Designing age-hardenable Al alloys using ANFIS and GA

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Abstract. Age-hardenable aluminium alloys have higher strength compared non-heat-treatable alloys due to strengthening by the precipitates. Increasing the toughness of such alloys require improved balance between strength and ductility. To improve both ductility and strength through modification of composition and heat-treatment parameters of age-hardenable Al alloys (2XXX, 6XXX and 7XXX) an artificial intelligence based computational design approach is employed. Published data on the alloys are used for developing the data-driven models for tensile strength, yield strength, and %elongation. Fuzzy C means clustering is used to cluster the variables in the database into different levels and to generate fuzzy rule correlating those variables. Adaptive neuro-fuzzy inference system (ANFIS) used the fuzzy rules to develop the data-driven fuzzy predictive models for the said properties of the alloys. These models in turn played the role of objective functions for the multi-objective optimization using genetic algorithm (GA) for handling the conflicting objectives of improving ductility as well as strength to design alloys. The generated Pareto solutions are analyzed for finding suitable composition and process parameters fulfilling the purpose.

1. Introduction

Aluminium is one of the most widely used metallic element. One can easily find its application in household items like aluminium foils, cans, kitchen utensils etc. The wide range of applications of aluminium alloys extend to automobile and aircraft industries. The reason for its popularity is due its low density and high corrosion resistance nature [1]. It has characteristics like easy workability, high electrical and thermal conductivity. Such characteristics provide these alloys with extra advantages than structural steels [2]. The high strength to weight ratio of aluminium alloys becomes the major reason for their design applications in automobile and aircraft industries [3]. The reason for their properties can be rooted back in their composition and microstructure. The mechanical, chemical and physical properties of aluminium are enhanced by alloying it with suitable one or more than one element at specific quantities [4]. Major elements that are generally preferred for combining are Silicon (Si), Copper (Cu), Magnesium (Mg), Zinc (Zn) etc. Certain aluminium alloys that respond to heat treatments like solution treatment and ageing based on their phase solubility. Those alloys are termed as heat treatable or precipitation hardened or age hardenable alloys [5]. The primary alloying elements that are considered for such age hardenable aluminium alloys are Cu (2XXX series), Zn and Mg (7XXX series) or Mg and Si (6XXX series) [6,7]. The process of age hardening involves dissolving of the second phase in the solid solution at elevated temperatures. Then, it precipitates upon aging at lower temperatures. The major condition to be taken into consideration is that the second
phase must be soluble when the temperature is elevated but should show decreasing solubility when there is decrease in temperature [8,9]. The above said condition proves to be a hindrance to the number of utilisable age-hardened alloy systems. With proper alloying, the strength of such alloys can be as high as 40times more than that of pure aluminium. To improve the properties of such age hardenable aluminium series like Al-Cu, Al-Mg-Si and Al-Zn-Mg attempts have been made previously [10,11]. The attempts, if restricted to trial and error method, to search for desirable chemical composition and optimum processing parameters, will be time consuming, costly and tedious. It might end up with no assured results. One might approach the problem mathematically and bring out the relationship between the necessary chemical composition with its associate process parameters [12].

The complex correlation, which was earlier difficult to describe through physical models, now being unveiled through data driven models. This will lead to effective material design. Computational designing of alloys as a preliminary step before experimental validation will provide us with lesser number of trials and more accurate results [13,14]. Along with computational intelligence used for designing, design optimization can be implemented to create complex designs and obtain optimized solutions. Artificial intelligence-based material designing tools that are generally used are artificial neural network (ANN) and fuzzy logic for predictive models and genetic algorithm (GA) for optimization [15]. There are several examples where the outputs of ANN or fuzzy inference system (FIS) can be used as an objective function of GA based optimization [16]. The present study provides design of aluminium alloys with higher strength and ductility at room temperature for three alloy series – 2XXX, 6XXX and 7XXX. Data-driven models for the tensile properties of the three Al alloys series are developed through Fuzzy C-means clustering followed by development Adaptive Neuro-Fuzzy Inference System (ANFIS). The developed ANFIS models are used as the objective functions for the multi-objective optimization of ductility and strength using GA.

