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(RESEARCH ARTICLE)

Prediction model for hardness and tensile strength of graphene reinforced AZ 61 alloy based composite using Metaheuristic Algorithm

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Abstract

It is possible to produce improved material performance through the utilization of computational intelligence approaches such as genetic algorithms optimization technique which are discussed in this paper. The optimization of processes and the development of models that are driven by data are the key uses of these technologies. This article offers a comprehensive introduction of the topic of materials and discusses the ways in which computational intelligence techniques might be utilized to develop new materials. The present study envisages the development of data driven model that enables to derive desirable properties of the said composite; so, in order to secure the optimized subset of requirements (process parameters), a metaheuristic optimization tool is employed. We invoke the use of the Genetic Algorithm (GA) optimizing tool in association with linear regression, so as to achieve the best combination of hardness and tensile strength of AZ61 graphene nanoplate (GNP) composite.

Keywords: Materials design; Optimization; Genetic algorithm

1. Introduction

Within the context of the new product development cycle, it is essential to create a limited number of functional prototypes or models in order to facilitate the rapid decision-making process regarding the production process, the verification of the product's marketability, and the ongoing evolution of the product through design iterations [1-3]. Methods of rapid prototyping (RP) were applied extensively in the past in order to accomplish these requirements. Fast prototyping techniques are currently being considered by manufacturers as a potential alternative to rapid tooling (RT) processes [4]. Developing many prototypes of a specific component that are economically viable is a situation in which this is especially true. When it comes to RT treatments, soft tooling (ST) is one of the solutions that is both the most effective and affordable [5-6].

According to Tiwari, A et al. [7], computational materials science provides a variety of resources for material creation. These instruments are made to cut down on the time and energy needed to make new materials that meet the standards of the industry. Models based on scientific data may predict how created materials will act on many different sizes of scales, from the atomic to the microstructural to the product or component level [8-11]. Many materials scientists use techniques like molecular dynamics and density functional theory to investigate materials at the atomic level. Thermodynamic principles are employed in order to model the phase transition and the resulting microstructure [12].

For the purpose of developing manufacturing processes [13-16] and materials for a variety of applications [17], the application of machine learning (ML) techniques is becoming increasingly widespread. The design of materials is yet another domain in which evolutionary algorithms have been successfully used [18-20]. Multiple attempts have been made to establish a link between the mechanical properties of titanium alloys, phase transition, and microstructure

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through the application of machine learning techniques [21-22]. ML approaches were utilized in order to enhance the mechanical characteristics of titanium alloy for the purpose of the additive manufacturing process [23]. Although there have been some attempts to apply machine learning techniques in the creation of new titanium alloys for use in biomedical applications, these efforts have been restricted.

Table 1 Comparison of present optimization result with some previously reported strategies

Author's	Technique	Results
Amit Tiwari [Present Work]	Regression model plus Genetic Algorithm	Genetic algorithm is employed to predict the hardness and ultimate tensile strength of graphene-reinforced AZ 61 alloy-based composite.
Tarek Emam et.al. [39]	Invokes Lateral Growth Rooted Tree Optimization (LGRTO) for better performance over Rooted Tree Optimization	LGRTO eliminates the influence of the best root to direct the search pattern of other roots. Investigate how LGRTO can solve multi-objective and combinatorial problems.
Di He et.al. [40]	A hybrid optimization algorithm has been proposed to solve the presented multi-objective models.	This paper Addresses the multi-objective steady-state optimization of a complex nonlinear system in glycerol metabolism
Leyva, H, et.al. [41]	Use of metaheuristic soft computing, GA to tackle combinatorial problem	Optimization of system reliability with the goal of maximizing reliability under resource restrictions.
Pankaj Rajak et.al. [42]	The combined neural network and genetic algorithm establish the mapping model between process parameters and rolling stability	Optimal rolling condition suggested Rolling width deviation and low stability in limit specification of hot strip rolling,
P. Rajak et.al. [43]	Data-driven models constructed by feeding the MD results to an evolutionary neural network.	Two important soft computing paradigms, genetic algorithms and neural nets. Gives better Pareto front
Baidurya Bhattacharya et.al. [44]	Use of Evolutionary Neural Network evolved through a multi-objective Genetic Algorithm. .	Various interfaces in Zn coated steel are examined on the basis of two conflicting requirements of minimum deformation at a maximum absorption of shear energy.
Yu Yoshida et al. [45]	Developing Neural Network generated meta-models of objective functions required in the subsequent Pareto-optimization task using a Multi-objective Genetic Algorithm.	Successful design of a coating that can absorb maximum energy prior to failure with minimum deformation.
Katoch, S et.al [46]	Application of the evolutionary technique based on genetic algorithms for structural design is demonstrated.	Improves the structural performance and is able to reduce the total structural cost of the buildings.

