ANN PREDICTION MODELS FOR MECHANICAL PROPERTIES OF AZ61 MG ALLOY FABRICATED BY EQUAL CHANNEL ANGULAR PRESSING

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ABSTRACT
Artificial Neural Network (ANN) based prediction models are developed to predict the mechanical properties of AZ61 Mg alloy fabricated by equal channel angular pressing (ECAP). A back-propagation (BP) algorithm is used to train the neural network prediction models. Grain size, yield strength, and tensile strength of the alloy are predicted based on the number of ECAP passes. The ANN predictions are shown to be in excellent agreement with experimental results, and the prediction error is shown to be minimal. The main advantage of using these ANN prediction models is that they can be used to decide the optimal number of ECAP pressings required to achieve the desired mechanical properties. These models can also be extended in the future to predict other properties, and possibly characterize other alloys.

Keywords: *Artificial Neural Networks, Magnesium, Tensile Strength, Yield Strength, Grain Size*

1. INTRODUCTION

Mechanical properties of alloys are significantly influenced by the underlying micro-structure and texture. The development of these properties is well-understood in conventional alloy-forming processes, such as rolling and drawing [1]. The behavior under more modern techniques like equal channel angular processing (ECAP) however, is relatively less-understood. This paper directly addresses this problem, by constructing an artificial neural network (ANN) based model to predict the development of mechanical properties under ECAP.

ECAP can produce ultra-fine-grain-sized bulk materials by introducing extremely large shear strain during deformation processing [2]. Experimental studies have been carried out in the past to characterize the mechanical properties of alloys like AZ61, when subjected to ECAP [3]. While such experimental studies are useful in estimating the general trend of the mechanical properties, a quantitative prediction model would prove very useful in precisely characterizing these properties.

Artificial Neural Networks are computational systems that emulate the behavior of a biological brain to predict/classify data. These techniques are extremely useful in modeling scenarios, where the underlying relationships are relatively unknown [4]. Various learning algorithms like back-propagation (BP) have been developed to automatically train such prediction networks. These networks are typically represented as a graph of processing elements (PEs), interconnected by weighted edges. Inputs to the PEs correspond to the actual dendrites of a biological neuron, while the outputs correspond to axons. The synapses are modeled by the weighted edges connecting the various PEs. The activation of each neuron is dependent on the weighted sum of its inputs, and an ANN specific transfer function. Learning algorithms typically determine the synaptic weights, and interconnection patterns required to accurately model the training data.

Recently, researchers have resorted to ANN based modeling techniques in material science. Corrosion fatigue behavior of DP steel has been predicted using neural networks [5]. Fatigue crack growth in DP steel has also been modeled [6]. Blast furnace hot metal temperatures have also been predicted using ANNs [7]. Neural network based techniques have also been successfully used in modeling, fracture toughness in micro-alloy steels [8], mechanical behavior of powder metallurgy steel [9], dry sliding wear in Fe-2%Ni based PM alloy [10], and the effect of heat treatment on mechanical properties in MIM alloy [11]. These studies suggest that ANNs are very effective in modeling the mechanical properties of materials.

In this paper, artificial neural network based prediction models are developed to predict the mechanical properties of AZ61 Mg alloy fabricated by equal channel angular pressing (ECAP). The experimental measurements observed in [3] are used to train these models, using a back-propagation training algorithm. The results from these models are verified against testing data. The effectiveness of ANNs in modeling the properties of the AZ61 Mg alloy, suggest that this approach can be extended to predicting the properties of other alloys.

The rest of this paper is organized as follows: First, a brief review of the experimental process used in [3] is presented. Following this, the corresponding data-set used in developing the ANN prediction models, is listed. Details of the training algorithm, parameter selection, and model generation are then presented. The actual ANN models are subsequently described, and their prediction accuracies, are analyzed. Finally, the paper concludes with a summary of the results, and possible directions for future work.

