of input nodes in the input layer will be same to the number of inputs considered in modeling artificial neural network. The input nodes send the values of the independent variables to the hidden layer. Selection of hidden layers plays a major role in the design of network topology as the hidden layers and nodes decide the efficiency of the model to a great extent. The over fitting and under fitting of the model is controlled mainly by the topology of nodes and layers. Even though these two factors play a major role in modelling a neural network, there is not a specified methodology in selecting the optimal number of nodes and layers. Two proposed aids for selecting the same is provided in equation 1 and 2.

N2 = (No of outputs +1) or (No of outputs +2) for a model with fewer outputs where N1 has to be found out by trial-and-error method and N1 and N2 indicates the number of nodes in first and second hidden layer respectively [35]. (1)

Number of hidden nodes = [0.5(no of inputs + no of outputs) + sqrt (No of training patterns)] which was put forward by neuroshell [36,37]. (2)

The output layer obtains its input from the hidden layers in a processed form. The outputs in the training section works as the target signals in the supervised form of neural network modeling.

In this research, the input comprises of 12 nodes of which the chemical composition of the different alloying elements in weight percentage make up the first eight nodes and processing parameters the rest four. The considered alloying elements in this research includes Aluminum (Al), Copper (Cu), Magnesium (Mg), Manganese (Mn), Iron (Fe), Lithium (Li), Zirconium (Zr) and Zinc (Zn) while, the process parameters considered are temperature (°C), time (Hrs), strain rate (s⁻¹) and current density (mA/cm²). The target data for training the ANN model consists of UTS (MPa) and YS (MPa) with the percent elongation. Approximately 40 readings were collected from various journals to train an ANN model and thereby predict the mechanical strength of hydrogen charged aluminum alloys. From these readings data set were used for training the network model and the rest for validating it. The statistical values of the training data and the target data are provided in Table 1 and 2 respectively.

Variable	Al	Cu	Mg	Mn	Fe	Li	Zr	Zn	Temp	Time	Strain	Current
	wt%	wt%	wt%	wt%	wt%	wt%	wt%	wt%	°С	hr	rate (s^{-1})	Density
Min	90.3	1.3	0.5	0.02	0.012	0	0	0.2	25	0	10 ⁻³	0
Max	94.31	4.46	2.2	0.8	0.6	2.59	0.13	5.4	150	48	10 ⁻⁶	17.5
Mean	92.91	2.5	1.29	0.24	0.16	1.01	0.05	1.39	88.71	9.91		5.37
Std. Dev	1.54	1.27	0.57	0.31	0.21	1.09	0.057	2.22	51.67	7.85		4.54

 Table 1 Range of input variables for training

Unification of the training data is a major step in ANN modeling were the normalization of the data are carried out. The collected data is undergone normalization process to make the data in the range of 0 to 1 so that the entire input factors have a similar authority over the output values. The equation (3) is utilized in this work for the normalization process.

$$N_{V} = \left[\frac{2 \times (N_{i} - N_{\min})}{(N_{\max} - N_{\min})}\right]$$
(3)

Where N_v stands for the normalized value, N_i denotes the value to be normalized, and N_{max} and N_{min} are the maximum and minimum values within the training set.

The training of a neural network model in a supervised condition is the process of changing the connection weights accordingly for the given inputs based on the target values such

that an exceptional value is obtained by the connection weights which allows the network to generate outputs close enough to the target outputs.

Variables	Minimum	Maximum	Mean	Standard Deviation
UTS (MPa)	338	596	441.37	79.5
YS (MPa)	289	571	383.94	81.89
Percent Elongation	1.7	23.6	13.48	7.44

 Table 2 Range of output variables for training

In this research a back propagation algorithm is engaged for the training purpose of network of feed forward multilayer perceptron. Back propagation training algorithm is used extensively throughout previous research for pattern recognition and forecasting problems with the available or back-up data [36]. The back propagation method is a gradient descent technique which has been found simple and reliable. The training rule which has been employed in this study to optimize the weights and bias was the Levenberg-Marquardt back propagation method effectively known as Trainlm in Matlab considering its reliability and speed. The tan sigmoid activation function was considered for the hidden layers and purelin for the output layer neurons of the model.

Based on the available data from literature, numerous models were tried out to evolve an ANN model that can predict the mechanical properties of aluminum. It was observed from Mean Absolute Value (MAE) and scatter diagrams of the developed models that great fluctuations occurred between the desired and predicted values. Hence to reduce the load on the models and to train with greater efficiency it was decided to develop two models, of which ANN Model I predicts the tensile and yield strength, while ANN Model II yields the value of percent elongation. It has been noted in the detailed literature surveys that optimizing the hidden layers and nodes is essential to achieve the best model and can be done mainly by trial and error. Even though a trial and error method was carried out, as explained above, based on equation 1 and 2 ANN models with varying topology were tested in this study with 25,000 iterations to find out the optimal model capable of predicting the mechanical properties with better precision and accuracy. The performance function Mean Square Error (MSE) value was considered in this to study the generalization of the model. The MSE value between the experimental and predicted value can be obtained employing equation 4.

