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Application of artificial neural networks for modelling correlations in age hardenable aluminium alloys

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Analysis and modelling

ABSTRACT

Purpose: This paper discusses some of the preliminary results of an ongoing research on the applications of artificial neural networks (ANNs) in modelling, predicting and simulating correlations between mechanical properties of age hardenable aluminium alloys as a function of alloy composition.
Design/methodology/approach: Appropriate combinations of inputs and outputs were selected for neural network modelling. Multilayer feedforward networks were created and trained using datasets from public literature. Influences of alloying elements, alloy composition and processing parameters on mechanical properties of aluminium alloys were predicted and simulated using ANNs models.Two sample t-tests were used to analyze the prediction accuracy of the trained ANNs.
Findings: Good performances of the neural network models were achieved. The models were able to predict mechanical properties within acceptable margins of error and were able to provide relevant simulated data for correlating alloy composition and processing parameters with mechanical properties. Therefore, ANNs models are convenient and powerful tools that can provide useful information which can be used to identify desired properties in new aluminium alloys for practical applications in new and/or improved aluminium products.
Research limitations/implications: Few public data bases are available for modelling properties. Minor contradictions on the experimental values of properties and alloy compositions were also observed. Future work will include further development of simulated data into property charts.
Practical implications: Correlations between mechanical properties and alloy compositions can help in identifying a suitable alloy for a new or improved aluminum product application. In addition, availability of simulated structure-process-property data or charts assists in reducing the time and costs of trial and error experimental approaches by providing near-optimal values that can be used as starting point in experimental work.
Originality/value: Since the simulated data provides near-optimal values, manufacturers of new and/or improved aluminum alloys can use the simulated data as guidelines for narrowing down extensive experimental work. This in turn reduces the process design cycle times. Designers of new and/or improved aluminum products can also use the simulated data as a guideline for correlating property-application information, which is useful in preliminary design phase.
Keywords: Artificial intelligence methods; Artificial Neural Networks (ANNs); Aluminum alloys; Mechanical properties

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1. Introduction

Aluminium is a very light metal whose strength can be adapted to the application required by modifying the composition of its alloys and/or by applying appropriate thermal and mechanical treatments. Uses of aluminium alloys are found in a wide range of applications including transportation, packaging, construction, household items, and electrical transmission to just mention a few [1]. High strength aluminum alloys (i.e. 2xxx, 6xxx, and 7xxx series) have found structural applications as well as applications in the automotive and aircraft industries. Each of these applications requires different properties of aluminium alloys. To meet these demands of a wide range of applications new aluminium alloys and new production techniques have been proposed as manufacturers seek more efficient and cost effective ways of producing aluminum alloys of desirable strength [2].

Most of the new techniques and new aluminium alloys are developed for specific process routes that are designed to produce a particular product [2-3]. In such developments, a very limited number of alloy types are extensively investigated mostly through trial and error experimentation, which is costly and time consuming. However, the methods used and the new techniques applied cannot predict or simulate: the required microstructure, the optimal processing parameters or the alloy compositions required for a new or improved application. There is, therefore, a need to develop methods of a general nature that can accurately predict as well as simulate processing-structure-property relations in aluminium alloys. Such predictive methods are even more important in applications of recycled aluminium for which trace elements may significantly affect the mechanical properties [4].

Most applications of aluminium alloys are related to mechanical properties. For age hardenable aluminium alloys (i.e. 2xxx, 6xxx and 7xxx series), the mechanical properties depend on the characteristics of the microstructure. The microstructure is developed during the various stages of production. Since the microstructure develops under specific conditions, it is important for designers, aluminium alloy developers and producers to know and understand the practical implications of kinetics of the phase transformations taking place during the various production stages. Of particular importance to age hardenable aluminium alloys are the transformations that take place during solution heat treatments.

Solution heat treatment processes involve heating the material to an elevated temperature (above the solvus) and soaking at this temperature for sufficient time followed by cooling [5-6]. This process affects the mechanical properties of age hardenable aluminium alloys by altering their microstructures. This in turn alters the mechanical properties of the alloys. Therefore, knowledge of solution heat treatment conditions is important in achieving desired mechanical properties. In addition to solution heat treatment conditions, an understanding of the correlationships between mechanical properties and processing parameters is vital. Such knowledge helps in optimizing processing parameters in a bid to achieve desired mechanical properties for a specific application. Therefore, an understanding of the process-structure-properties relationship is essential in the design and development of new aluminium alloys for new or improved applications.

