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Ceramics International 41 (2015) 1631–1639

CERAMICS INTERNATIONAL

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Rapid synthesis of nanopowders in high energy ball milling; Optimization of milling parameters

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Received 28 July 2014; received in revised form 17 September 2014; accepted 17 September 2014
Available online 28 September 2014

Abstract

An important factor in high energy ball milling process is to speed up the synthesis of metal/ceramic nanocomposites. In this work, for the first time, particle swarm optimization (PSO) as a new powerful algorithm was used for optimization of milling parameters in order to minimize the synthesis time of metal/ceramic nanocomposites in planetary mills. Accordingly, it is important to find a mathematical model to correlate the milling parameters with the synthesis time of metal/ceramic nanocomposites and then optimize the mentioned model. In this work, Burgio's mathematical model was chosen because it describes the energy supplied by a planetary mill using only analytical expressions. Based on Burgio's model eight design parameters in milling, namely, number of balls, ball diameter, vial radius, vial height, ball diameter distribution coefficient, plate spinning rate, vial spinning rate and distance between the center of the plate and the center of the vial, were optimized by the PSO algorithm. By optimizing the milling parameters and given the Burgio model, the synthesis time was minimized. At the end two test cases were solved to demonstrate the effectiveness and accuracy of the proposed design. Computational results showed that the proposed optimization algorithm is quite effective and powerful in optimizing the planetary mills to speed up the metal/ceramic nanocomposites synthesis.

Keywords: A. Milling; Metal/ceramic nanocomposites; Optimization; Planetary mill; PSO algorithm

1. Introduction

Mechanical alloying (MA), which is generally achieved through high-energy ball milling has been widely utilized for producing supersaturated solid solutions, (non-equilibrium) intermetallic compounds, or the formation of stable or unstable carbides, borides, nitrides, silicides, etc. [1,2].

Many studies have confirmed that changing the milling conditions influences the energy transferred to the milled nanopowders and hence duration of product synthesis [3,4]. Accordingly, a mathematical model in which the milling parameters are correlated with the syntheses time of nanostructured powders is very important. The aim of constructing a model is to be able to design the mechanical alloying process and to predict the formation of the desired products in the least possible time by adjusting the milling parameters appropriately.

So far the mechanical alloying process has been simulated in terms of ball velocity, frequency of impact and power/kinetic energy transferred to the raw materials during milling [5–11]. By the same token a set of kinematic equations was formulated by Burgio et al. [12] to evaluate the velocity and acceleration of a ball in a planetary mill and, thereby, investigate the energy transferred to the nanopowders.

Since in the present study the optimization process is done on a mathematical model, it is necessary to build the mentioned model initially. The Burgio model [12] is chosen in this research because the energy during milling with planetary mills has been described only in terms of analytical expressions without any numerical calculation. Therefore, it was possible to more easily compare the quantitative forecasts of the model with our observational data.

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http://dx.doi.org/10.1016/j.ceramint.2014.09.101
0272-8842/

The optimization problem can be described as finding an argument x whose relevant cost $f(x)$ is optimum, and it has been extensively used in many different situations such as industrial planning, resource allocation, scheduling, and pattern recognition. Different methods have been proposed to solve the optimization problem [13]. Evolutionary algorithms such as genetic algorithm(GA) [14,15], biogeography based optimization (BBO) [16,17], taboo search [18–20], ant colony optimization [21–23], bees algorithm [24–26], simulated annealing [27,28], artificial bee colony [29,30] and firefly optimization [31,32] are a set of algorithms that were suggested in the past decades for solving optimization problems in different branches of engineering.

When an algorithm is inspired by the intelligent collective behavior of some animals, a PSO takes place. Two of the obvious advantages of the PSO are its ease of implementation and few parameters for adjustment. What is desirable in PSO is encouraging individuals to wander through the entire search space, without clustering around local optima, during the early stages of the optimization. On the other hand, enhancing convergence in the global optima is very important to find the optimum solution efficiently (exploitation). Generally, the performance of the standard PSO depends almost entirely on its parameters.

