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Modeling the mean grain size of synthesized nanopowders produced by mechanical alloying

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Abstract

Gene expression programming (GEP) optimization tool has been utilized to predict the mean grain size of nanopowders synthesized by mechanical alloying. 86 data were collected from the literature, randomly divided into 65 and 21 sets and then, respectively, were trained and tested by 11 different GEP models. The differences between the models were in their linking functions (addition and multiplication) and sub expression trees (3, 4, 5, 6, 7 and 8). The method of calculation of the mean grain size, milling time, annealing temperature, produced phases after mechanical alloying, vial speed and ball to powder ratio were considered as input variables to predict mean grain size of nanopowders as output. The obtained results from training and testing of the different models showed that some of them are capable to predict mean grain size of the synthesized nanopowders in the considered range. However, the best results were obtained by using 7 sub expression trees addition as linking function. R^2 value of the trained and tested suggested model showed this situation.

Keywords: Gene expression programming; Mechanical alloying; Nanopowder; Modeling

1. Introduction

Mechanical alloying (MA) is a solid state technique used for fabrication of nanocrystalline alloys and intermetallic compounds. MA allows materials scientists to overcome material limitations and to manufacture alloys that are difficult or impossible to be produced by conventional melting and casting techniques. Through this technique, the fine-grained powders can be formed [1]. During the last decade, many equilibrium and/or non-equilibrium materials have been successfully synthesized through this technique like those were done in the previous works [2–13], where several alloys and compounds were synthesized successfully through MA. In all of the previous works, mean grain size of the synthesized MA-nanopowders was calculated as a critical factor by the acquired XRD patterns. 3 main methods which were used for determining mean grain size of the synthesized nanopowders include Reitveld refinement [14], Williamson–Hall [15] and Scherrer methods [16].

Genetic programming (GP) garnered considerable attention due to its ability to model nonlinear relationships for input–output mappings. Several studies have utilized GP derivatives for construction industry problems. Baykasoglu et al. [17] applied GEP to determine concrete strength, cost, and slump. Yeh and Lien [18] developed a genetic operation tree (GOT) to investigate concrete strength. The GOT uses a tree topology (as does GEP) and optimized coefficients that differ from other GP derivatives. Coefficients do not frequently appear in formulas programmed using any of these GP models. Tsai [19] proposed a weighted GP (WGP) to introduce weight coefficients into tree connections and generate a fully weighted formula. Jabeen and Baig [20] presented an approach to classify mixed attribute data using two layered GP. The presented approach does not transform data into any other type and combines the properties of arithmetic expressions (using numerical data) and logical expressions (using categorical data).

The authors' literature survey shows that utilizing soft-computing techniques for evaluation the properties of synthesized nanopowders is rarely reported. Therefore, in the present study, GEP has been employed to predict the

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Table 1
The gathered data as input and target for training, testing and validating sets from the previous works [2–13].