2. Database

Around 200 numbers of data are collected from standard sources about Al alloys of 2XXX, 6XXX and 7XXX series. Various input parameters and output parameters are considered [9]. Elements comprising the composition of alloys are taken as the input parameters. Silicon, copper, magnesium and zinc are taken as the major constituents. Other constituting elements are manganese, chromium, nickel etc. The ‘other’ elements are also included in the parameters. Physical parameters those are included as inputs are aging temperature, aging time and cold work. Tensile strength, yield strength and elongation are taken as outputs. The correlation between the input and output variables are established. These correlation forms a model by using fuzzy inference system and these models serve as objective function for optimization using genetic algorithm. Table 1 gives the complete data for the process.

| Input/Output | 2XXX Series | 6XXX Series | 7XXX Series |
|--------------|-------------|-------------|-------------|
|              | Min. | Max. | Average | Std. Dev. | Min. | Max. | Average | Std. Dev. | Min. | Max. | Average | Std. Dev. |
| Si (wt%)     | 0.18 | 0.90 | 0.493   | 0.2733     | 0.40 | 1.40 | 0.783   | 0.3416     | 0.1  | 0.4  | 0.261   | 0.1375   |
| Cu (wt%)     | 2.30 | 6.30 | 4.695   | 1.1872     | 0.10 | 1.0  | 0.288   | 0.2561     | 0.1  | 2.3  | 1.509   | 0.7216   |
| Mg (wt%)     | 0.0  | 1.60 | 0.844   | 0.6977     | 0.50 | 1.10 | 0.743   | 0.1909     | 2.3  | 2.8  | 2.518   | 0.1945   |
| Zn (wt%)     | 0.10 | 0.30 | 0.212   | 0.0756     | 0.05 | 0.25 | 0.180   | 0.0812     | 4.0  | 6.8  | 5.709   | 0.9385   |
| Other (wt%)  | 0.70 | 3.30 | 1.626   | 0.9249     | 0.20 | 1.90 | 1.010   | 0.4951     | 0.262 | 1.3  | 0.836   | 0.4405   |
| Aging Temp. (°C) | 24  | 240 | 122.95  | 83.239     | 24  | 205 | 120.133 | 74.021     | 120 | 170 | 139.090 | 18.850   |
| Aging Time (hr) | 6   | 72  | 37.5    | 28.661     | 1   | 72  | 31.333 | 31.148     | 22  | 72  | 49.454  | 24.703   |
| Cold Work (Y/N) | 0 | 1 | 0.500 | 0.4899 | 0 | 1 | 0.500 | 0.3999 | 0 | 0 | 0 | 0 |
|----------------|---|---|-------|--------|---|---|-------|--------|---|---|---|---|
| Yield strength (MPa) | 186 | 450 | 328.1 | 74.473 | 90 | 379 | 226.500 | 92.2188 | 380 | 540 | 472.545 | 53.5916 |
| Tensile strength (MPa) | 345 | 485 | 427.75 | 47.381 | 152 | 400 | 280.133 | 75.3298 | 450 | 605 | 535.727 | 51.5100 |
| %Elongation | 7 | 22 | 13.75 | 4.7104 | 6 | 24 | 15.733 | 5.3162 | 11 | 14 | 12.090 | 1.1642 |

3. Computational Procedure

3.1. FIS and ANFIS
Fuzzy Inference System (FIS) concerns with fuzzy logic that deals with relative importance of precision and does not consist of clearly defined boundaries [12,17]. FIS maps a set of inputs to the outputs of the data set. It primarily consists of membership functions, linguistic if-then rules and the fuzzy implication operator. A membership function maps each point within the input space to a membership value and can be of several types where gaussian function is the most used one. Triangular, trapezoidal, gaussian, sigmoidal et cetera are few more examples. The linguistic rules are used to describe the relationship between the inputs and the outputs in an imprecise way and hence creates a system knowledge base [18]. Adaptive Neuro-Fuzzy Inference System (ANFIS) is a technique for learning from the dataset, such that it can calculate membership functions parameters in order to map the dataset and to construct a FIS. The parameters of the membership functions and the number of rules can be customized by a back propagation algorithm. The FIS forms a network structure that plots inputs and outputs through input membership functions and output membership functions. The parameters change by means of learning process and their computation is aided by a gradient vector which measures the quality of modelling the input or output data for the given set of parameters by the FIS. ANFIS can be used to train the FIS model using the training data through modifications the membership functions, next to which model validation is performed. ANFIS is always Sugeno type system [19]. In this work Fuzzy logic toolbox of Matlab is used for the modelling.