In the process of developing new alloys, information for selecting the appropriate solution heat treatment conditions for an alloy of desired properties must be available. Despite the large number of existing aluminium alloys and alloy databases, identifying proper alloys for specific applications still remains a challenge. This is because there is a general lack of information on factors correlating mechanical properties of aluminium alloys with processing variables and alloying elements composition [7]. In addressing the mentioned deficiencies, the idea proposed in this work is to utilize computational modeling and simulation capabilities of neural networks to provide the necessary information through predictive methods. The challenge lies in obtaining accurate predictions that can be used in optimizing the processing parameters and alloy composition in order to achieve the desired combination of properties for any particular application.

In this paper, artifial neural networks (ANNs) modelling is used to predict correlations between mechanical properties of aluminium alloys with alloy composition as well as processing parameters. The objective is to develop artificial neural network models that can provide data regarding the influence of processing parameters and alloy composition on mechanical properties of age hardenable aluminium alloys for new or improved applications.

2. Neural network modelling method

In order to facilitate the predictions of the processing-structure-property relations in age hardenable aluminium alloys, a multilayer feedforward neural network modeling approach was used. The key to predictions was the determination of relationships between alloy properties, alloy composition and process variables. In practice, the underlying mechanisms that determine the processing-structure-property relations are not fully understood and the physical phenomenon are difficult to describe [8]. Since ANNs are capable of computing and generalizing non-linear complex relationships, their suitability in simulating correlations in processing-structure-property relations were investigated in this paper.

In general, neural networks are characterized by their architecture, activation functions, and learning algorithms [9]. In the design and training of the implemented ANNs the following aspects were considered; structure of the ANNs, training algorithms; and the transfer function.

2.1. Model description

An Artificial Neural Network (ANN) is a “black box” to which inputs are supplied and it gives outputs after some computational processing. Multilayer feedforward neural networks were used to develop the various simulation models for predicting correlations in processing-structure-properties of age-hardenable aluminum alloys. ANNs are suitable for simulating physical phenomena such as processing-structure-properties

relations since the phenomena are characterized by multiple inputs and have nonlinear and complex relationships between the input and output variables.

The structure or architecture of ANNs is usually specified by the number of the layers in the ANN model and the number of the neurons in each layer. As shown in Figure 1, the general structure of the implemented ANN models consists of an input layer, a hidden layer and an output layer.

2.2. Neural network training

The neural network modelling and simulation procedures implemented in this paper were done in five steps as follows: (i) data collection, (ii) pre-processing of collected data, (iii) neural network training, (iv) testing of the trained neural network model and (v) predictive simulations using the trained neural network models.

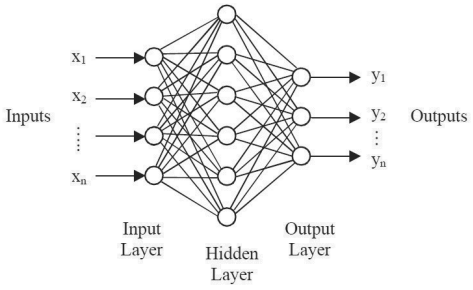

Fig. 1. General Architecture of the implemented Artificial Neural Network Models

In the ANN model development process, training of the models was performed in order to find the error by comparing the output value of the network with the target value and then minimizing the difference (error) by modifying the weights. Four (4) learning algorithms were tested for suitability. These include; (i) resilient back propagation (RPROP) which implements a first order optimization rule, (ii) QuickProp which implements a second order optimization rule, (iii) Batch and (iv) Incremental learning algorithms. Except for the incremental learning algorithm, the other three learning algorithms calculate the error for the entire data set and update the weights. On the other hand, incremental training calculates the error and updates the weights after each input/output pair is presented. In trial experiments, it was found out that the most appropriate learning algorithm for the available data sets was the RPROP algorithm [10]. This was because it was fast and efficient in comparison to the others.

