Designing Fe-based high entropy alloy – a machine learning approach

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Abstract. High Entropy Alloys (HEAs) are constituted by at least five elements and can even increase to seven or eight different elements. Due to high entropy of mixing, the solid solutions of so many elements become stable and the tendency to form intermetallic compounds decrease. As a result, it is possible to develop alloys with high strength and high hardness using this approach. Changing the composition of such alloys, the mechanical properties of the alloy can be varied widely. In this work HEAs with high toughness are designed computationally using machine learning and artificial intelligence approaches. With so much potential in this new breed of alloys, iron-based alloys (having high iron content) is designed in the present work to reduce the cost of the alloy. Here we have used supervised machine learning technique to map the relation between composition and properties of HEA. Multi-objective optimization is employed to search suitable composition for Fe-based HEA having increased strength and ductility, which will lead to improved toughness of the alloy.

1. Introduction

High Entropy Alloys (HEAs) are a new breed of alloys that are much different than conventional alloys presently used. Their composition, number of constituting elements, formation process, characteristics (like yield strength, elongation, hardness, etc.) are much different than normal alloys. Moreover, since they are composed of 5 to 8 elements, which do not form intermetallic compounds and remain in stable solid solution due to their high entropy configuration, they can be easily varied in composition and concentration to obtain an alloy with the desired needs [1]. An alloy may have high hardness as well as good ductility, or, high ductility with high yield strength owing to its multiphase design structure [1-5]. The combinations are limitless, and this is attracting current researchers who are studying extensively in this field; but still only a small portion of such possibilities have been uncovered successfully [6].

Traditional lab experimentation can take up much time and resources, even more when there are so many constituents in HEAs. But with the advent of virtual simulations in different fields of study, artificial intelligence has successfully replaced most of the live experiments. Now proper results can be achieved in a short time through such methods, which can be even fine-tuned through optimization techniques [7-9]. Different types of computational procedures or algorithms are applied in different studies depending on the raw data, process objectives, and the end results; and based on these, effort and time spent for further lab analysis can be significantly reduced. Computational designs are the
formation of different algorithms and methods for various concerned problems [10-13]. Some methods like approximation algorithms can be used to compute large simulations, requiring fewer interactions to evaluate at any point [14]. Heuristic algorithms provide faster and efficient ways to solve a problem, but lack in accuracy, precision or optimality [15, 16]. Many such algorithms have been introduced and are used substantially in many interdisciplinary fields achieving outstanding results.

In this paper we have worked towards producing a mathematical model which can successfully arrange each composition element, in definite concentrations, ultimately defining the desired characteristics of yield strength, hardness, etc. We have formed a few such combinations while keeping high ductility as the common goal in all. In this type of study we have can follow some approaches, like a scientific approach, and a data driven approach. A scientific approach can deduce the model successfully for a smaller number of elements by applying the logic behind formulations and derivations to obtain the end model. But a data-driven approach or a statistical approach uses pre-recorded data and trends to fabricate the logic behind characteristics’ dependencies on element mixing entropies and features of each constituent [17, 18]. We have utilized Artificial Neural Network (ANN) to study these data virtually and map the relationship between inputs and outputs. The developed predictive models for the mechanical properties of the alloys are used as objective functions for multi-objective optimization using Genetic Algorithm (GA). In the present work alloys having a minimum 30% Fe content with optimum combination of mechanical properties are designed.

2. Database
A database is formed by observing numerous papers and about 600 HEAs are recorded, each with different compositions and different properties [19-41]. This gave an insight on the behavior of each element and their contributions to the end characteristics. From these observations a total of 13 elements, or input variables are chosen. The output variables or desired characteristics are taken as yield strength (YS), hardness (H), Young’s modulus (E) and %elongation (%El). The detail about the database is described in Table 1. This data set is used to develop the ANN models for the properties. These models correlate the input and output variables. For different output properties, each respective ANN model is developed which are used as objective functions for the multi-objective optimization later.

| Variables          | Minimum | Maximum | Average |
|--------------------|---------|---------|---------|
| **Inputs**         |         |         |         |
| Al (wt%)           | 0       | 42.85   | 14.3783 |
| Co (wt%)           | 0       | 33.30   | 16.5776 |
| Cr (wt%)           | 0       | 25.00   | 16.5156 |
| Cu (wt%)           | 0       | 25.00   | 8.1715  |
| Fe (wt%)           | 0       | 34.88   | 19.3299 |
| Mo (wt%)           | 0       | 20.00   | 0.2758  |
| Mn (wt%)           | 0       | 33.30   | 2.8721  |
| Ni (wt%)           | 0       | 38.46   | 18.3473 |
| Ti (wt%)           | 0       | 26.67   | 1.9395  |
| V (wt%)            | 0       | 26.60   | 1.1907  |
| Si (wt%)           | 0       | 16.67   | 0.3815  |
| **Outputs**        |         |         |         |
| Young’s Modulus (GPa) | 136     | 230     | 186.90  |
| Hardness (HV)      | 105     | 1050    | 464.38  |
| Elongation (%)     | 0.24    | 77.80   | 23.0692 |
| Yield Strength (MPa) | 100     | 2877   | 954.63  |
3. Computational Methods

3.1. Artificial Neural Network (ANN) Modeling

ANN models are computer-based programs that are inspired by the human neural system. ANN studies the patterns and relationships in the input data and trains itself from experience. It is formed of a network of nodes, also called neuron; and each of these nodes are internally connected with weighted links arranged in layers [7, 8]. The weights are adjusted by the model itself as its training progresses. In this work we have used a feed forward multi-layered perceptron structure and this is trained with scale conjugate gradient back propagation algorithm. This algorithm contains several hidden layers each containing the nodes. The inputs pass through these layers as the different weights are multiplied with the inputs. This gives different outputs which are compared with preset preferred values, and the remaining errors are fed back into the model according to which the weights are adjusted to match the values as desired. This process repeats itself as the program continues to minimize the error and train itself [9, 10, 11].