Because of the significant advancements that have been made in the capabilities of the materials sector in terms of testing and characterization, an overwhelming amount of data is being produced on a global basis. The pure existence of data, on the other hand, is entirely pointless in the absence of the formation of any type of meaningful interaction. At this point in time, it is very simple to accomplish this task by utilizing sophisticated software and high-end machines [24-26]. On the other hand, there is the problem of knowledge extraction. In reality, the objective is to discover the underlying pattern that underlies the relations in the data. According to Teng Long et al. [27], the results of data mining and knowledge discovery techniques that are based on statistical or artificial intelligence technologies may have a substantial impact on the assignment. It is possible to create materials that possess the required characteristic or performance level by making use of the knowledge that was received. Incorporating this materials design strategy might be as simple as lowering the chance of failure while also saving both time and money [28]. Furthermore, the other group should strongly examine the materials informatics area's findings. This kind of finding might be made as a result of the discovery process, which would help to partially remove the constraints of models based on physics. Finding better materials in the future will depend on creating hybrid systems that combine scientific and technological models [29]. Combined approaches using various types of modeling and AI/ML should be used in domains where data is unreliable or when experimental observations are the sole source of knowledge. All of the methods combined may not be as successful as these models [30]. Additionally, they will improve the overall look of the different materials.

In order to iteratively refine a collection of solutions, evolutionary algorithms (EAs) employ principles inspired by biology and the notion of survival of the fittest. They are population-based meta heuristic optimization algorithms [32-33]. As a subtype of evolutionary algorithms (EAs), genetic algorithms (GAs) use binary strings or arrays of other elementary kinds as search space elements. Biological creatures that have evolved to thrive in dynamic, competitive environments serve as inspiration for genetic algorithms (GAs), which are search algorithms implemented in computers [34-35]. Genetic algorithms (GAs) have made tremendous strides in the past decade for optimizing process control system solutions. For efficient, precise, and dependable optimization of challenging problems, genetic algorithms (GAs) are the way to go. There has been an exponential growth in the number of applications of genetic algorithms (GAs) in response to the increasing complexity of real-time controllers [36-38].

The purpose of global optimization is to identify the global optimum, which may be thought of as the highest or least value of the goal function. In the process of solving optimization problems, one might discover parameters or designs for components or plans that are intended to be implemented by people or robots. Utilizing genetic algorithms for the purpose of optimizing process controllers is the subject of this analysis. Included in the article is a summary of genetic algorithms as well as the process by which they are optimized. At this point, a comprehensive description of the operating mechanism, algorithm, and flowchart depiction of the genetic algorithm is supplied. In the present work models for ultimate tensile strength (UTS), and hardness are developed. The models are used for improving the understanding the graphene reinforced AZ 61 alloy-based composite system, and also used as multi-objective genetic algorithm for strength optimization. The developed non-dominated Pareto solutions are analysed to find the trend of the input variables towards achieving the optimum performance. Genetic algorithm was used in Matlab 2021a platform. Within the constraint of input parameters, GA was utilized to forecast the maximum hardness and ultimate tensile strength values of the composite. Rolling temperature, number of passes and the initial thickness have been used as the variables. Genetic algorithm is employed to predict the most significant variables as well as for the validation purpose by means of the real- life experimental results. Comparison of present optimization result with some previously reported strategies are discussed in Table 1.

2. Principle of the genetic algorithm

Genetic algorithm is founded on Darwin's theory of evolution. A chromosome, a gene, the population, fitness function, breeding, mutation, and selection are all involved genetic algorithms (GAs) [7]. A population, or set of solutions represented by chromosomes, serves as the starting point for the genetic algorithm. The idea that the new population will be superior to the previous one motivates the utilization of solutions form one population to create a new population. Additionally, solutions are chosen on the basis of its capacity to produce offspring, that is, new solutions. Until a certain specified condition is met, the aforementioned procedure is repeated. The fundamental genetic algorithm (GA) is briefed below: algorithm: -