Before training, the data set was randomly divided into two groups. 65% of the data were used for training and 35% for testing. At the start of training, the network creates a set of random weights between the neurons in the successive layers and computes the outputs. The calculated outputs are compared with the target values and the differences are the errors. According to the magnitude of the error, each weight is adjusted so as to reduce the total error. Then the calculation is performed once again using the adjusted weights in order to get a new set of outputs. These in turn are compared with the targets, and the weights are adjusted again. This process is repeated until an acceptable criterion is reached. For experiments in this paper, the total error (i.e. error based on the Mean Squared Error (MSE) between the network output and target), was used as a criterion for terminating the training session.

In ANNs, a transfer function transforms the neuron input value into the output value. For all cases, a linear transfer function was used in the output layers. In the hidden layers the tan-sigmoid transfer function and the log-sigmoid transfer function were employed [11-12]. After satisfactory training, the neural network models were used for further simulations and predictions of different correlations and phenomena in processing-structure-properties relationships.

2.3. Input data modelling

The input parameters for studying the processing-structure-property relationships in age hardenable aluminium alloys (designated as 2xxx, 6xxx and 7xxx) were the chemical composition of the alloys i.e. different types, quantities and combinations of alloying elements. In the above designation, the first digit indicates the series, and the second digit indicates alloy element modifications of an already existing alloy. The third and fourth digits identify a specific alloy element, without physical significance, and they only serve to differentiate between various alloys. Three ANN models, based on the architecture shown in Figure 1, were developed for each of the three alloy series.

The major alloying elements in the 2xxx series are Copper (Cu) and Magnesium (Mg). The major alloying elements in the 6xxx series are Magnesium (Mg) and Silicon (Si), while the major alloying elements in the 7xxx series are Zinc (Zn), Magnesium (Mg) and Copper (Cu). Lists of alloying elements used in this analysis are shown in Tables 1-3.

In addition to the summary of data represented in Tables 1-3, solution heat treatment parameters and various mechanical properties for various alloys were collected from public databases. The mechanical properties included; ultimate tensile strength, yield strength, shear stress, fatigue strength, shear strength and proof stress.

3. Results and discussions

ANN models were developed for the analysis and prediction of the correlation between processing (heat treatment) parameters and mechanical properties in aluminium alloys. The ANN models were then used to predict and simulate the correlations between processing parameters and working conditions as well as mechanical properties. Typical types of heat treatment of age hardenable aluminium alloys were considered in the analysis [13].

Table 1.
Input Parameters for the 2xxx series

	Major alloying elements			Others					
Alloying element	Cu	Mg	Si	Zn	V	Ti	Fe	Mn	Cr
Number of alloys containing this element	27	20	10	10	6	5	10	11	6
Range, (% weight)	0-6.8	0-1.8	0-1.2	0-0.25	0-0.15	0-0.15	0-0.70	0-1.2	0-0.2

Table 2.
Input Parameters for the 6xxx series

	Major alloying elements			Others					
Alloying element	Mg	Si	Cu	Zn	V	Ti	Fe	Mn	Cr
Number of alloys containing this element	40	30	21	14	0	12	16	13	12
Range, (% weight)	0-1.4	0-1.8	0-1.2	0.0.25	0	0-0.2	0-0.70	0-1.1	0-0.5

Table 3.
Input Parameters for the 7xxx series

	Major alloying elements				Others				
Alloying element	Cu	Mg	Zn	V	Si	Ti	Fe	Mn	Cr
Number of alloys containing this element	21	40	27	5	17	10	16	13	12
Range, (% weight)	0-2.4	0-2.9	0-7.3	0-0.05	0-0.7	0-0.2	0-0.5	0-0.3	0-0.3

