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Ignition time of nanopowders during milling: A novel simulation

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ABSTRACT

Detecting the sudden temperature increase of the milling vial, detecting the sudden total pressure increase inside the vial as well as XRD analysis from the synthesized phases are techniques that can be used to determine the ignition time in mechanically self-sustaining reactions (MSRs) induced by ball milling. In the present study a novel technique based on the Gene Expression Programming (GEP) algorithm is presented to estimate the ignition time in MSRs induced by high energy planetary mills, without any experimental testing. In other words, only by knowing some of the milling and reaction parameters comprised of $\Delta H/C_P$, ball to powder weight ratio (BPR), vial spinning rate, arithmetic mean of melting points of reactants, average diameter of balls and amount of used process control agent (PCA), one can predict the ignition time in the mentioned systems. Accordingly, most of the systems that are based on the MSR mode were gathered from the literature, and the data obtained from them are trained and tested by the GEP modeling algorithm. The results indicated a very good agreement between the experimental data and the predicted ones. The biogeography based optimization (BBO) was also utilized to optimize the milling parameters. 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 are fully functional to accurately estimate the optimal conditions for planetary mills experiments which show the potential application of these calculations and analysis in materials science and engineering.

1. Introduction

Mechanical alloying or the high-energy milling of (elemental) powders is a very low cost technique to obtain amorphous or nanostructured materials [1,2]. In this process, a powder mixture placed in a ball mill usually at room temperature is subjected to high-energy collisions from the balls [3,4].

Ball milling can also produce mechanically induced self-sustaining reactions (MSRs) in many highly exothermic powder mixtures [5,6]. An MSR mode, similar to any other mechanical alloying process (gradual mode), is associated with an activation period, during which size reduction, mixing, and defect formation take place. But at a critical time, called the ignition time (t_{ig}), the reaction rate begins to increase. As a result, the temperature rises, and the reaction rate increases further which leads to a self-sustaining process. Since these events occur at a fraction of time, most of the reactants are consumed within seconds [7]. The ignition time of nanopowders depends on the milling parameters as well as thermodynamic and kinetic properties of the system under study [8].

It should be noted that t_{ig} can be detected with the sudden temperature increase of the milling vial [9] or the total pressure inside it [10] resulted from the heat released from the highly exothermic reaction. Since in many systems containing MSR mode, the ignition time is equal to the synthesis time of products [5,6,9,11], these systems have a major advantage of predictability of the synthesis time, in comparison with other ones. In other words, without any phase analysis, which is common in other systems to determine the synthesis time, one can predict the synthesis time only by measuring the temperature or pressure of the milling vial. Therefore, the ignition time of nanopowders can be utilized as a reference point because its variation with milling conditions reflects changes in the mechanical dose rate of the mill. This parameter also simplifies the comparison of reaction kinetics data obtained using different milling equipment and, consequently, their efficiencies [12]. On the other hand, if the appropriate situation can be provided to optimize the milling parameters, the ignition time occurs faster resulting in a rapid synthesis of products.

In this paper, Gene Expression Programming (GEP) and biogeography based optimization (BBO) algorithms as powerful tools have been utilized for modeling and optimizing of milling process, respectively.

BBO was developed by Dan Simon in 2008 in the form of a computational algorithm [13]. The BBO algorithm shares information among solutions with the migration operator [14]. According to Simon [13] the

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performance of BBO algorithm is better than or similar to that of the other algorithms although it uses less control parameters so that a potential for solving multi-modal and multidimensional optimization is obtained.

As a generalization of genetic algorithm (GA), Genetic programming (GP) was proposed by Koza [15]. Three basic genetic operators exist in GP including reproduction, crossover and mutation. In the present work, we have utilized APS 3.0 [16], and Gene Expression Programming (GEP) software developed by Candida Ferreira. GEP is an extension of GP that evolves computer programs of different sizes and shapes encoded in linear chromosomes of fixed length [17,18].