- Step 1[Begin] Create a chromosomal population at random, i.e. the appropriate answer to the issue.
- Step 2 [Fitness] Determine each chromosome's population fitness.
- Step 3 [New population] Repeat the subsequent stages until the new population is created.
  - [Selection] Choose two parent chromosomes from a population according to how well-adapted they are. Greater fitness increases the likelihood of being chosen as a parent.
  - [Crossover] The parents with a crossover probability may create new offspring, or children. If no crossover occurrs, the child is treated as the replica of the parents.
  - [Mutation] Create new mutant offspring at each locus with a mutation probability.
  - [Accepting] Add additional children to the existing population.
- Step 4 [Replace] Use the newly created population in a subsequent algorithm run.
- Step 5 [Test] Stop and run the top response from the current population if the end condition is met.
- Step 6 [Loop] Step 2 is next

The crossover and mutation have a significant impact on the performance of genetic algorithm Fig 1. depicts the block diagram for genetic algorithms (GAs). We must create the algorithm's code, fitness function, and a genetic operator in order to run an efficient and successful genetic algorithm optimization method. The population of potential solution used by the genetic algorithm is represented by chromosomes. Genes that represent encoded information are carried on each individual chromosome (solution). Typically, a variable is allocated to each gene. Genetic algorithm alters the population of solutions through iterative process. It chooses the member of the existing population to act as parents and bear the future generation's offspring at each stage. Numerous organism selection techniques exist, including roulette wheel select and tournament select. The various solution is assessed using a fitness function, and the fitter solution is the one with a higher fitness value. The global function may be the same as the fitness function.

Genetic operator is used to generate a fresh population of solutions. Crossover operator and mutation operator are the two most common genetic operators. In crossover, two chromosomes that are typically referred to as parents join together to create new chromosomes called offspring; mutation introduces random change into chromosome characteristics that helps in order to avoid convergence to a local optimum [7]. When a termination requirement is satisfied, this evolutionary process come to an end. It can be done by specifying a set of a number of iterations, a set runtime, a set fitness value, or it can be terminated when further improvement cease to take place.