3.1. Prediction of mechanical properties of aluminum alloys

In practice, variations in mechanical properties of aluminum alloys arise due to differences in thermo-mechanical processing (mainly heat treatment-temper) of the alloy either during the production process or post-production fabrication. For age hardenable aluminum alloys, many tempers are possible since changing the heat treatment temperature and/or heat treatment time results in different microstructures that exhibits a wide variety of mechanical properties. In the ANN modelling, microstructures were input in the model by a decimal digit that corresponds to the alloy temper(T) designation, i.e. 1, 2, 3...where 1 stands for T1, 2 stands for T2 and 3 stands for T3 etc. Alloys in nine (8) different tempers were experimented with. Data on mechanical properties of alloys was collected for different working temperatures in the range 15ºC to 560º C. The outputs from the ANN models were the various mechanical properties of which strength properties are most important in the high strength alloys considered in this work. A comparison of the predicted and experimental data on fatigue strength of selected aluminum alloys from the 2xxx, 6xxx and 7xxx series for commonly used temper designation are shown in Figure 2.

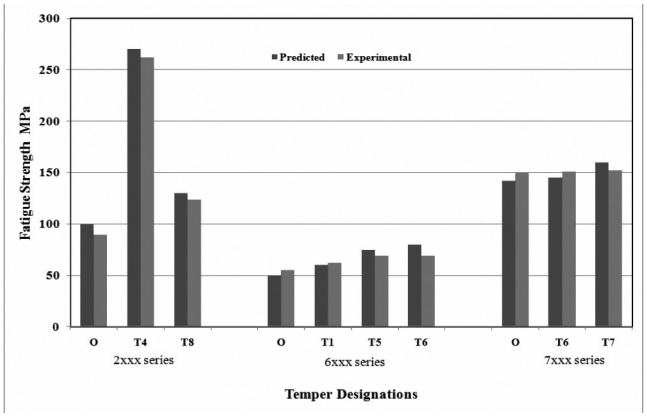

Fig. 2. Comparison of ANN predictions and experimental data on fatigue strength of various aluminum alloy series with different temper designations

The results in Figure 2 show that there is close agreement between the predicted and experimental data. A two-sample t-test, conducted in Minitab, for the predicted versus experimental data

gave the following *p-values* for the 2xxx, 6xxx and 7xxx series respectively: 0.918, 0.214 and 0.001 all based on a 95 % confidence level and assuming equal variances. Since the *p-values* for the 2xxx and 6xxx series data are greater than 0.05, it can be inferred that there is no significant difference (statistically) between the predicted and experimental data for the fatigue strength. However, the differences in the predicted and experimental data for the 7xxx series are statistically significant.

Figures 3-5 show comparisons between predicted and experiment data on the shear strength of various commercial alloys from the 2xxx, 6xxx and 8xxx series respectively. Error bars indicating regions of 5% errors associated with the data predicted by the ANNs models are also shown. It can be observed from these figures that the ANN prediction is within 5% error of the experimental data.

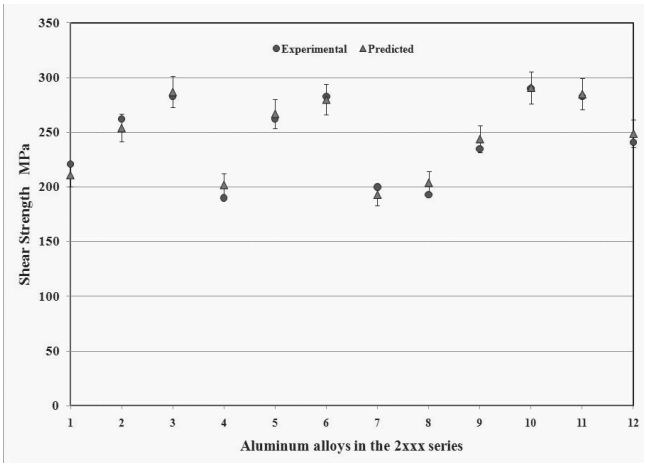

Fig. 3. Comparison of predicted and experimental shear strength values of aluminum alloys belonging to the 2xxx series