2. EXPERIMENTAL PROCESS

The AZ61 alloy is extruded to pieces of length 100mm and diameter 17mm. The equal channel angular pressing is carried on this as-extruded material through a die made of SKD 61 with an internal angle of 90^0 between the vertical and horizontal channels, and a curvature angle of 30^0. Molybdenum disulphide is used as a lubricant. The rod is held at 275^0 for 20min and then pressed through the die preheated to 275^0, with a speed of 4mm/sec. The pressings are made after rotating each sample about the longitudinal axis by 90^0 in the same direction between consecutive passes. While the experimental process provides the context for interpreting the measurements used in this paper, the main contribution of this work is the ANN-based prediction model. An interested reader is referred to [3] for more details on the actual experimental setup.

The experimental measurements as observed in [3] are given in Table I.

TABLE I: Mechanical Properties of the AZ61 Mg Alloy

ECAP Pass no.	Grain size d(μm)	YS (MPa)	UTS (MPa)
0	24.4	215	322
1	15.8	193	302
2	12.5	202	317
3	11.2	208	329
4	10.6	191	317
8	8.4	154	310

In all the subsequent discussions regarding the prediction models, these measurements are assumed to constitute the governing data-set, unless otherwise explicitly stated.

Prior to describing the process used to construct ANN-based models, it is useful to understand the trends presented in this data-set. The grain-size appears to be decreasing with increasing number of ECAP passes, however the actual rate of decrease seems to be exponentially decreasing with the number of passes. The corresponding yield strength presents a more mixed picture by rapidly reducing on the first pass, steadily increasing till 3 passes, and then subsequently decreasing with increasing number of passes. The main challenge of any prediction model would be to absorb this behavior, and generalize this complex relationship between the number of ECAP passes and yield strength (YS). Tensile strength (UTS) appears to follow a very similar trend like yield strength, but the magnitude of changes are seen to be much lower. This correspondence between UTS and YS also needs to be reflected in the corresponding prediction models.

3. ANN PREDICTION MODELS

Experimental measurements presented in the previous section, clearly illustrate that the mechanical properties of AZ61 are dependent on the number of ECAP passes. The entire extrusion process is maintained as a constant, and hence the variations in resulting properties should strictly be functions of the pressings. These characteristic functions are relatively less understood in literature, and hence there is no known set of governing equations. Although the underlying physical relationships are not accurately available, prediction models can guide engineers in optimizing for particular mechanical properties. Artificial Neural Networks (ANNs) have been proven to be very successful in characterizing such unknown functions, where only a set of input/output observations are available.

The ANN prediction models developed in this paper were developed using the FANN Library [12]. This library is freely available as an open-source toolkit for ANN model developers.

A. Model Characteristics

Artificial neural network models can be visualized as graphs G: (V, E), each vertex in this graph is a neuron, with a model-specific transfer function. The interconnections between the neurons and the weights of the edges govern the behavior of the model. The individual neuron (show in Fig. 1) is activated based on the input values, weights on the input links, and the model-specific transfer function.

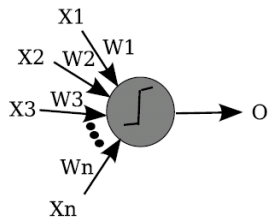

Fig. 1: Individual Neuron in an ANN

The sigmoid activation function used in this paper, is given by the relationship:

$$O = \frac{1}{1 + e^{-2\sum X_i * W_i}}$$

This activation function is highly non-linear in nature. The activation function behavior is such that if the total sum of the weighted inputs is zero, then the output is 0.5. Whenever the weighted input sum is negative, the output exponentially approaches 0. On providing with a positive weighted input sum, the output exponentially approaches 1. This non-linear activation function of the neuron, approximately models a threshold element, whose output is 0 for negative, and 1 for positive weighted input-sums.