3.2. Genetic algorithm based multi-objective optimization

Genetic algorithms are adaptive heuristic algorithms that are based on the idea of natural selection in genetics study. They are used in optimization techniques to generate high quality solutions towards the given search-space [13]. It simulates the process of natural selection, or, ‘survival of the fittest’ among the chosen inputs; and then continues the process with only those values which can adapt according to the simulation. Initially the population or values are computed arbitrarily. But then the fitness is defined and it selects the parents from the initial population. The second generation of population created by the parents are crossed over and mutation occurs. This finally determines the fittest population. These steps are repeated until the best individuals are obtained. In the case of multiple objectives, a negotiation is made between the best solutions for each case and those solutions, all of which can be considered optimum solution, are chosen as the final result. These values form a Pareto set, which can be plotted as a scatter graph to form a Pareto front [11, 18]. This graph shows all the optimum solutions for the multiple objectives selected.

4. Results and Discussions

Several multi-layer perceptron ANN models are developed using single hidden layer. The number of neurons were varied to find best models for mapping the correlations between the variables for all three properties. A couple of representative scatter-plots showing the predictions made by the ANN models are given in figure 1. It may be noted here that the database was generated from different sources, and in such cases the amount of noise in the data was expectedly quite high. In such situations the predictions made by the trained ANN models are acceptable.

The ANN models for Young’s modulus (E), hardness (H), yield strength (YS) and %elongation (%El) are used as objective functions for multi-objective optimization. The properties related to strength, viz. E, H and YS, are placed separately with ductility (%El) as objective functions for three different bi-objective optimizations. In each case one strength component with ductility is optimized for their expected conflicting nature for maximizing both the properties. The Pareto fronts generated due to the optimization are given as figure 2. As mentioned before, the Fe content of the alloys being designed through this process is restricted to 30 wt%, whereas the other alloying elements are allowed to be varied within the limits of the elements present in the database from which the ANN models are generated, as mentioned in table 1. The only constraint employed for the optimization process was that the summation of the weight percentages of the elements to be 100. The results show that the designed alloys could achieve quite high strength/hardness/modulus, but the ductility is quite low, less than 10% for all cases of optimization. This clearly shows that the presence of Fe to this extent (30%) will reduce the ductility and thus toughness of the alloy. But for alloys with such high strength, low
ductility is expected. The Fe content may be varied in future designs to find the optimum Fe content for achieving adequate ductility of the alloy.

Figure 1. Scatter plots showing the predictions of selected ANN models for (a) Young’s modulus and (b) Hardness.
Figure 2. Pareto fronts generated from the multi-objective optimization of (a) Young’s modulus and %elongation, (b) hardness and %elongation and (c) yield strength and %elongation.

The range of elements selected in all the non-dominated solutions for all three multi-objective optimizations are given in Table 2. It shows that for simultaneous optimization of E and %El, the preferred major elements in the alloy, other than Fe, are Mn, Mo, Co, Ni and Ti. A few more elements are also present with low amount. In case of improving H along with %El, the major elements are Mo, Cr, Co, Ni and Ti, and Fe of course. For the third and final optimization process, where Ys and %El have been optimized, the elements are found to be Fe, Ni, Cu, Si and Nb, with some amount of C. This shows that for achieving better combination of properties, the elements preferred are different for different combinations.

| Elements (wt%) | E and %El | H and %El | YS and %El |
|---------------|-----------|-----------|-------------|
| Al            | 1.96      | 1.96      | 0.01-0.02   |
| C             | 0.01      | 0         | 2.62-9.59   |
| Co            | 2.57-11.31| 9.97-10.69| 0.01        |
| Cr            | 2.00-2.03 | 11.49-12.45| 0.01       |
| Cu            | 2.56-4.80 | 2.56      | 11.27-12.18|
| Fe            | 34.87     | 30.00     | 30.00       |
| Mo            | 11.68-14.92| 12.78-14.99| 0.37-2.82  |
| Mn            | 14.89-21.02| 2.40      | 0.01-0.02   |
| Ni            | 5.99-6.09 | 8.34-10.08| 23.12-29.93|
| Ti            | 5.79-6.59 | 7.11-10.11| 0.01-0.96   |
| V             | 3.50      | 3.50      | 0.01        |
| Nb            | 0         | 1.96      | 7.18-8.60   |
| Si            | 3.84      | 3.84      | 15.58-16.65 |

5. Conclusion
The results achieved can push us to deduce certain conclusions:
 i. ANN models can be used successfully as objective functions.
 ii. The Pareto fronts show that for high Fe content the ductility of the alloy could not be much high (<10%).
 iii. The alloying elements preferred for the different alloys designed in the process differed from case to case, depending on the combination of conflicting mechanical properties considered for the optimization.

6. References
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