MSE =
$$\frac{1}{M \times N} \sum_{x=0}^{N} \sum_{y=1}^{N} [E_y(x) - P_y(x)]^2$$
 (4)

Where N is the number of samples, M is the number of training parameter, E is the experimental output and P is the predicted output by the network. Out of the 25,000 models developed for each ANN network topology, the one with the lowest MSE value was considered to be the best model. These models of various topologies were then validated to find the preeminent ANN model that predicts the results with the best efficiency.

Results and Discussion

Evaluating the developed models is one of the most important process to establish their efficiency. It is a known fact from the journals that the performance of an ANN model can be evaluated by computing the MAE value and plotting the scatter diagram of the desired and the model's output. MAE value of a model can be calculated using the formulae 5.

Where t=T-T' and p = P-P' in which the T and P are target and predicted output, T' and P' are its mean with n being the number of samples. [25].

The MAE value of the developed models were computed and highlighted in Figure 2 and 3 for model I and II respectively. From figure 2 and 3 it can clearly be viewed for the various network topology of feed forward ANN model trained with back propagation algorithm. The figures show a clear image of the network topologies studied for both Model I which predicts the UTS, YS and Model II which forecasts percent elongation. Network topology for both the models includes single and double hidden layer were the nodes were varied accordingly for single hidden layer models and when considering the double hidden layer models the nodes for the first layer were varied and second layer was kept constant at a value of n+1 and n+2 where n stands for number of outputs. It is a known fact that model with single hidden layer has the capability to train successfully and predict the results as proved by Hornik et al, but in this study to predict the tensile properties of aluminum alloys before and after hydrogen charging a model with double hidden layer proved to be more efficient as seen in Figure 2. Thus, out of the different ANN models developed, a feed forward ANN model trained with back propagation algorithm having a network topology of 12-13-3-1 proved to be more efficient.



Figure 2. MAE for Different Nodes for Model I (UTS&YS)



Figure 3. MAE for Different Nodes for Model II (%Elongation)

Similarly, Figure 3 points out the best model from the models developed with varying nodes in both single and double hidden layer topology. The MAE values of the ANN models to predict the elastic percentage of the aluminum alloys of various grades before and after hydrogen charging are shown in Figure 3. It gives a clear image which obeys the statement of Hornik et al that a model with single hidden layer with optimized hidden nodes is more appropriate to make an efficient ANN model [38]. From the Figure 3, network topology of the ANN model trained with back propagation algorithm is viewed to be 12-11-1.



Figure 4. Schematic diagram of model I (UTS&YS)



Figure 5. Schematic diagram of Model II (%Elongation)

MAE based valuation of the various models has been carried out to establish the best topology based ANN model, and to find out the ability of the model to accurately predict the UTS, YS and percent elongation. Evaluation of the ability of the feed forward back propagation ANN model with network topology 12-13-3-2 to predict the UTS is done through scatter diagram and shown in Figure 6. It can be clearly viewed from the figure that the model has the ability to be trained to predict as per the given inputs. The same model also predicted the YS for the trained data with high correlation as shown in Figure 7. This proved that the developed feed forward back propagation ANN model with 12-13-3-2 network topology can be a good support in judging the UTS and YS after hydrogen charging the aluminum alloys of various grades.

The scatter diagram for the evaluation of model that predicts the UTS and YS (Model I) has been used to confirm its accuracy in prediction. The same process must be carried out for Model II which predicts the percent elongation of the aluminum alloys to evaluate the computing accuracy. The scatter diagram, Figure 8 showcases the accuracy of the 12-11-1 ANN model in predicting the percent elongation of the aluminum alloys after charging. It is clearly visible from the figure that most of the experimental values and the predicted values are very close.



Figure 6. Scatter diagram for UTS



Figure 7. Scatter diagram for YS



Figure 8. Scatter diagram for Percent Elongation

										Strain	Current
Al	Cu	Mg	Mn	Fe	Li	Zr	Zn	Temp	Time	Rate	Density
92.5	4.46	1.44	0.6	0.13	0	0	0.2	150	48	10-3	10
93.6	1.3	1.1	0.09	0.012	2.59	0.13	0.2	25	0	10^{-3}	0
94.31	2.1	1.1	0.05	0.04	1.8	0.1	0.2	150	10	10^{-3}	7
93.4	4.4	0.5	0.8	0.6	0	0	0.2	45	10	10^{-3}	8

Table 3. Inputs for the validation of the developed model

Even though validating the models through scatter diagram is a valid method, to study the efficiency of the model a set of unknown data that has not used for the training process is provided to the developed model. This gives a clear view of the efficiency of the model. The inputs that have been provided to the models are as provided in Table 3.