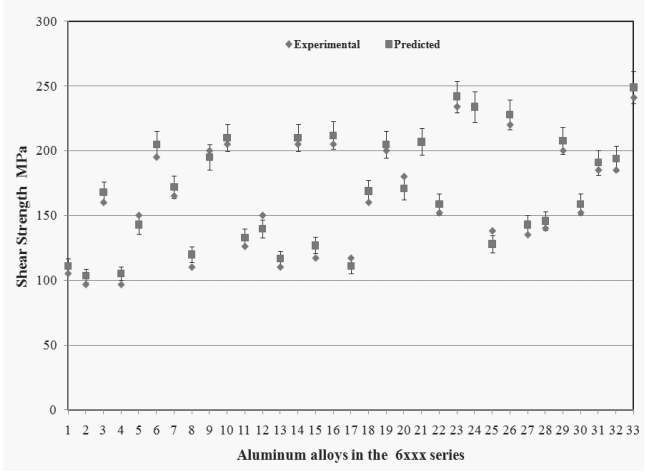

Fig. 4. Comparison of predicted and experimental shear strength values of aluminum alloys belonging to the 6xxx series

Two-sample t-tests for the predicted and experimental shear strength data for the 6xxx and 7xxx series aluminum alloys gave *p-vales* of 0.477 and 0.639 respectively. Based on these values it can be inferred that there is no significant difference (statistically) between the ANN predicted and experimental shear strength data for the 6xxx and 7xxx series aluminum alloys.

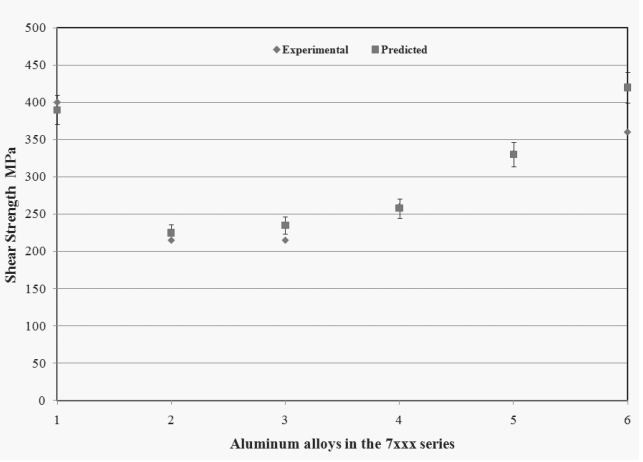

Fig. 5. Comparison of predicted and experimental shear Strent values of aluminum alloys belonging to the 7xxx series

3.2. Effects of alloying compositions

The effects of major alloying elements on the mechanical properties of the 2xxx, 6xxx, and 7xxx alloy series was simulated from values predicted by the ANN models. Figures 6-8 show a simulation of the effects of alloying compositions on the ultimate strength and proof stress of the various alloy series.

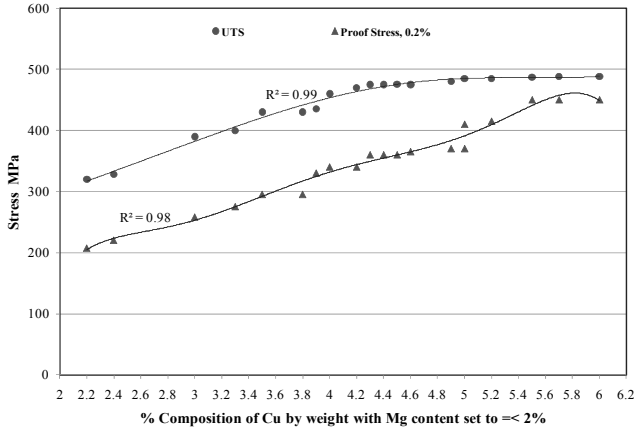

Fig. 6. Simulated effects of copper content on mechanical properties of 2xxx series aluminum alloys

Unlike Figure 8, the data points from scatter plots in Figures 6 and 7 were fitted with the most appropriate trendline. Values simulated by the trendlines are approximations of the generalized trends in the ultimate tensile strength and proof stress for alloys in the 2xxx and 6xxx series. R^2 values of the fitted curves are also shown. These R^2 values show a high degree of mapping accuracy of the the various data points on ultimate tensile strength and proof stress. Such simulation curves contain information on generalized and predicted values of ultimate tensile strengths and proof stress as a function of alloying compositions (or vice-versa). In practice, simulated values from these curves can be used to approximate the required alloy compositions that meet certain desired mechanical properties (or vice-versa). Obtained approximations can also be used to narrow down the cost and time required in carrying out trial and error experimental methods for alloy characterization.