Method of calculation mean grain size	Milling time (h)	Annealing temperature (°C)	Produced phase	Vial speed (rpm)	Ball to powder ratio	Mean grain size (nm)	Reference
Reitveld refinement method	10	As milled	Mo	750	5 to 1	22.3	[2]
Reitveld refinement method	10	900	Mo	750	5 to 1	23.3	[2]
Reitveld refinement method	20	As milled	Mo	750	5 to 1	14.6	[2]
Reitveld refinement method	30	As milled	$MoSi_2$	750	5 to 1	13.2	[2]
Reitveld refinement method	30	700	$MoSi_2$	750	5 to 1	15.2	[2]
Reitveld refinement method	30	900	$MoSi_2$	750	5 to 1	21.5	[2]
Williamson–Hall	20	As milled	α-$MoSi_2$	750	15 to 1	31.8	[3]
Williamson–Hall	45	As milled	Flaky-SiO_2	500	10 to 1	35	[4]
Scherrer	30	As milled	Spherical-FeSi	500	10 to 1	13	[4]
Scherrer	45	As milled	Spherical-FeSi	500	10 to 1	11	[4]
Scherrer	70	As milled	Spherical-FeSi	500	10 to 1	9	[4]
Scherrer	45	600	Spherical-FeSi	500	10 to 1	11	[4]
Scherrer	45	800	Spherical-FeSi	500	10 to 1	12	[4]
Scherrer	45	1000	Spherical-FeSi	500	10 to 1	34	[4]
Williamson–Hall	30	1000	Mo–15%Cr	540	10 to 1	30	[5]
Williamson–Hall	50	1000	Mo–15%Cr	540	10 to 1	20	[5]
Williamson–Hall	50	800	Mo–25%Cr	540	10 to 1	37	[5]
Williamson–Hall	50	1400	β-$MoSi_2$–15%Cr	540	10 to 1	29	[5]
Williamson–Hall	70	1400	β-$MoSi_2$–15%Cr	540	10 to 1	26	[5]
Williamson–Hall	100	1400	β-$MoSi_2$–15%Cr	540	10 to 1	23	[5]
Williamson–Hall	10	700	Mo	525	15 to 1	24	[6]
Williamson–Hall	70	700	Mo	525	15 to 1	31	[6]
Scherrer	5	As milled	Bi_2Te_3	525	10 to 1	15	[7]
Scherrer	10	As milled	Bi_2Te_3	525	10 to 1	13.5	[7]
Scherrer	15	As milled	Bi_2Te_3	525	10 to 1	12.5	[7]
Scherrer	20	As milled	Bi_2Te_3	525	10 to 1	11.5	[7]
Scherrer	25	As milled	Bi_2Te_3	525	10 to 1	10	[7]
Scherrer	3	As milled	Al_2O_3	700	10 to 1	22.6	[8]
Scherrer	6	As milled	Al_2O_3	700	10 to 1	22.6	[8]
Scherrer	10	As milled	Al_2O_3	700	10 to 1	22.6	[8]
Scherrer	20	As milled	Al_2O_3	700	10 to 1	22.6	[8]
Scherrer	40	As milled	Al_2O_3	700	10 to 1	22.6	[8]
Scherrer	70	As milled	Al_2O_3	700	10 to 1	13.8	[8]
Scherrer	100	As milled	Al_2O_3	700	10 to 1	12.3	[8]
Scherrer	3	As milled	β-$MoSi_2$	700	10 to 1	15.7	[8]
Scherrer	6	As milled	β-$MoSi_2$	700	10 to 1	15.2	[8]
Scherrer	10	As milled	β-$MoSi_2$	700	10 to 1	11.3	[8]
Scherrer	20	As milled	β-$MoSi_2$	700	10 to 1	9.7	[8]
Scherrer	40	As milled	β-$MoSi_2$	700	10 to 1	6.9	[8]
Williamson–Hall	70	As milled	α-$MoSi_2$	700	10 to 1	19.2	[8]
Williamson–Hall	100	As milled	α-$MoSi_2$	700	10 to 1	17.3	[8]
Williamson–Hall	5	As milled	Mo	700	10 to 1	26.7	[9]
Williamson–Hall	10	As milled	Mo	700	10 to 1	24.8	[9]
Williamson–Hall	20	As milled	Mo	700	10 to 1	23.9	[9]
Williamson–Hall	30	As milled	$MoSi_2$	700	10 to 1	27.7	[9]
Williamson–Hall	50	As milled	$MoSi_2$	700	10 to 1	24.3	[9]
Williamson–Hall	70	As milled	$MoSi_2$	700	10 to 1	20.1	[9]
Williamson–Hall	100	As milled	$MoSi_2$	700	10 to 1	15.8	[9]
Williamson–Hall	150	As milled	$MoSi_2$	700	10 to 1	11.7	[9]
Scherrer	5	As milled	Al–5%carbon	500	10 to 1	23	[10]
Scherrer	10	As milled	Al–5%carbon	500	10 to 1	10	[10]
Scherrer	10	800	Al–5%carbon	500	10 to 1	18	[10]
Scherrer	5	As milled	Al–10%carbon	500	10 to 1	18	[10]
Scherrer	5	As milled	Al–12.5%carbon	500	10 to 1	16	[10]
Scherrer	5	As milled	Al–15%carbon	500	10 to 1	16	[10]
Scherrer	5	As milled	Al–17.5%carbon	500	10 to 1	13	[10]
Scherrer	5	As milled	Al–20%carbon	500	10 to 1	14	[10]
Scherrer	35	As milled	Al_2O_3–TiC	500	10 to 1	12	[11]
Scherrer	55	As milled	Al_2O_3–TiC	500	10 to 1	8	[11]
Scherrer	80	As milled	Al_2O_3–TiC	500	10 to 1	7	[11]

Table 1 (*continued*)

