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The best conditions for minimizing the synthesis time of nanocomposites during high energy ball milling: Modeling and optimizing

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Abstract

The present study is an accurate estimate of the milling parameters in order to maximize the energy transferred to the synthesized nanopowders. The maximum energy represents the leading stage for minimizing the synthesis time of nanocomposites during high energy ball milling. Accordingly, 271 dataset were collected from the literature and then by a modeling algorithm called gene expression programing (GEP), a mathematical relation between the grain size and milling parameters is developed. Afterwards by an optimization algorithm called Artificial Bee Colony (ABC), the milling parameters including amount of reinforcement, type and amount of process control agent (PCA), type of mill, type of vial, type of ball, vial spinning rate, BPR, milling atmosphere and milling time were optimized in order to achieve minimum grain size. Minimizing the mean grain size is equal to maximize the energy transferred to the nanopowders during high energy ball milling. Experiments were performed at the optimized parameters to proof the validity of the analysis. Given the broad range of the parameters used, it was found that our analysis and model is fully functional to accurately estimate the optimal conditions for ball milling experiments which shows the potential application of these calculations and analysis in materials science and engineering.

Keywords: A. Milling; B. Nanocomposites; Optimization; Powders; Synthesis time

1. Introduction

In high energy ball milling, a suitable powder charge (typically, a blend of elemental) is processed in a high energy mill, along with a suitable milling media. The objective of milling is to reduce the particle size and blending of particles to produce a fine grained blend and/or new phases. The kinetics of mechanical milling or alloying depends on the energy transferred to the powder from the balls during milling. The energy transfer is affected by many parameters such as the type of balls, the ball to powder weight ratio (BPR), milling speed, size of the balls, temperature of milling and the milling time [1].

It is well known that by estimation of grain size we can predict the energy transferred to the nanopowders during various times of milling. In other words, finer grains imply that more milling energy has been available during milling [2]. Therefore, if we optimize the milling parameters, we would be able to maximize the energy transferred to the synthesized nanopowders and hence, minimize the synthesis time of nanocomposites. Accordingly, it is important to find a mathematical model to correlate the milling parameters with the mean grain size of nanostructured powders and then optimize the mentioned model. It should be noted that the aim of constructing a model is to be able to simulate the mechanical alloying process and to predict the mean grain size of nanopowders by adjusting the milling parameters appropriately and the aim of optimizing is to find an optimum milling parameters $x,y,z,\ldots$ whose mean grain size or relevant cost $f(x,y,z,.)$ is minimum.

In this paper, gene expression programming (GEP) and Artificial Bee Colony (ABC) algorithms as powerful tools, have been utilized for modeling and optimizing of mechanical alloying process, respectively.

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The basic gene expression programming (GEP) [3] algorithm was developed by Ferreria in 2001 that has the benefit of simple coding, fast convergence speed and strong problem solving ability [4–6]. Symbolic regression or function finding is one of the promising applications of the GEP. The goal of this application is to find an expression that performs well for all fitness cases within a certain error of the correct value [3]. Due to the complexity of the relationships between response variables and casual factors, prediction of the response variables based on mathematical expressions by using empirically observed values or measurements is critically important.

Inspired by the behavior of a bee colony, the Artificial Bee Colony (ABC) algorithm was proposed in 2005 by Karaboga for real-parameter optimization [7]. Despite the fact that the ABC algorithm uses less control parameters, it was found that its performance is better or similar than other algorithms such as genetic algorithm, (GA), particle swarm optimization (PSO), differential evolution (DE), and evolution strategy (ES) [8]. To the best knowledge of the authors, the ABC algorithm has not been used in materials science and engineering applications.

There are some reported work using the Gene expression programming to predict the mean grain size of nanopowders synthesized by mechanical alloying [6], however there are opportunities for improving these models considering that:

1. Several milling parameters such as type of mill, type of ball, type of vial, type and amount of PCA, amount of reinforcement and milling atmosphere affecting on mean grain size were not considered.
2. Systems under study were very limited, led to a very low number of data and therefore the obtained results do not cover a wide area.
3. The squared regression of training and testing sets was not significant. This can drastically reduce the accuracy of the model.
4. The proposed model was not evaluated in experimental conditions so that it is not clear that this model is effective in practice or not.
5. Optimizing was not performed on the milling parameters so that we finally did not have an optimal system.

In this work, for the first time, all mentioned shortcomings were addressed and resolved and as a new work in material science and especially mechanical alloying, a targeted synthesis of nanopowders was simulated, modeled and optimized. Our experimental results prove that by considering all determining parameters, the GEP and ABC are promising technique to simulate ball milling process and optimize the parameters for enhanced performance.

2. Materials and methods

2.1. Data collection

The collected data from the previous works are listed in Table 1. Mean grain size of several MA-synthesized nanomaterials has been considered as the main objective or cost function of this study for prediction by GEP model. The input parameters were consisted of the amount of reinforcement, type of mill, type of balls, type of vial, type of PCA, amount of PCA, milling type, ball to powder weight ratio and milling atmosphere with the given ranges in Table 2. Further details about the values in Table 1 have been listed in the Table 3. For example, in the Column of "Milling atmosphere", number (1) is the argon atmosphere.

2.2. Genetic programming and gene expression programming theory

Genetic programming (GP) is simply consisted of three stages called, reproduction, crossover, and mutation. The problem-independent approach in GP is inherited from the genetic algorithm proposed by Koza [93,94]. In a selection strategy, reproduction, small percentage of trees that have the worst fitness should be removed and then the remaining are the survived trees according to the accepted selection mechanism [93]. Subsequently, the crossover stage involves swamping of randomly selected parts of two trees and combining good information from the parents to develop the fitness of the next generation [94]. At last, the mutation step protects the model against premature convergence and helps developing the non-local properties of the search [94].

In GEP approach, individuals are considered as linear strings with fixed sizes, genome. The genomes will be treated later as non-linear entities with different size and shapes, expression trees (ET). The selection procedure that is guided by the fitness value, is applied to the ETs in order to generate new individuals [95]. The mathematical code of a gene is expressed in Karva language [8] such as the language of the genes and the language of the ETs. Fig. 1 demonstrates an encoded chromosome as linear string with one gene. The ET and the corresponding mathematical expression are also shown in this figure. Reading from left to the right in the top line and from top to bottom, we can see how the ET is translated to Karva language. Similar to the sequences of biological genes, this method uses coding and noncoding parts.

In this study, as seen in Fig. 2 the expression trees of GEP approach model was constructed for mean grain size (MGS) values of synthesized nanopowders. $d(0)$, $d(1)$, $d(2)$, $d(3)$, $d(4)$, $d(5)$, $d(6)$, $d(7)$, $d(8)$ and $d(9)$ in Fig. 2 represent the values for input layers, i.e. amount of PCA, amount of reinforcement, type of atmosphere, type of ball, ball to powder ratio (BPR), type of mill, milling time, type of PCA, vial spinning rate and type of vial, respectively. The number of genes were seven (Sub-ETs), and linking function was addition "+". In the training and testing of GEP model, $d(0)$, $d(1)$, $d(2)$, $d(3)$, $d(4)$, $d(5)$, $d(6)$, $d(7)$, $d(8)$ and $d(9)$ were considered as input data and MGS as independent output data. Among 271 experimental sets, 222 sets were randomly chosen as a training set for the GEP modeling and the remaining 49 sets were used as testing the generalization capacity of the proposed model.

The first step in a GEP-based formulation is to choose the fitness function. For this purpose, Eq. (1) measures the fitness,