3.2. Multi-objective optimization employing GA
Genetic Algorithm (GA) is an efficient optimization tool that follows the principle of natural genetic selection. GA consists of three steps: (a) Selection of individual based on their fitness from a current population. (b) Crossover of genetic information among the individuals by using the new population in iterations of the algorithm. It stops when the generation has reached the maximum or satisfactory fitness level. (c) Mutation occurs at last which is basically a small change in the last generation as deemed necessary [13]. Multi objective GA follows the concept of Pareto optimality and represents the optimized solution in the form of Pareto front which presents the best compromised solution to any conflicting set of objective data sets. In order to perform such operation non-dominated sorting genetic algorithm (NSGA-II) code has been used [20]. During the multi-objective optimization, the number of chromosomes in the population and the number of generations are considered as 100. The crossover and mutation probabilities are 0.95 and 0.05 respectively.
4. Results and discussions

4.1. Rule Base

Fuzzy rules in a fuzzy set are if-then statements that provide conditional factors of fuzzy logic. The fuzzy rules assume: if x is A and y is B then z is C. Here the fuzzy rules used for Yield Strength (YS) are shown in Table 2, Table 3 and Table 4. It may be noted here that fuzzy C means clustering method is employed to develop fuzzy clusters of the data for each variable. Later, the fuzzy clusters represented by their membership functions were customized by naming them ‘Low’, ‘Medium’, ‘High’, ‘Low-Medium’ and ‘High-Medium’ as per their values. Table 2 and Table 4 show that there are 5 rules for YS of 2XXX and 7XXX aluminium alloys series respectively while Table 3 suggests 7 rules for YS of 6XXX series. It has been observed that with increase in number of rules the optimized solution has improved. Number of rules for Ultimate Tensile Strength (UTS) for 2XXX, 6XXX and 7XXX aluminium alloy series are 5, 7 and 5 respectively. For percentage elongation (%Elongation), number of rules for 2XXX and 7XXX series are 5 for each series while in the case of 6XXX series 12 rules are considered.

Table 2. Rule base for Al-Cu (2XXX series) alloys on yield strength.

| Si          | Cu    | Mg   | Zn   | Others | Aging temperature | Aging time | Cold Work | YS   |
|-------------|-------|------|------|--------|-------------------|------------|-----------|------|
| High        | Medium| High | High | High   | High              | Low        | Low       | Low  |
| Medium      | Medium| Medium| High | Medium | Low               | High       | Low       | Low-Medium |
| Low         | Medium| High | High | Low-Medium | High          | Low       | High       | Medium |
| Low         | High  | Low  | Low  | Low    | High              | Medium     | Low       | High-Medium |
| Low         | High  | Low  | Low  | Low    | High              | Medium     | Low       | High-Medium |

Table 3. Rule base for Al-Mg-Si (6XXX series) alloys on yield strength.

| Si           | Cu       | Mg     | Zn     | Others    | Aging temperature | Aging time | Cold work | YS           |
|--------------|----------|--------|--------|-----------|-------------------|------------|-----------|--------------|
| Low-Medium   | Low      | Low    | Medium | Low-Medium | High              | Low        | Low       | Medium       |
| Medium       | Medium   | Low    | High   | Medium   | High              | Low        | Low       | High-Medium 1 |
| Medium       | Medium   | Low    | High   | Medium   | Low               | High       | Low       | High-Medium 2 |
| Low          | Low-Medium| Low-Medium | Low   | Low      | Low               | High       | Low       | High         |
| Low-Medium   | Low      | Medium | Medium | Low-Medium | Medium           | Low        | High       | Low          |
| High         | High     | High   | High   | High     | High              | High       | Low       | Low-Medium 1 |
| High         | High     | High   | High   | High     | Low               | Low        | Low       | Low-Medium 2 |
Table 4. Rule base for Al-Zn-Mg (7XXX series) alloys on yield strength.

| Si       | Cu      | Mg       | Zn       | Others | Aging temperature | Aging time | YS     |
|----------|---------|----------|----------|--------|-------------------|------------|--------|
| Low      | Medium  | Low      | Medium   | Low    | Medium            | High       | Low    |
| High     | High    | High-Medium| High    | High   | Low               | Low        | Low-Medium|
| Medium   | Low     | High     | Low      | Medium | Low               | Low        | Medium |
| High     | Medium  | Medium   | Medium   | High   | High              | High       | High-Medium|
| Low      | Medium  | Low      | Medium   | Low    | Medium            | Low        | High   |

