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Intelligent design optimization of age-hardenable Al alloys

Swati Dey[a], Nashrin Sultana[a], Partha Dey[b], Susanta Kumar Pradhan[a,c], Shubhabrata Datta[d,*]

[a] Indian Institute of Engineering Science and Technology, Shibpur, Howrah 711103, India
[b] Academy of Technology, Hooghly 712121, India
[c] National Institute of Technology Sikkim, South Sikkim 737139, India
[d] SRM Institute of Science and Technology, Kattankulathur, Kanchipuram Dist 603203, India

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ABSTRACT

Softening at elevated temperatures is known to be a serious problem in aluminium alloys which restricts its wide span of application. Existing database on age-hardenable aluminium alloys (2XXX, 6XXX and 7XXX) is utilized in consolidation to design Al alloy with superior performance measured in terms of the mechanical properties, viz. yield strength, ultimate tensile strength and %Elongation, at different temperature regimes. Data on all three alloy groups are merged to a single database for developing the data-driven rough-fuzzy model, to utilize the effect of all possible precipitations and achieve stability of microstructure at elevated temperatures, without significantly compromising the ductility. The database consists of fifteen compositional and processing variables as the input variables, and three mechanical properties as the outputs. Rough-fuzzy approach is employed for modelling the complex alloy system due to its capability to bring out the most significant variables (removing redundant ones), and to formulate if-then rules to explain the system by adding a fuzzy element to it. This makes the model transparent also. The problem with conflicting objectives of increasing strength as well as ductility, is solved through multi-objective optimization using genetic algorithm to design alloys. The alloy is designed from the Pareto solutions and when developed experimentally shows promising results for further exploration.

1. Introduction

The age-hardenable aluminium alloys, i.e. 2XXX (Al-Cu), 6XXX (Al-Mg-Si) and 7XXX (Al-Zn) series of alloys, have higher strength and toughness due to precipitation strengthening. For an alloy to be age-hardenable, it should show a sloping solvus where solid solubility of one or more of the alloying elements decreases with decreasing temperature— a condition that puts a restriction on the number of these alloys [1]. Hardness of the age-hardenable alloys can be increased even up to 40 times in comparison to pure aluminium by proper alloying and heat treatment, thus making this the principal strengthening mechanism in case of Al alloy systems. Attempts to improve the properties of alloys within the above three series are restricted to minor additions [2–4], or to thermal [5,6] or thermo-mechanical processing [7,8]. The motivation of the present research lies in the notion that if the effect of the precipitates from all the three series could be simultaneously included, crossing the barrier that differentiates these individual series, then possibly the performance of alloy could be made better through the complementary effects of the different precipitations. Instead of the experimental trial and error, in this work the data generated from experiments is used to design and thereafter develop alloys having good strength-ductility combination. To search for alloys with desired properties, experimental trial and error, when implemented, is a time and cost intensive process with no warranted results. Computational designing of the alloy prior to experimental validation leads to lesser number of trials and increases the possibility of success manifold. Among the computational approaches design informatics [9] and design optimization [10] can be utilized together for designing complex multi-variate alloy systems. Soft computing based materials design, using tools like artificial neural network (ANN), fuzzy logic and genetic algorithm, has been successfully implemented previously [10–12]. In case of Al alloys these tools are applied successfully by several authors [13–15], including the present authors [16–18].

Rough set analyses (RSA) is a soft computing tool having certain advantages over other data-driven modeling techniques, e.g. ANN, for finding the significant variables (in the form of a 'reduct') from a high dimensional data and generating relationship between the variables in the form of if-then rules [19,20]. The formation of if-then rule can be utilized to extract useful knowledge from the data in a perceptible form, and makes the model transparent, compared to most of the other empirical modeling techniques. This entails a trade-off with accuracy, where useful knowledge in the form of if-then rules replaces complex

* Corresponding author.
E-mail address: shubhabrata.p@ktr.srmuniv.ac.in (S. Datta).

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functional dependencies. Thus, the present modelling paradigm focuses more on transparency and interpretability, rather than trying to be highly accurate but not revealing a grain of knowledge. The technique has been applied successfully in the field of materials engineering [21,22]. In the present work, the database of all three series is created from standard sources, consisting of compositional and processing variables as the input parameters and mechanical properties (yield strength, ultimate tensile strength and %Elongation) as the output variables. The data of the three series is used in combination to form rough-fuzzy rules and search for a superior alloy. The cuts generated from rough set analysis discretizes the variables in a crisp manner. But such crisp discretization rarely occurs in real life scenario. Fuzzy logic has the capacity to make set boundaries soft and make it more like human reasoning. The inconsistency of rough set can thus be resolved using the concept of rough-fuzzy hybridization, where rules generated in the RSA is used to generate a fuzzy inference system (FIS) [10,11]. Thereafter the conflicting multi-objective problem of designing an alloy with superior strength-ductility combination is solved using genetic algorithm (GA) [23,24]. The FIS thus generated is used as the objective function in GA for the simultaneous optimization of strength and ductility of the Al alloy. Such methodologies have been applied successfully for the design of complex materials systems [25–27] with encouraging results. The Pareto non-dominated solutions, generated through multi-objective optimization, provide valuable information regarding the alloy system and clue for designing the alloy for experimentation. A similar approach has been applied in the design of Al alloys for cryogenic applications and has been reported previously [28]. In the present work, the alloys for ambient and high temperature regimes are designed using this hybrid approach using rough-fuzzy-GA in tandem. The designed alloy is experimentally developed, which provides promising results for future investigation.