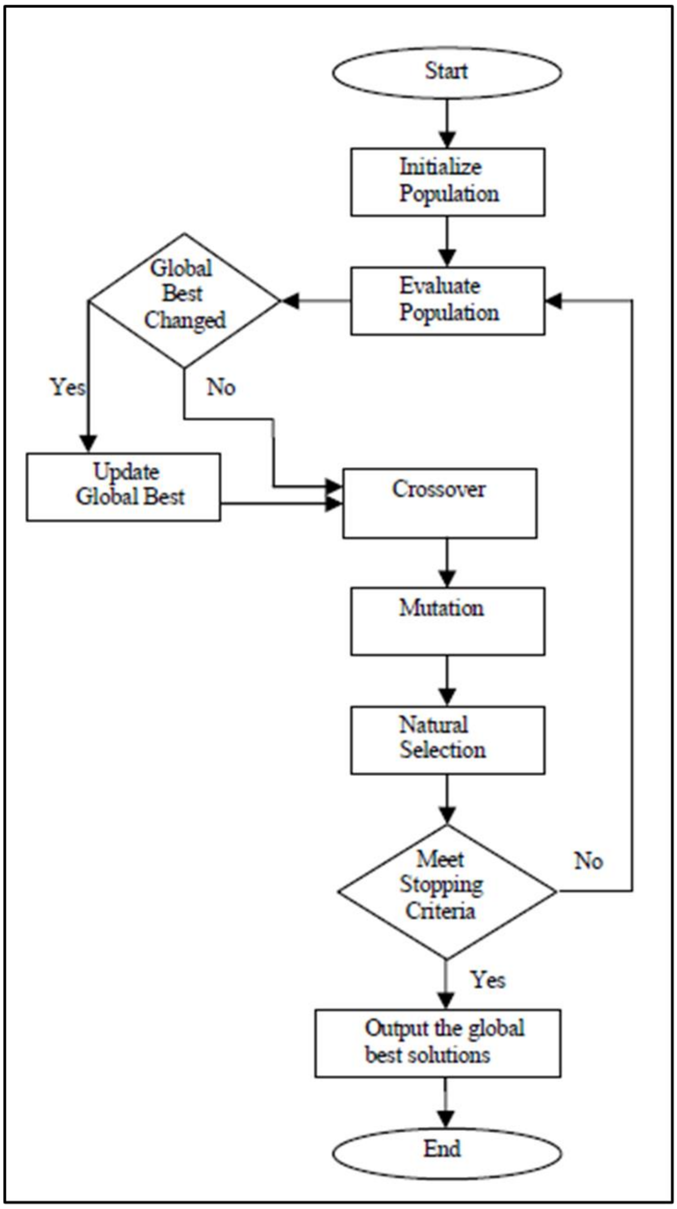

Figure 1 Flow chart of genetic algorithm

3. Optimization procedure with genetic algorithm

The goal of the study's optimization procedure is to identify the optimal input parameters that can give rise to the best possible combination of hardness value and tensile strength of graphene reinforced AZ 61 alloy-based composite. The objective functions for the cases of hardness and tensile strength are respectively defined by Eq. [1], and Eq. [2]. These functions are obtained by regression analysis carried out on the basis of experimentally determined values. The maximum hardness value and tensile strength in the input parameters were predicted by using the Matlab software 2021a version for GA tool. A conventional mathematical design with an empirical quadratic mathematical model was used to create the optimization. (Table 4); displays the predictive output of GA (predictive error 5%).

In this research, rolling process parameters have been considered as independent variables in accordance with the optimization principles, and genetic algorithm has been applied for optimization. Real coded genetic algorithm (GA) is used to optimize the input process parameters that yield the desired features. Every generation has a certain number of chromosomes that makes up the population and this number never changes. In this study, the rolling temperature(x_1), number of passes(x_2), and initial rolling stock thickness(x_3) are represented by chromosomes. The parameters ($x_1, x_2, and\ x_3$) are selected to confirm the genetic algorithm predicted best values. The identical GA prediction criteria are used for multiple runs. To access the prediction's accuracy, the obtained mean values are contrasted with the test values carried out by following the predicted process parameters.

3.1. Chromosomes representation

The variables (chromosomes) take values at random from the ranges assigned to each of the input parameters. (Table 2) describes chromosome representation for the contemplated multi-objective optimization.

Table 2 Chromosomes representation

Temperature °C	No of Passes	Thickness before rolling in (mm)
250	3.46	9.16
250	3.77	7.11
300	3.46	9.20
300	3.46	9.20
350	3.81	7.08
350	3.60	7.33

- *Evolution Process:* Due to stochastic nature of responses, the fitness values are modified by iterative process and the process continues until the desirable value is achieved. The genetic search may explore a large state space because of genetic operators including reproduction, crossover, and mutation.
- *Crossover*: The crossover operation is divided into point crossovers and uniform crossovers. A point crossover occurs when the chromosomal string of the parents is arbitrarily cut at one or more spots, whereas, uniform crossover give way to joining of gene forming chromosome to that of the kid.
- *Mutation*: To preserve the population variety, this operator introduces a new genetic material into the population. It is essentially a random change in a bit value at a specific bit location on a chromosome. For the study the optimal mutation rate is take as 0.05.
- *Reproduction operator*: The reproduction operator has been used to maintain a consistent population size while emphasizing excellent solutions and eliminating undesirable ones.

3.2. Fitness function

The genetic algorithm uses the mathematical model created by Minitab statistical software 2019 version developing the desired linear regression equation; accordingly, the derived equations are used as the fitness functions.

Hardness Value as objective function

$$y_1 = -(122.1 - 0.070 * x_1 + 3.10 * x_2 - 1.25 * x_3) \ldots\ldots\ldots\ldots\ldots \text{ Eq...(1)}$$

Tensile Strength as objective function

$$y_2 = -(-93 + 0.661 * x_1 + 33.6 * x_2 - 5.2 * x_3) \ldots\ldots\ldots\ldots \text{ Eq...(2)}$$

Here,
x_1 = Rolling temperature

x_2 = Number of passes
x_3 = Rolling initial thickness

Table 3 The Genetic Algorithm parameters selected for the current problem

Population size	200
Number of generations	600
Crossover Probability	0.95
Mutation Probability	0.05

4. Results and discussion

The GA parameters used for the present study is summarized in (Table 3). The output of GA provides the optimal process parameters which when used in practice should yield the maxima in hardness and yield strength. With the help of fitness function, it is easy to find out the values of response variables viz. hardness and strength. (Table 4). Shows the optimized process parameters and the corresponding values of hardness and tensile strength as are predicted by GA.