4.2. Plots for Prediction
The prediction plots for each aluminium alloy series naming 2XXX, 6XXX and 7XXX series for each output traits are obtained using ANFIS. Three different prediction models for Tensile Strength (UTS), Yield Strength (YS) and %Elongation are obtained for each of the alloys. Prediction plots are obtained by loading the database into the ANFIS, training of the loaded data under specified number of rules and then testing of the trained data. The plots are created against training data. figure 1 showing the prediction plot for 2XXX series containing 8 input parameters and 5 rules with YS as output parameter. figure 2 representing 6XXX series having 8 input parameters and 7 rules with YS as output parameter. and lastly, figure 3 showing 7XXX series having 7 input parameters due to the absence of Cold Work as a parameter and 5 rules with YS as output parameter. Here YS suggests Yield Strength. Similarly plots for UTS and %Elongation are also done. The plots suggest the amount of error in the model. For example, the mean square error for Al-Cu alloy model with YS as output is calculated as 0.33 by the software, which is within limit as evident by the plot.

Figure 1. Prediction of YS of 2XXX aluminium alloys series by ANFIS.
Figure 2. Prediction of YS of 6XXX aluminium alloys series by ANFIS.

Figure 3. Prediction of YS of 7XXX aluminium alloys series by ANFIS.

4.3. Pareto Front
The Pareto front obtained from optimization using multi-objective genetic algorithm is listed in figure 4, figure 5 and figure 6. The plots are plotted against YS representing Yield Strength, UTS representing Ultimate Tensile Strength and %Elongation for ambient/room temperature for 2XXX, 6XXX and 7XXX aluminium alloy series. The Pareto front follows the fundamentals of Pareto optimality and shows of the set of all Pareto efficient allocation graphically. Here, the UTS and YS are conflicting properties against %Elongation. These properties taken as output parameters acted as multi-objectives when optimization has taken place.
Figure 4. Pareto front for 2XXX series Al alloys.

Figure 5. Pareto front for 6XXX series Al alloys.

Figure 6. Pareto front for 7XXX series Al alloys.
4.4. Solutions
One hundred non-dominated optimum solutions (Pareto solutions) are generated for three aluminium alloy series (2XXX, 6XXX, and 7XXX) through the multi-objective optimization. Table 5 represents the maximum and minimum values of the design variables (inputs) of all the solutions. The solution table shows the minimum and maximum values of the input parameters. The solution maps the compositions of the alloys along with aging temperature, aging time and cold work. The table shows that among the major four elements, in case of 2XXX series alloys Cu and Mg has been most important along with some amount of Si. Si, Mg and Cu are also important for 6XXX series alloys. For 7XXX series alloy only Zn and Mg are found to be important. For this alloy series the amount of those two elements are also found to almost same for all non-dominated solutions. The elements other than the major four elements also have their contributions, particularly to the 6XXX and 7XXX alloys.

Table 5. Solution table for all three series showing the minimum and maximum values for each entity in room temperature.

| Input/Output | 2XXX Series | 6XXX Series | 7XXX Series |
|--------------|-------------|-------------|-------------|
|              | Maximum     | Minimum     | Maximum     | Minimum     | Maximum     | Minimum     |
| Si (wt%)     | 0.1953      | 0.0034      | 0.9731      | 0.4004      | 0.3175      | 0.3063      |
| Cu (wt%)     | 6.2999      | 0.0015      | 0.6747      | 0.3386      | 0.1137      | 0.1000      |
| Mg (wt%)     | 1.5999      | 0.0065      | 0.7909      | 0.7810      | 2.8000      | 2.7999      |
| Zn (wt%)     | 0.3000      | 0.000024    | 0.0501      | 0.0500      | 4.000023    | 4           |
| Other (wt%)  | 0.7022      | 0.0005      | 0.9992      | 0.2971      | 1.2999      | 1.2683      |
| Aging Temp. (°C) | 226.9350    | 7.3690      | 139.5910    | 39.2051     | 136.1871    | 135.3371    |
| Aging Time (hr) | 71.999      | 0.0010      | 49.9999     | 27.9815     | 72          | 71.9999     |
| Cold Work (Y/N) | 1           | 0           | 1           | 0           | 1           | 0           |

5. Conclusion
The experiment deals with designing of aluminium alloys of three different series (2XXX, 6XXX, and 7XXX) under room temperature using computational methods. It can be concluded that:

The FIS models generated through ANFIS can be used as objective function for performing optimization using genetic algorithm.
The Pareto front generated through GA shows the trend for YS, UTS and %Elongation for different alloy series that showcase the preferability of different alloying elements.
The preferred alloy series can be varied along with constrains in the application process.
The results provide us with future experimental scope for developing the alloys and experimenting under various temperature regimes.
6. References

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