2. Database

A database consisting of 259 data objects is generated from standard source [29] for the three series of age-hardenable aluminium alloys. The input variables consist of chemical composition and processing parameters and output variables comprise the three mechanical properties, viz. yield strength (YS), ultimate tensile strength (UTS) and % Elongation (%El). The data is first searched for significant variables using rough set analysis. Further, rough-fuzzy hybrid models are generated, that serve as objective functions for the optimization study. Separate models are developed for the two cases where the testing temperature is kept as the room temperature in one case, and considerably higher than the room temperature in the other. The list of input and output variables along with their ranges, mean values and standard deviations in case of the two different temperature ranges are presented in Table 1.

3. Computational itineraries

3.1. Modeling using rough set

Rough Set Theory is a relatively new concept in Information Science proposed by Zdzisław Pawlak in 1982 [30]. It is essentially an extension of the classical Set Theory, allowing an element to 'possibly belong' to a certain set, in addition to the well-known faculties of belonging or not-belonging to it. A data set or an information system may be represented in the form of a table, with each row representing an observation or, more formally an object. Each of the corresponding columns denote a variable or an attribute, whose values for each object comprise the entire information. Usually there are several independent variables or conditional attributes, on which the value of the decision attribute depends. The information system used in the present problem may be represented in the form of a table illustrated in Fig. 1.

Rough set theory can be used to achieve the following objectives [31]—

- reduction of data sets and discretization;
- finding hidden data patterns;
- generation of decision rules.

Rough set analysis is carried out in the present investigation considering the data in the two temperature regimes separately. The conditional attributes are categorized with the help of cuts, which define boundaries of the distinct categories into which each attribute is discretized. The essence of the MD-Heuristic algorithm [32] is adopted in dynamic discreduction [22] of the variables, which considers repeated samples from the data to discretization of the attributes as well as the reduct. A code in Visual C++ has been developed that implements the above algorithm and applies it to the present problem. According to the sharp cuts from rough set analysis, variables are assigned a low category if its value falls just below the cut, and a high value if it falls just above it. Such crisp distinction does not corroborate to a real life scenario, where quality is observed to change gradually with quantity. To resolve the inconsistency, the positions of the obtained cuts are fuzzified by considering Gaussian membership functions. With the fuzzy categories thus obtained, if-then rules are formed, which build up a Fuzzy Inference System.

3.2. Fuzzy inference system

Fuzzy logic and fuzzy set theory deal with the relative importance of precision, propounded by Lotfi A. Zadeh in his seminal paper [33]. Fuzzy logic is a fascinating area of research as it opens the arena for a tradeoff between significance and precision. A fuzzy set does not have a crisp or clearly defined boundary. Any element within the set has a degree of membership, which is mapped in the variable space between 0 and 1 by a membership function. Formally, a fuzzy set is a set of ordered pair $B = \{(x, \mu_B(x))|x \in X\}$, where X is a universal set and $\mu_B(x)$ is the grade of membership of object x in B. The membership functions can be triangular, trapezoidal or may have a Gaussian distribution. In the present work Gaussian membership function has been used, as it characterizes the normal distribution followed by majority of the random variables. The Gaussian membership function is defined in Eq. (1).

$$y = f(x, \sigma, c) = e^{-\frac{(x-c)^2}{2\sigma^2}} \quad (1)$$

where c is the mean and σ is standard deviation.

Here fuzzy if-then rules are generated from the database through RSA.

A fuzzy inference system (FIS) consists of the fuzzifier, the inference engine (where the fuzzy knowledge base is embedded in the form of fuzzy rules), and the defuzzifier [34–36]. A schematic diagram is shown in Fig. 2.

3.3. Rough-Fuzzy hybridization

The process of crisp discretization in RSA generates a set of values or 'cuts' on the variables or attributes. The intervals between the adjacent values of the cuts develop the discrete groups for the attributes. However, the methodology adopted by RSA makes these positions of cuts very sensitive to the classification accuracy. To avoid this problem and make classes or sets more practical from the standpoint of design of the alloy system, we use the concept like the fuzzy discretization as proposed by Roy and Pal [37], which uses the cuts obtained from rough set and transforms them to a fuzzy discretized decision table. While they used a trapezoidal function for the fuzzy memberships, we here use Gaussian membership functions defined in the previous section and using the if-then rules from rough set analysis, Mamdani FIS is implemented.