The entire neural network is a collection of these neurons (vertices), interconnected by weighted edges. The entire process of generating ANN models, therefore only involves choosing the appropriate interconnection patterns, and edge weights. A wide variety of training algorithms are available, to assist in this process of adapting the weights to learn the underlying input/output relationships. The following sub-section details the training algorithm used in this paper.

B. Training Algorithm

The first step in developing prediction models is to divide the available data-set randomly into training-data and testing-data. The randomness of selection ensures that neither the testing-data, nor the training data are biased, and are faithfully representative of the entire data-set. The ANN is then trained repetitively on this training data-set, in order to accurately learn the underlying model characteristics.

In this paper, all the models were developed using the back-propagation training algorithm. This algorithm operates by starting with an initial network configuration, and iteratively refining it to fit the provided training data-set. Individual iterations in turn comprise of two phases: (i) Forward propagation of the input training data (ii) Backward propagation of the errors from the output.

1) Forward Propagation: During this phase, the training inputs are applied to each neuron, and the outputs are generated based on the activation function. This phase propagates layer-by-layer, from the ANN-inputs to the ANN-output, thus ensuring that each neuron has all the available inputs before proceeding with its activation.

2) Backward Propagation: The final output value generated from the forward propagation phase is compared with the actual expected output for the corresponding training input. The difference in values is computed as the estimate of the model-error. This error-estimate is back-propagated along the network till the inputs. Each neuron along the backward path, updates the weights appropriately to reduce the error. This adjustment is done according to (i) magnitude of the error, (ii) direction of error, (iii) slope of the activation function, and (iv) learning factor. A learning factor of 0.7 was used to generate the models developed in this paper. The learning factor was chosen carefully, since a low learning value needs a very large data-set, while a higher learning factor is susceptible to data-noise.

As the algorithm proceeds, the output error of the ANN model starts decreasing. The ANN model thus gradually learns the training data-set by using the back-propagation learning algorithm.

C. Parameter Selection

Analysis of experimental measurements suggests a simple relationship between the number of ECAP presses and the resulting grain-size. Yield strength and tensile strength however, exhibit a more complex relationship with the number of passes. Based on these observations, it is prudent to first develop the ANN model to predict the grain-size of AZ61 Mg alloy. Using a simple network configuration with 1 input layer, 1 output layer, and 1 hidden layer, it is possible to develop a prediction model for the grain-size (See Fig. 2).

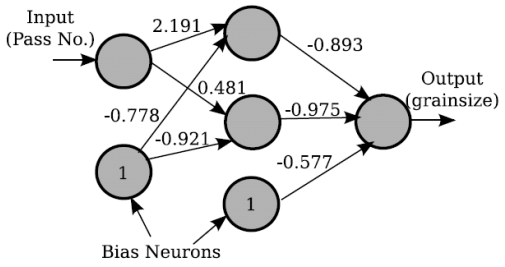

Fig. 2: ANN Prediction Model for Grain Size

The prediction model for yield-strength is significantly more complex than that of the grain-size. In the process of developing an ANN model for yield-strength, it would be wasteful to re-learn the relationships already characterized by the grain-size model. The input parameters for the yield-strength model therefore consist of both (i) number of ECAP passes, and (ii) grain-size. The learning time is significantly reduced, and the resulting model complexity is also minimized (See Fig. 3).

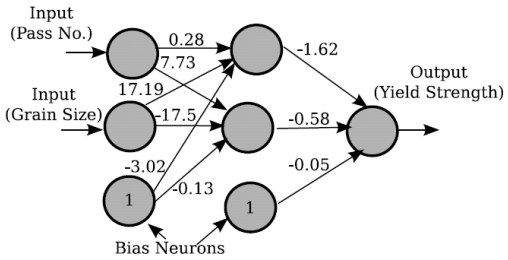

Fig. 3: ANN Prediction Model for Yield Strength

In selecting the input parameters for predicting tensile strength (UTS), (i) number of ECAP passes and (ii) grain size are chosen as the important features. (See Fig. 4). Adding yield-strength does not result in any significant improvements, and ends up adding more noise at the input stage. This behavior results from the fact that the grain-size prediction errors influence the predicted yield-strength errors. These errors get further magnified, if used as input to a subsequent stage to predict the tensile-strength. Adding an extra input parameter would also result in a significantly complex network configuration.

