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Optimization of process parameters to maximize hardness of metal/ceramic nanocomposites produced by high energy ball milling

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Abstract

In our previous work [Abdellahi, J. Mater. Res. 28 (2013) 3270], a novel method was used to predict the hardness of Aluminum matrix nanocomposites synthesized by high energy ball milling. In the mentioned work, however, systems under study were very limited, the squared regression of training and testing sets was not significant and optimizing was not performed on the milling parameters so that we finally had not an optimal system with a maximum value of hardness. In this work, for the first time, all mentioned shortcomings were addressed and resolved and as a new work the process parameters, namely, amount of reinforcement, amount of process control agent, type of mill, type of vial, type of ball, vial spinning rate, ball to powder weight ratio, type of process control agent, type of atmosphere, milling time, sintering time, sintering temperature and compact pressure were optimized to maximize the hardness of metal/ceramic nanocomposites produced by high energy ball milling. To evaluate the efficiency of the proposed optimization, a system based on the optimized parameters was established (system 2) and the obtained results were compared with those in system that was established based on the parameters used by Akbarpour et al. (system 1). The results showed two things: first, the use of system 2 brings a maximum value of hardness for the produced nanocomposites and second, the optimized system is really consistent with what actually happens in practice.

Keywords: A. Milling; C. Hardness; Metal/ceramic nanocomposites; Modeling; Optimization

1. Introduction

Mechanical alloying (MA) or high energy ball milling as a powder processing technique involves repeated deformation, welding and fracturing of powder particles. MA has been widely used to synthesize a variety of materials, such as supersaturated solid solutions, (non-equilibrium) intermetallic compounds, or to the formation of stable or unstable carbides, borides, nitrides, silicides, etc. [1–3]. It is well known that the addition of ceramic hard particles to metal alloys increases the strength, micro-hardness, and wear resistance during high energy ball milling [4]. But, it is essential to have an optimal milling parameters (in this study, sintering time, sintering temperature and compact pressure were also considered as milling parameters) to achieve excellent mechanical properties. Otherwise, agglomeration or inhomogeneous distribution of reinforcement can lead to lower ductility, strength, and toughness of the composites. Enhanced mechanical properties can be obtained when the milling parameters are optimal.

Accordingly, it is important to find a mathematical model to correlate the milling parameters with the hardness of metal/ceramic nano-composites and then optimizing 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 harness of metal/ceramic nano-composites by adjusting the milling parameters appropriately and the aim of optimizing is to find an optimum milling parameters x, y, z,… whose hardness or relevant cost $f(x, y, z,..)$ is maximum.

In this paper, Gene expression programming (GEP) and Artificial Bee Colony (ABC) algorithms as powerful tools

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have been utilized to modeling and optimizing of mechanical alloying process, respectively.

Ferreira developed the basic Gene expression programming (GEP) [5] algorithm in 2001, which has inherited the advantages of the traditional genetic algorithm (GA) and genetic programming (GP). It has been applied to many fields [6–9] for its simple coding, fast convergence speed and strong ability of solution problems. One important application of GEP is symbolic regression or function finding, where the goal is to find an expression (equation) that performs well for all fitness cases within a certain error of the correct value [5]. The "function finding" application of GEP can be extremely important within the pharmaceutical field. In general, the relationships between response variables and causal factors are not simple and the prediction of response variables on the basis of mathematical expressions using empirically observed values or measurements is a common and important problem to be solved.

The Artificial Bee Colony (ABC) algorithm, proposed by Karaboga in 2005 for real-parameter optimization, is a newly presented optimization algorithm which simulates the foraging behavior of a bee colony [10]. Karaboga et.al [11] compared the performance of the ABC algorithm with that of genetic algorithm (GA), particle swarm optimization (PSO), differential evolution (DE) and evolution strategy (ES) algorithms on a large categories of unconstrained test functions, and found that its performance is better than or similar to that of other algorithms although it uses less control parameters and it can be efficiently used for solving multi-modal and multi-dimensional optimization problems. ABC like ICA and BBO is a new and powerful optimization technique which has rarely been used in materials engineering [12–14].

In our previous work [9], Gene expression programming was utilized to predict the hardness of Aluminum matrix nanocomposites synthesized by mechanical alloying; however there were three flaws in the research.

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 hardness were not considered.
2. Systems under study were very limited (only Al matrix nanocomposites), 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. Optimizing was not performed on the milling parameters so that we finally had not 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, modelled and optimized. Our experimental results prove that by considering all determining parameters, the GEP and ABC are promising techniques 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 [15–33] are listed in Table 1. The hardness of several MA-synthesized nano-composites has been considered as the main objective or cost function of this study for prediction by a GEP model. The input parameters were consisted of the amount of reinforcement, amount of PCA, type of mill, type of vial, type of ball, vial spinning rate, BPR, type of PCA, type of atmosphere, milling time, sintering time, sintering temperature and compact pressure with the given ranges in Table 2. Further details about the values presented in Table 1 have been listed in the Table 3. For example, in the column of "type of atmosphere", number (1) is the argon atmosphere.

2.2. Genetic programming and gene expression programming theory

Genetic programming (GP) is proposed by Koza [34]. It is a generalization of genetic algorithms (GAs) [35]. The most general form of a solution to a computer-modelled problem is a computer program. GP takes cognizance of this and endeavors to use computer programs as its data representation.

In GEP, individuals are encoded as linear strings of fixed size (genome), which are expressed later as non-linear entities with different size and shapes. These entities are known as expression trees (ETs). Usually, these individuals are composed by only one chromosome, which, in turn, can have one or more genes, divided in head and tail parts. ETs are the expression of a chromosome, and they undergo the selection procedure, guided by their fitness value, so as to generate new individuals. During reproduction, the chromosomes, rather than the respective ET, are modified by the genetic operator. In GP, the expression trees act both as phenotype and as genotype, while in GEP the phenotype is obtained through a translation process from the genotype. This way, an important advantage of GEP over classical GP is clear separation between phenotype and genotype. The chromosomes may be consisted of one or more genes which represents a mathematical expression. The mathematical code of a gene is expressed in two different languages called Karva Language [5] such as the language of the genes and the language of the ETs. The genes have two main parts addressed as the head and the tail. The head includes some mathematical operators, variables and constants ($+$, $-$, $*$, $/$, $\sqrt{}$, sin, cos, 1, a, b, c) which are used to encode a mathematical expression. The tail just includes variables and constants (1, a, b, c) named as terminal symbols. Additional symbols are used if the terminal symbols in the head are inadequate to define a mathematical expression. A simple chromosome as linear string with two genes is encoded as shown in Fig. 1. Its ET and the corresponding mathematical equation are also shown in same figure. The translation of ET to Karva Language is done by beginning to read from left to right in the top line of the tree and from top to bottom. Joining