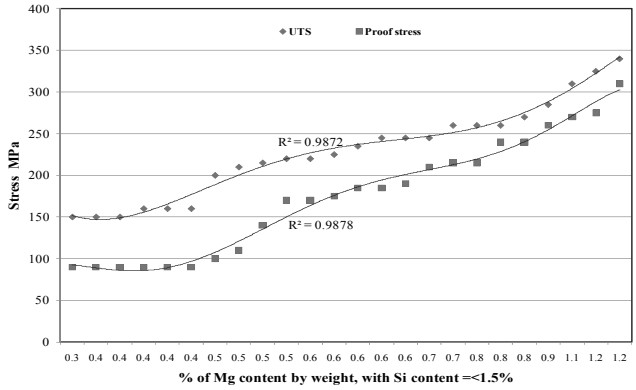

Fig. 7. Simulated effect of magnesium content on mechanical properties of 6xxx series aluminum alloys

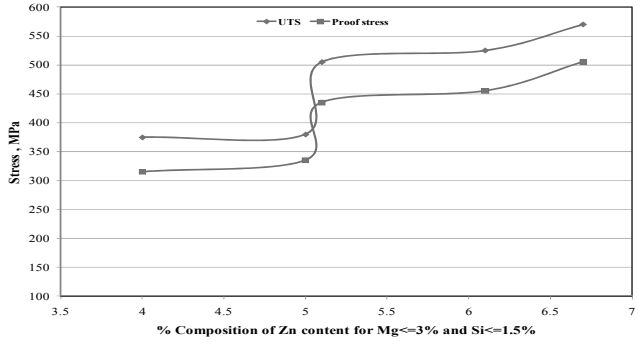

Fig. 8. Simulated effect of zinc content on mechanical properties of the 7xxx series aluminum alloys

3.3. Example applications of simulated data

Figures 9-11 demonstrate three examples of using the ANNs models for simulation of the influence of alloying compositions on mechanical properties. In Figures 9-11, the influence of major alloying composition for selected aluminum alloys from the 2xxx, 6xxx and 7xxx series, respectively are show for specific alloy tempers.

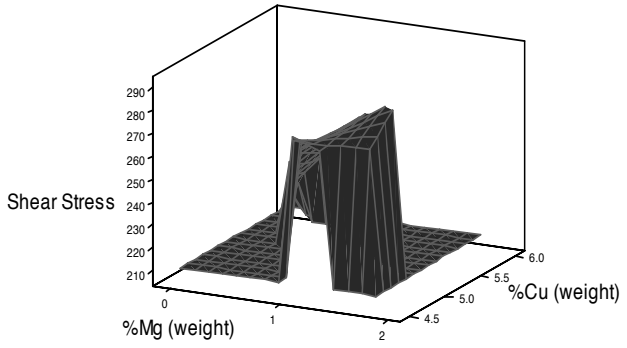

Fig. 9. Neural network model simulations for the influence of alloy compositions in 2xxx aluminum alloy series on shear stress for T4 temper

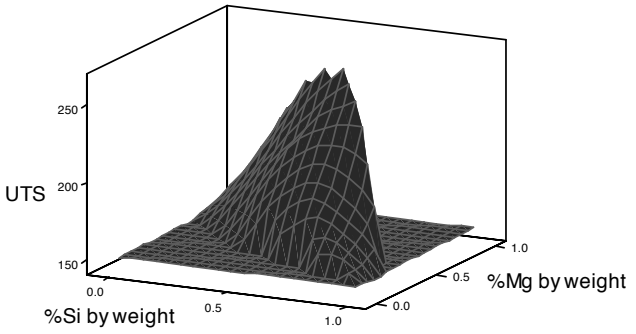

Fig. 10. Neural network model simulations for the influence of alloy compositions in 6xxx aluminum alloy series on ultimate tensile strength for T1 temper

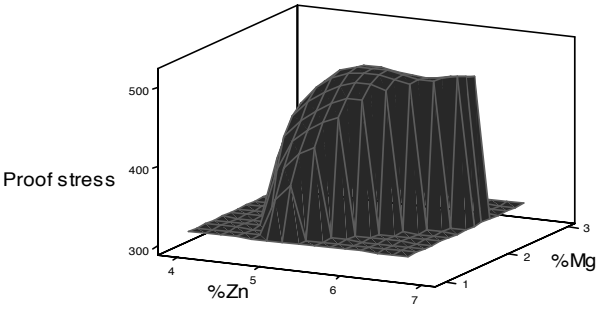

Fig.11. Neural network model simulations for the influence of alloy compositions in 7xxx aluminum alloy series on proof stress.