D. Model Generation

After deciding on the training algorithm to be used in generating the model and selecting the appropriate input parameters for each model, the actual model generation phase can proceed. In this phase, the input parameters from the training data-set are applied, and the corresponding output values are used to estimate the error. The estimated error is used to refine the model, as specified by the training algorithm.

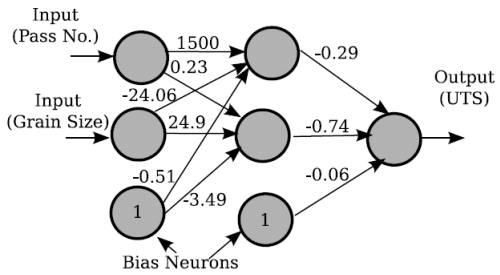

Fig. 4: ANN Prediction Model for UTS

The main objective of any training algorithm is to reduce a specific error-metric aggregated over the training data. The back-propagation algorithm used in this paper optimizes the mean-squared error value. Iterative reduction in the aggregate mean-squared error during the grain-size model generation is shown in Fig. 5. As expected, the initial error is quite high, as the number of iterations increases the estimated error is successfully reduced using the back-propagation algorithm. The error estimate is not a strictly decreasing function, since during model generation the training algorithm has to recover from local-minima. The aim is to obtain the global-minimum mean squared-error hence there are slight disturbances in the decreasing nature of the error-estimate.

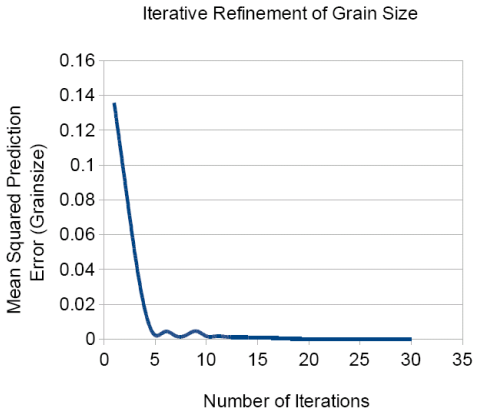

Fig. 5: Grain-Size Model Generation

The minimization of mean-squared error during the yield-strength and tensile-strength model generation phases, is shown in Fig. 6 and Fig. 7. The first observation here is that the initial error value for the grain-size model is greater than the yield-strength model, which is in turn greater than the tensile-strength model. This behavior is attributed to the difference in relative output ranges, expected from each of these models. The relative range is clearly much larger for grain-size, than it is for yield-strength, which is in turn greater than that of tensile-strength. This relationship is clearly reflected in the initial error estimates of each model. Otherwise, the behavior of mean-squared error is quite similar, as it gets successively reduced with increasing number of iterations.