The GEP has been utilized as a new tool several times in the field of mechanical alloying. Predicting and maximizing the hardness of metal matrix nanocomposites produced by mechanical alloying [19,20] and minimizing the synthesis time of nanocomposites during milling [21], are some applications of GEP in this field.

In the present work, the ignition time of nanopowders in mechanically induced self-sustaining reactions has been estimated in high energy planetary mills (Given the significant differences between the mills [22], this research has been developed only for planetary mills). Since in many combustion systems, the synthesis time is equal to the ignition time of nanopowders, this work can be a very novel and interesting work. Henceforth, it is not necessary to measure the vial temperature and pressure for determining the ignition time of nanopowders produced by MSR mode. In other words, only by knowing the milling parameters and without performing any experimental work, one can predict the ignition time of nanopowders or synthesis time in highly exothermic powder mixture during milling with planetary mills. Moreover, we were able to obtain the best conditions for minimizing the ignition time (synthesis) during high energy ball milling. To assess the theoretical model of what happens in practice, a few case studies have been undertaken.

2. Materials and methods

2.1. Data collection

The collected data from the previous works [23–49] are listed in Table 1. Ignition time of several mechanically induced self-sustaining reactions in high energy planetary mills has been considered as the main objective of this study for prediction by GEP model. The input parameters consist of $\Delta H/C_P$, ball to powder weight ratio (BPR), vial spinning rate, average melting point of reactants, average diameter of balls and amount of used PCA, with the ranges given in Table 2. The ignition time of nanopowders has been calculated with three different methods including detecting the sudden temperature increase of the milling vial, detecting the sudden total pressure increase inside the vial and the XRD of analysis the synthesized phases.

2.2. Gene Expression Programming structure & parameters

The GEP encodes the individuals of the created computer programs as linear strings of fixed length (the genome or chromosomes) which are afterwards expressed as nonlinear entities of different sizes and shapes called as expression trees (ET). Accordingly, two languages comprised of the language of the genes and the language of ETs, are utilized in GEP. A significant advantage of GEP is that it enables us to infer exactly the phenotype given the sequence of a gene, and vice versa which is termed as Karva language [18]. The genes (SUB-TEs) have two main parts: the head and the tail. The head includes some mathematical

Table 1
The gathered data as input and target for training and testing sets from the previous works.