PSO is a powerful optimization technique which has been never used in materials engineering so far. In the present study we have introduced PSO as an interesting algorithm to minimize the synthesis (ignition) time of nanopowders in high energy planetary mills. This method can be easily used in many engineering problems that are concerned with the time. At the end a case study was conducted to evaluate the effectiveness of the mentioned optimization algorithm in the field of materials science and especially in mechanical alloying. Results showed a new achievement in engineering materials.

2. Problem definition

As mentioned in the introduction, the Burgio model [12] was chosen for optimization process. Initially it is good to know how a planetary mill works. Fig. 1 shows a schematic diagram of the planetary ball mill and the vial indicated by W_p and W_v, the absolute angular velocity of the plate of the mill and of one vial, respectively, and by R_v and R_p the vectorial distances from the center of the mill to the center of the vial and from the center of the vial to its periphery (vial radius). According to Burgio [12], the absolute velocity of one ball after a short succession of hits is obtained from

$$V_S = [(W_p R_p)^2 + W_v^2(R_v - d_b/2)^2 + 2W_p W_v R_P(R_v - d_b/2)]^{1/2} \quad (1)$$

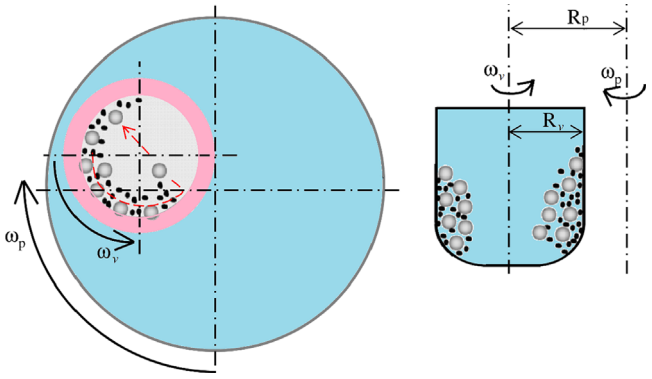

Fig. 1. Schematic diagram of the planetary ball mill and the vial.

where d_b is ball diameter. At the same time, kinetic energy of ball is released so that the balls residual energy becomes

$$E = 1/2\ m_b V_S^2 \quad (2)$$

where m_b is mass of the ball. Accordingly the total energy released by the ball during the series of collision events is given by

$$\Delta E_b = -m_b[W_v^3(R_v - d_b/2)/W_p + W_p W_v R_p](Rv - d_b/2) \quad (3)$$

Now, if we assume that the total energy transferred by the planetary mill per gram of reactant mixture and required synthesis of nanostructured powders is a constant value, A, the Burgio model defines this amount of energy by the following expression:

$$E_t/\mathrm{g} = \frac{(N_b \varphi_b f_b K_a m_b)[W_v^3(R_v - d_b/2)/W_p + W_P W_v R_P](R_v - d_b/2)t}{m_{ch}} = A\ (J/g) \quad (4)$$

where N_b is the number of balls; φ_b is a parameter that accounts for the degree of filling of the vial; f_b is the frequency with which the balls are launched against the opposite wall of the vial (s^{-1}); K_a is a constant that accounts for the elasticity of collisions, and a value of 1 represents perfectly inelastic collisions; m_{ch} is the mass of the powder charge; and t is the synthesis (ignition) time measured (s).

According to the literature [12,33]

$$\varphi_b = 1 - \left(\frac{d_b^3 N_b}{\pi R_v^2 H_v}\right)^{\varepsilon} \quad (5)$$

$$f_b = \frac{K(W_p - W_v)}{2\pi} \quad (6)$$

$$m_b = \frac{\pi \rho_b d_b^3}{6} \quad (7)$$

where H_v, ρ_b are respectively the height of the vial and the density of balls. K is a proportionality constant and is approximately equal to unity [33] and ε is a parameter called ball diameter distribution coefficient depending on the balls diameter.

Using Eqs. (5)–(7), formula (4) can be rewritten as where t is the synthesis (ignition) time measured (s).

$$t = \frac{12}{A\rho_b K_a K} m_{ch} \frac{1}{-N_b\left(1 - \left(d_b^3 N_b/\pi R_v^2 H_v\right)^{\varepsilon}\right)(W_p - W_v)\left(d_b^3\right)\left(W_v^3(R_v - d_b/2)/W_p + W_P W_v R_P\right)(R_v - d_b/2)} \quad (8)$$