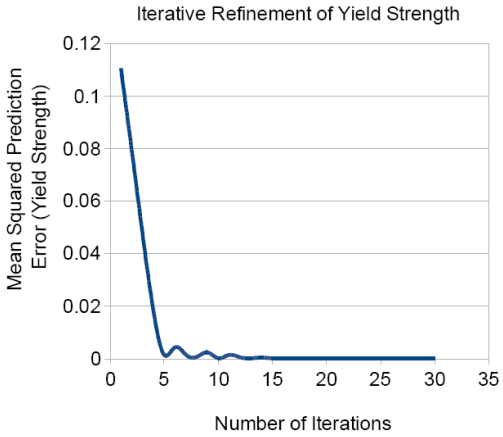

Fig. 6: Yield-Strength Model Generation

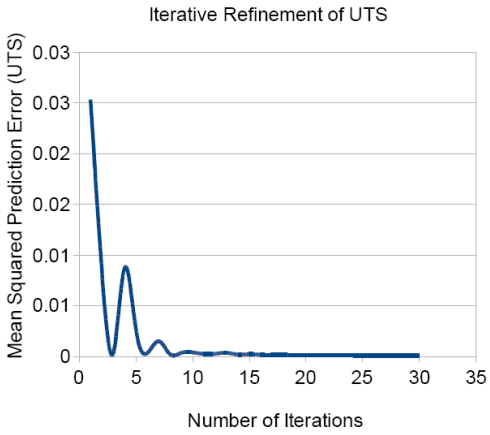

Fig. 7: Tensile-Strength Model Generation

4. RESULTS

As described in the previous section, the data-set was randomly divided into training data and testing data. The predication accuracy of each individual model is analyzed in this section.

TABLE II: Prediction-Model for Grain Size

ECAP Pass No.	Measured Grain size A_g (μm)	Predicted Grain Size P_g (μm)	Relative Error ($\frac{\lvert P_g - A_g \rvert}{A_g}$)
0	24.4	24.3	0.004
1	15.8	15.7	0.006
2	12.5	12.5	0.000
3	11.2	11.1	0.009
4	10.6	10.1	0.047
8	8.4	8.3	0.012

The grain-size model results are summarized in Table. II. The relative error is very low (< 0.05), and this shows that the model has successfully learned the underlying pattern of decreasing grain-size, with increasing number of ECAP presses. As can be seen from the results, the initial rate of decrease is quite high, and the rate reduces with increasing number of ECAP passes. The maximum relative error occurs at 4 ECAP passes, while all the other estimates have a much lower error (< 0.01).

TABLE III: Prediction-Model for Yield Strength

ECAP Pass no.	Measured Yield Strength A_y (M Pa)	Predicted Yield Strength P_y (M Pa)	Relative Error $(\frac{\lvert P_y - A_y \rvert}{A_y})$
0	215	215	0.000
1	193	193	0.000
2	202	211	0.044
3	208	207	0.005
4	191	196	0.026
8	154	154	0.000

The yield-strength model results are summarized in Table. III. The relative error is again seen to be very low (< 0.05), and this shows that the model has absorbed the complex pattern of initial decrease, followed by another increase, and subsequent decrease. The maximum prediction error occurs at 2 ECAP passes, and this can be attributed to the fact that the yield-strength changes direction at this point (decreasing to increasing). The estimated yield strength has successfully predicted the change (193->211) while there is a slight error in its magnitude (actual yield strength is 211). The other noticeable error is at 4 ECAP passes, and this can be attributed to similar reasons. The overall error otherwise is very low (< 0.001), and the model is therefore highly successful in predicting the yield-strength. This best illustrate the suitability of artificial neural network based models to predict the mechanical properties of alloys like AZ61 Mg.

TABLE IV: Prediction-Model for UTS

ECAP Pass no.	Measured UTS A_u (M Pa)	Predicted UTS P_u (M Pa)	Relative Error $(\frac{\lvert P_u - A_u \rvert}{A_u})$
0	322	321	0.003
1	302	302	0.000
2	317	324	0.022
3	329	328	0.003
4	317	325	0.025
8	310	310	0.000

The tensile-strength (UTS) results are presented in Table. IV. It can be seen that here again the resulting relative error is very low (< 0.03). Achieving such excellent agreements between predicted values and actual measurements, suggests the powerfulness of ANNs in modeling these varied properties. The main reason for the lower relative error of UTS is the smaller relative range of UTS values, compared to the other output parameters. At 2 ECAP passes, and 4 ECAP passes, the tensile-strength trend changes directions, and this results in the slightly increase error values at these points.