Raw materials → products	$\Delta H/C_p$ (K)	Arithmetic mean of melting points (k)	BPR	Velocity (rpm)	Mean diameter of balls (mm)	PCA (%)	Ignition time of nanopowders (h)	Ref.
$3ZrO_2 + 3B_2O_3 + 10Al \rightarrow 3ZrB_2 + 5Al_2O_3$	4134	1548	5	750	15	0	22.5	[23]
$3ZrO_2 + 3B_2O_3 + 10Al \rightarrow 3ZrB_2 + 5Al_2O_3$	4134	1548	15	750	15	0	20	[23]
$3ZrO_2 + 3B_2O_3 + 10Al \rightarrow 3ZrB_2 + 5Al_2O_3$	4134	1548	25	750	15	0	17.5	[23]
$Ti + C \rightarrow TiC$	3855	2993	10	300	17.4	2	8	[24]
$CuO + Mg \rightarrow Cu + MgO$	7120	1274	15	250	8.6	0	0.5	[25]
$WO_3 + 3\,Mg \rightarrow W + 3MgO$	6898	1274	15	250	8.6	0	0.5	[25]
$4Al + 3TiO_2 + 3C \rightarrow 2Al_2O_3 + 3TiC$	3560	2365	20	600	10	0	10	[26]
$10Al + 3TiO_2 + 6H_3BO_3 \rightarrow 3TiB_2 + 5Al_2O_3 + H_2O$	4620	1164	20	600	20	0	1.5	[27]
$10Al + 3TiO_2 + 6H_3BO_3 \rightarrow 3TiB_2 + 5Al_2O_3 + H_2O$	4620	1164	10	250	–	1.5	30	[28]
$10Al + 3TiO_2 + 3B_2O_3 = 3TiB_2 + 5Al_2O_3$	5000	1257	10	250	–	1.5	10	[29]
$MoO_3 + 2SiO_2 + 14/3Al \rightarrow MoSi_2 + 7/3Al_2O_3$	4285	1291	10	700	15.8	0	3	[30]
$3Co_3O_4 + 8Al \rightarrow 9Co + 4Al_2O_3$	8089	1050	15	600	–	0	0.8	[31]
$3V_2O_5 + 28Al \rightarrow 6Al_3V + 5Al_2O_3$	3960	951	10	500	20	0	0.5	[32]
$3Ti + Al + 2C \rightarrow Ti_3AlC_2$	4721	2306	5	600	12	0	3	[33]
$Ni + 3NiO + 6Al \rightarrow 4NiAl + Al_2O_3$	5485	1429	–	–	20	0	10	[34]
$4Al + 2B_2O_3 + C \rightarrow 2Al_2O_3 + B_4C$	6600	1900	20	500	20	0	4	[35]
$0.65Mo + 0.35\,W + 2Si \rightarrow 0.65MoSi_2 + 0.35WSi_2$	2003	2759	25	350	15.5	0	80	[36]
$14Ti + 2BN + 2Si_3N_4 \rightarrow 10TiN + TiB_2 + 3TiSi_2$	3296	2453	30	600	9	0	0.18	[37]
$15Ti + 4BN + Si_3N_4 \rightarrow 8TiN + 2TiB_2 + Ti_5Si_3$	3523	2453	30	600	9	0	0.18	[37]
$Si + C \rightarrow SiC$	2654	2896	10	700	12	0	10	[38]
$3SrSO_4 + 8Al \rightarrow 3SrS + 4Al_2O_3$	6500	1269	40	600	20	0	0.75	[39]
$MoO_3 + 2Al + 0.5C \rightarrow 0.5Mo_2C + Al_2O_3$	6128	2016	20	300	–	1	10	[40]
$MoO_3 + 2Si + 2Al \rightarrow MoSi_2 + Al_2O_3$	5732	1409	35	600	–	0	0.25	[41]
$MoO_3 + 2Si + 2Al \rightarrow MoSi_2 + Al_2O_3$	5732	1409	35	600	–	1	22	[41]
$MoO_3 + 2Si + 2Al \rightarrow MoSi_2 + Al_2O_3$	5732	1409	20	600	–	0	0.36	[41]
$MoO_3 + 2Si + 2Al \rightarrow MoSi_2 + Al_2O_3$	5732	1409	20	600	–	1	0.58	[41]
$MoO_3 + 2Si + 2Al \rightarrow MoSi_2 + Al_2O_3$	5732	1409	10	600	–	0	1	[41]
$MoO_3 + 2Si + 2Al \rightarrow MoSi_2 + Al_2O_3$	5732	1409	10	600	–	1	1.25	[41]
$Cr + 3Al + Fe_2O_3 \rightarrow (Fe,Cr)_3Al + 3Al + Al_2O_3$	3021	1648	10	500	20	0	135	[42]
$3Fe_2O_3 + 8Al \rightarrow 2Fe_3Al + 3Al_2O_3$	3093	1381	10	250	10	0	2.25	[43]
$Cu + In + Se \rightarrow CuInSe_2$	2189	760	10	600	–	0	0.75	[44]
$ZnO + Ca \rightarrow Zn + CaO$	4220	1681	30	230	–	0	1.45	[45]
$2Al(s) + 3ZnO(s) \rightarrow Al_2O_3(s) + 3Zn(s)$	4006	1690	15	600	–	0	5	[46]
$2Al + B_2O_3 + Ti \rightarrow Al_2O_3 + TiB_2$	5214	1437	10	500	20	0	32	[47]
$WO_3 + 3\,Mg + C \rightarrow WC + 3MgO$	6856	2238	15	200	10	0	4.5	[48]
$Ti + Si \rightarrow TiSi$	2875	1814	17	800	15	0	0.3	[49]