Table 4 GA predicted optimized input parameters for maximizing hardness and tensile strength of the composites along with the GA predicted values of response variables

Temp (°C)	Passes	Thickness before rolling in (mm)	Hardness (HV)	Tensile Strength (MPa)
250	3.46	9.16	103.41	145
250	3.77	7.11	107.41	162
300	3.46	9.20	100.23	174
300	3.46	9.20	98.64	189
350	3.81	7.08	101.08	253
350	3.60	7.33	99.71	186

The calculation of fitness value is accomplished by using GA tool box in MATLAB platform. For calculating the fitness value of each chromosome, the lower bound and upper bound have been taken as [250, 1, 6.96] and [350, 4, 10.7] respectively (Table 3). Chromosome representation in genetic algorithm optimization tool box has been selected. The objective function of hardness and tensile strength are individually used; moreover, the variables, three in number, are required to be selected and obviously, these happen to be the rolling temperature, number of passes and initial thickness. ‘Optimize best fitness’ option is selected from the said tool box. Running the program gives rise to the best fitness curve as the output and is shown Fig 2 (a) and 2 (b). three number of variables in the present case for calculated fitness value. Before run the optimization best fitness value option was selected to draw a best fitness curve in GA optimization tool box.

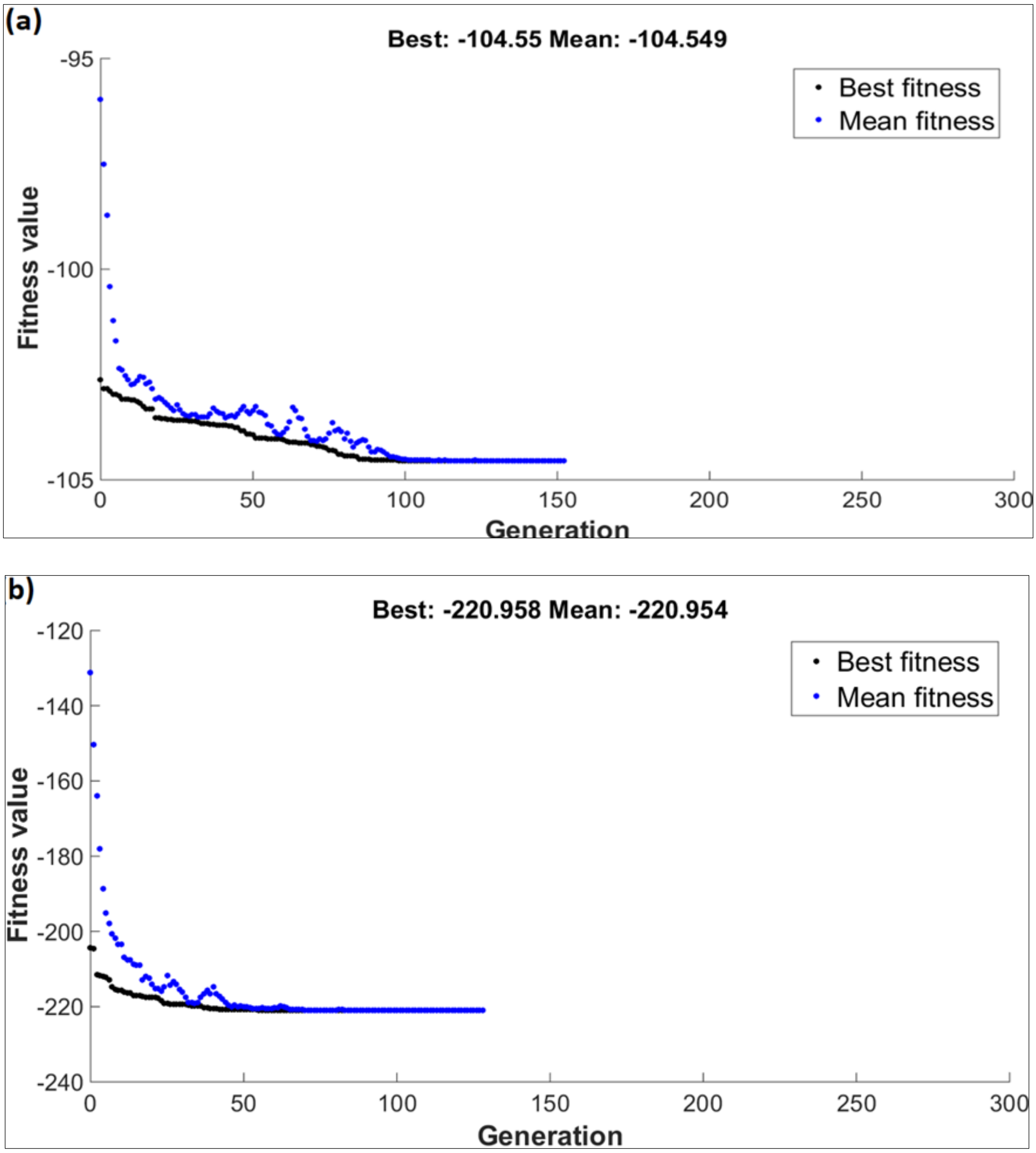

Figure 2 Fitness Curves for (a) Vickers hardness value, (b) Tensile strength value