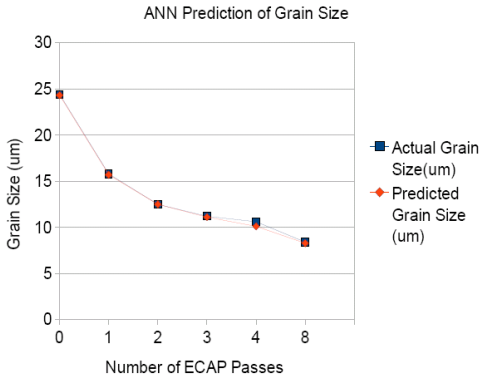

Fig. 8: ANN Prediction Accuracy for Grain Size

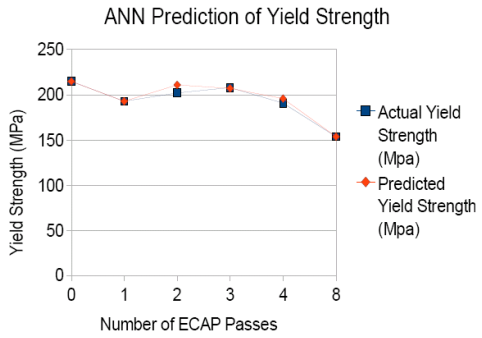

Fig. 9: ANN Prediction Accuracy for Yield Strength

Based on the results of each individual prediction model, it is evident that artificial neural network based models are a lucrative choice for estimating the mechanical properties of alloys. All the models presented in this paper, have a very low relative-error (< 0.05), this is proof that they are fairly accurate. The usefulness of these models stems from the fact that they are immensely valuable, when optimizing for different mechanical properties. Material-science engineers looking for particular yield-strengths and tensile-strengths can use these models to determine the optimal number of ECAP presses. These mathematical models help avoid extensive experimentation.

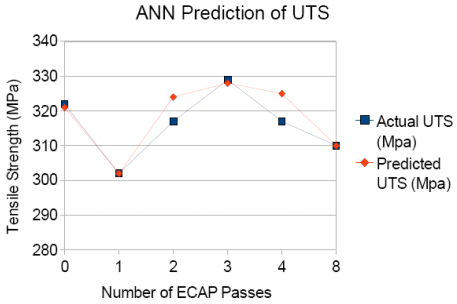

Fig. 10: ANN Prediction Accuracy for UTS

In a pure experimental approach, the designer has to apply different number of presses, and measure the target mechanical properties. It may also be required to apply invasive and destructive tests to measure some of these mechanical properties. When the target properties are not achieved, the extrusion process needs to be repeated with a different number of passes. It may also be possible that some strength values are not achievable on particular alloys. In such situations, all the experimentation on the alloy may be wasted. Using the artificial neural network prediction model, avoids all these disadvantages. The prediction model can be used to estimate the optimal number of presses required for the desired property. Based on the number of presses, one can determine whether it is practically feasible to use the alloy, or to choose another material altogether. The extrusion process can then be carried out to form the actual alloy.

Although artificial neural network models are effective in reducing the error-estimate, and accurately predicting mechanical properties, they pose certain difficulties during construction. The choice of appropriate parameters like learning factors and number of layers, involves significant insights into the target properties. The parameter selection process also involves important decisions regarding which input parameters are best at determining each output parameter. After resolving these initial issues, it is quite easy to generate fairly accurate and robust ANN prediction models for mechanical properties.

5. CONCLUSION

This paper has developed artificial neural network based prediction models, to estimate the mechanical properties of AZ61 Mg alloy fabricated by equal channel angular pressing. The results show that the relative prediction error is very low (< 0.05), and mostly occurs at locations where the output change is irregular. This close correlation between estimated measurements and experimental data, suggests that ANN-based models are very effective in predicting the mechanical properties of the AZ61 Mg alloy.

An important future work is to examine the extensibility of ANN-based models to other mechanical properties. Promising results also suggest the applicability of these models to other alloys, beyond AZ61 Mg. The ability of ANNs to generalize presented input/output patterns, make them the ideal candidates for constructing such models.

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