		1	1	0					
Ultimate '	Tensile Stren	gth	Yield Str	ength		% Elongation			
ANN Mo	del with topo	ANN Model with topology 12- 13-3-2 (Model II)							
Desired	Predicted	Error %	Desired	Predicted	Error %	Desired	Predicted	Error %	
392	383	2.3	362	371	2.49	1.7	1.71	0.59	
350	366	4.6	305	319	4.59	4.55	4.63	1.76	
402	398	1	329	329	0.02	19.5	19.60	0.51	
408	406	0.49	348	350	0.57	7.6	7.65	0.66	

 Table 4. Desired and predicted outputs along with its error%

It can be clearly understood from Table 4 that developed models have the capability to predict the mechanical properties with high accuracy. Table 4 gives a strong comment on the potential of the models developed in this research both for predicting the UTS, YS and the percent elongation of the hydrogen charged aluminum alloys. It can be clearly noted from Table 3 that the inputs delivered to both the Model I and II are of different aluminum alloys. From this it can be stated that the models developed have the capability to predict the tensile properties of various aluminum grades which falls under the probabilistic distribution of the trained data.

The results from the validation proved that the hence developed ANN models can be preferred for further prediction process. The R –value plays a major role in proclaiming the accuracy of an analytical model. R-Value is a statistical term which showcases a linear correlation between the desired value and the predicted value. In this study the R-value of the model developed is calculated for the outputs so as to understand the accuracy of the developed model.



Figure 9. Correlation between the observed and predicted UTS and YS values

The R-value in Figure 9 represents the linear correlation between the experimental and ANN predicted YS and UTS which showcased a value of 0.99. This value denotes that Model I, a feed forward artificial neural network with topology 12-13-3-2 trained with back propagation algorithm can predict the UTS and YS for the given chemical composition and process parameters which lie under the probabilistic distribution of the trained value. Thus it can be stated that the developed model can be able to predict the UTS and YS of the hydrogen charged aluminum alloys which comes under the probabilistic distribution with better accuracy than other traditional methods by extrapolating and interpolating accordingly



Figure 10. Correlation between the observed and predicted % elongation values

The R-value of Model II, an ANN model to predict the percent elongation of aluminum alloys charged with hydrogen was computed. The model with network topology 12-11-1 showcased an R Value of 0.9932 which clearly gives an idea of the high accuracy of the predictions made by this developed model. It can be clearly stated that the feed forward ANN model with network topology 12-11-1 has the capability to predict the percent elongation of the aluminum alloys with high efficiency for the inputs which lies under the probabilistic distribution of the trained data.

Al	Cu	Mg	Mn	Fe	Li	Zr	Zn	Temp	Time	Strain Rate	Current Density
92.5	4.46	1.44	0.6	0.13	0	0	0.2	150	0	10-3	10
92.5 92.5	4.46 4.46	1.44 1.44	0.6 0.6	0.13 0.13	0 0	0 0	0.2 0.2	150 150	7 24	10 ⁻³ 10 ⁻³	10 10

Table 5. Inputs for the testing of the developed model

From the above it has been made clear that the model can be employed to model the tensile properties of aluminum alloys after hydrogen charging. The models, Model I and Model II were made to predict the UTS, YS and percent elongation respectively for 2 series aluminum alloys of grade 2024. The brief input data is provided in Table 5 [1]. The data used for testing the models was different from the data used to train them.

Ultimate Tensile Strength Yield Strength % Elongation ANN Model with topology ANN Model with topology 12-13-3-2 (Model I) 12-13-3-2 (Model II) Error Error Error Desired Predicted Desired Predicted Desired Predicted % % % 430 372 290 287 7.2 7.19 13.5 1.04 0.14 359 359 0 289 290 .04 3.4 3.44 1.18 355 355 0 316 316 0 1.7 1.68 1.18

Table 6. Desired and predicted outputs along with its error%

The models provided the results shown in table 6 which shows a good correlation between the experimentally validated values and ANN predicted values. Even though one of the UTS values showcased a high deviation in the predicted value when considered with the desired value, the other reading produced by the model has a good confidence with desired values. Hence these models can be effectively considered for the study on the mechanical properties of aluminum alloys which undergoes through the hydrogen charging process.

Conclusions

A feed forward back propagation algorithm based ANN model was employed in this research to predict the tensile properties of aluminum alloys of varying grades after hydrogen charging. The chemical compositions of the aluminum alloys along with the processing parameters were considered for training the model as input and the tensile properties which includes UTS, YS and percent elongation as the target outputs. The results are as below:

- i) The developed ANN models were able to create a strong relationship between the input and target parameters.
- ii) ANN models, Model I and Model II were developed to predict the strength (UTS&YS) and percent elongation respectively.
- iii) Model I; an ANN model with double hidden layer yields the least mean absolute error value at the network topology 12-13-3-2 and showcased a high accuracy in predicting the tensile properties for the given inputs
- iv) Model II, developed in this study to predict the percent elongation of the hydrogen charged aluminum alloys, yielded a network topology of 12-11-1 which made accurate predictions.
- v) The scatter diagram for evaluating the computing ability of both the models proved promising
- vi) Values predicted by ANN model and the desired experimental values showcased high correlation to each other.
- vii) Verification and testing of both the model with the unknown input values proved successful and hence the developed models can be used for other research purpose on hydrogen charging of aluminum alloys.

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