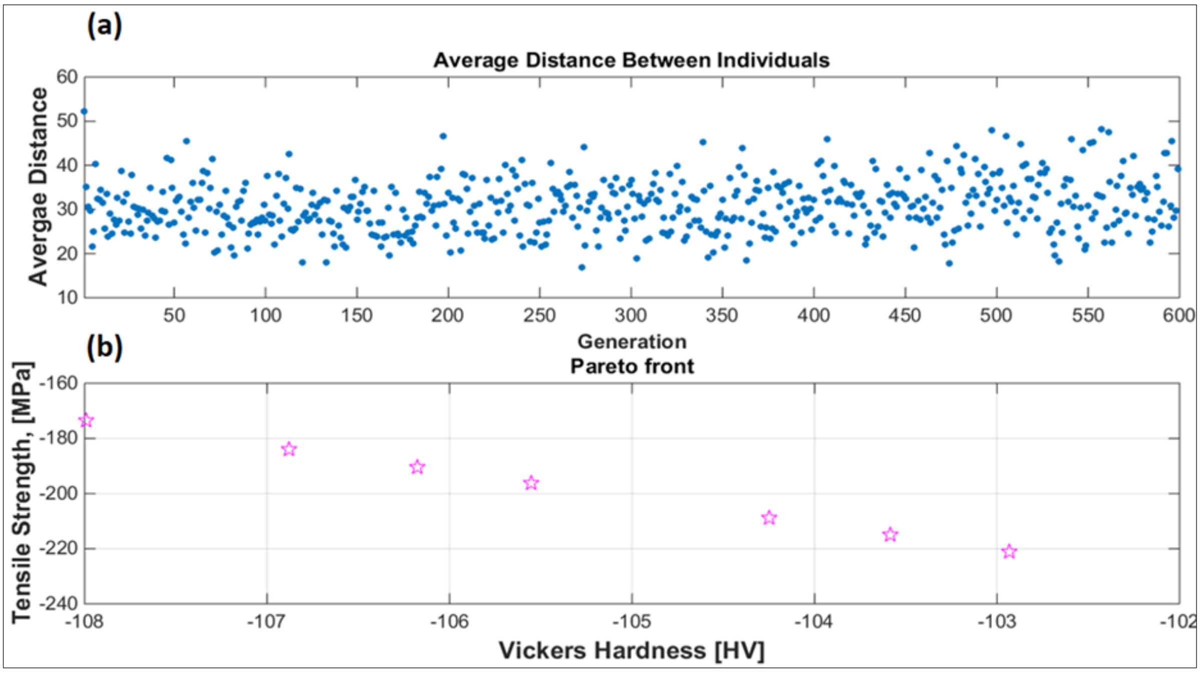

Figure 3 (a) Average distance between individuals and generation, and (b) Pareto front of predicted Vickers hardness and Tensile strength value

Fig 3(a), shows that when the maximum generation is attained during optimization, the optimal data output will be provided by the algorithm; in the present case 600 generation is found to fetch the best results. Moreover, the pareto front in Fig 3 (b) clearly demonstrates that the optimal hardness and tensile value as provided by genetic algorithm identifies with the best obtainable set of results noticed from validation when put as input parameters in the positive pareto front.

5. Conclusion

To conclude that the rolling parameters, viz. temperature of rolling, reduction percent per pass and the initial thickness of the rolling stock significantly influence the experimental hardness and tensile strength values. It is further concluded that the model proposed in the present investigation can be conveniently utilized with 95% confidence limit, for estimating the tensile strength and hardness value of AZ 61-GNP composite. Moreover, genetic algorithm is an effective tool to predict the combined strength and hardness value of the experimental composite. It is concluded that for the experimental material an inverse relationship exists between tensile strength and hardness.

Compliance with ethical standards

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Disclosure of conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The data that support the findings of this study are available from the corresponding author, upon reasonable request.

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