Figures 9-11 also show regions for which the combined effects of alloying compositions results in specific values of mechanical properties. Such relationships can be used as general guidelines in the conceptual phases of developing new and/or improved applications of aluminum alloys.

4. Concluding remarks

ANN models for predicting and simulating correlations in structure-process-property phenomena in the processing of age hardenable aluminium alloys were created trained and used to predict mechanical properties as a function of alloy composition. In using the created ANN models, the alloying compositions and processing parameters are the inputs while the mechanical properties are the outputs. In practice, however, it is usually desirable to find combinations of mechanical properties that would be used as inputs, to obtain specific alloying composition for a particular product application. In the work presented in this paper, this can be achieved by using the ANN models to simulate the required mechanical properties as a function of alloy composition. The results from the simulation can be used as a starting point in determining the optimal alloy compositions, processing parameters and conditions required to produce a high-quality and functional product. Unlike the experimental approach, which is time consuming and yet does not allow what-if simulations and analysis (for new and improved alloys), the ANN method is capable of generalizing the complex relationships and provide approximate solutions. This helps in simulation and analysis of customized product applications as well as new or improved product applications. Information obtained from the ANN predictions and simulations can also be used as guidelines during the conceptual design and optimization of manufacturing processes thus reducing the time and costs that would otherwise be incurred by experimental methods.

Future work related to this research includes; modeling and analysis of the effects of trace elements in recycled aluminum and further developement and extension of the simulated data into property charts.

References

[1] R.A. Sielski, Research Needs in Aluminum Structures, 10th International Symposium on Practical Design of Ships and Other Floating Structures, Houston, Texas, USA, 2007.
[2] J. Buha, R.N. Lumley, A.G. Crosky, K. Hono, Secondary precipitation in an Al-Mg-Si-Cu alloy, Acta Mater 55 (2007) 3015-3024.
[3] S. P. Ringer and K. Hono, Microstructural Evolution and Age Hardening in Aluminium Alloys: Atom Probe Field-Ion Microscopy and Transmission Electron Microscopy Studies, Materials Characterization 44 (2000) 101–131.
[4] AluMatter Electronic Database, http://aluminium.matter.org.uk accessed July 10 2010
[5] J. Buha, R.N. Lumley, A.G. Crosky, Microstructural development and mechanical properties of interrupted aged Al-Mg-Si-Cu alloy, Journal of Metallurgical and Materials Transactions A 37A (2006) 3119-3130.
[6] J.R. Davis and Associates (ed.), ASM Specialty Handbook on Aluminum Alloys, ASM International, Materials Park, Ohio, USA, 1993.
[7] D. Emadi, M Sahoo, T. Castles, H. Alighanbari, Prediction of mechanical properties of as-cast and heat treated automotive Al alloys using artofial Neural networks, TMS Light Metals (2001) 1069-76.
[8] C. Jose, R. Neil, R. Euliano, and W. C. Lefebvre. Neural and Adaptive Systems: Fundamentals Through Simulations, John Wiley and Sons, 2000.
[9] S. E. Fahlman, M. Lebiere, An Empirical Study of Learning Speed in Back-Propagation Networks, Tech Report CMU-CS-88-162, Carnegie Mellon University, September 1988
[10] T. M. Mitchell. Machine Learning, WCB-McGraw-Hill, 1997.
[11] J. Higham and N.J. Higham, MATLAB Guide 2nd edition: Soc for Industrial & Applied Math, Philadelphia, PA, 2000.
[12] Z. Wang, R. Tian, in: Manufacture Handbook of Al Alloy, Central South University of Technology Press, Changsha, 1989.