Method of calculation mean grain size	Milling time (h)	Annealing temperature (°C)	Produced phase	Vial speed (rpm)	Ball to powder ratio	Mean grain size (nm)	Reference
Scherrer	80	600	Al_2O_3–TiC	500	10 to 1	13	[11]
Scherrer	80	800	Al_2O_3–TiC	500	10 to 1	21	[11]
Scherrer	1	As milled	NiAl(IB)	600	12 to 1	9	[12]
Scherrer	8	As milled	NiAl(IB)	600	12 to 1	5.3	[12]
Scherrer	16	As milled	NiAl(IB)	600	12 to 1	3.8	[12]
Scherrer	30	As milled	NiAl(IB)	600	12 to 1	2.1	[12]
Scherrer	45	As milled	NiAl(IB)	600	12 to 1	1.8	[12]
Scherrer	1	As milled	NiAl(FWHM)	600	12 to 1	8.6	[12]
Scherrer	8	As milled	NiAl(FWHM)	600	12 to 1	5.4	[12]
Scherrer	16	As milled	NiAl(FWHM)	600	12 to 1	3.6	[12]
Scherrer	30	As milled	NiAl(FWHM)	600	12 to 1	2	[12]
Scherrer	45	As milled	NiAl(FWHM)	600	12 to 1	1.7	[12]
Scherrer	1	As milled	TiC(IB)	600	12 to 1	28	[12]
Scherrer	8	As milled	TiC(IB)	600	12 to 1	10.8	[12]
Scherrer	16	As milled	TiC(IB)	600	12 to 1	5.4	[12]
Scherrer	30	As milled	TiC(IB)	600	12 to 1	3.3	[12]
Scherrer	45	As milled	TiC(IB)	600	12 to 1	2	[12]
Scherrer	1	As milled	TiC(FWHM)	600	12 to 1	21	[12]
Scherrer	8	As milled	TiC(FWHM)	600	12 to 1	8.8	[12]
Scherrer	16	As milled	TiC(FWHM)	600	12 to 1	4.5	[12]
Scherrer	30	As milled	TiC(FWHM)	600	12 to 1	2.7	[12]
Scherrer	45	As milled	TiC(FWHM)	600	12 to 1	1.4	[12]
Scherrer	10	As milled	Sb_2Te_3	525	10 to 1	15	[13]
Scherrer	15	As milled	Sb_2Te_3	525	10 to 1	13.5	[13]
Scherrer	20	As milled	Sb_2Te_3	525	10 to 1	12.6	[13]
Scherrer	25	As milled	Sb_2Te_3	525	10 to 1	12.7	[13]

mean grain size of these materials. The data were collected from the previous works [2–13], trained and tested by eleven different GEP models. 6 independent input parameters that cover the method of calculation of the mean grain size, milling time, annealing temperature, produced phases after mechanical alloying, vial speed and ball to powder ratio were considered for predicting the mean grain size of nanopowders.

2. 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 of this study for prediction by different GEP models. The input parameters were consisted of the method of determining mean grain size, milling time, annealing temperature, produced phases, vial speed and ball to powder ratio with the given ranges in Table 2. The mean grain size of the nanopowders was calculated with 3 different methods including Reitveld method [14], Scherrer [15] and Williamson–Hall [16] methods with different method of calculation the mean grain size. For detailed description on the estimation techniques please refer to [14–16].

3. Genetic programming

Genetic programming (GP) approach is an extension to genetic algorithms proposed by Koza [21] who defines GP as a domain independent problem solving approach in which computer programs are evolved to solve, or approximately solve, problems based on the Darwinian principle of reproduction and analogs of naturally occurring genetic operations such as reproduction, crossover and mutation. GP reproduces computer programs to solve problems by executing the steps in Fig. 1. This figure is a flowchart showing the executional steps of a run of GP. The flowchart demonstrates the genetic operations in addition to the architecture chancing operations. Also, this flowchart demonstrates a two offspring version of the crossover operation.

Table 2
The range of the input parameters in GEP models.

Input	Range
Method of calculation mean grain size [a]	1–3
Milling time (h)	1–150
Annealing temperature (°C)	25–1400
Produced phase [b]	1–27
Vial speed (rpm)	360–750
Ball to powder ratio[c]	5–35

[a] 1,2 and 3, respectively, denotes Reitveld refinement, Williamson–Hall and Scherrer methods.

[b] 1, 2, …, 27, respectively, denotes Mo, $MoSi_2$, α-$MoSi_2$, β-$MoSi_2$, Flaky-SiO_2, Spherical-SiO_2, Spherical-FeSi, Mo–15%Cr, Mo–25%Cr, Si–15%Cr, β-$MoSi_2$–15%Cr, β-$MoSi_2$–25%Cr, Bi_2Te_3, Al, Al_2O_3, Al–5%carbon, Al–10%carbon, Al–12.5%carbon, Al–15%carbon, Al–17.5%carbon, Al–20%carbon, Al_2O_3–TiC, NiAl(IB), NiAl(FWHM), TiC(IB), TiC(FWHM) and Sb_2Te_3.

[c] 5, 10, 12, 15 and 35, respectively, denotes 5:1, 10:1, 12:1, 15:1 and 35:1 ball to powder ratios.

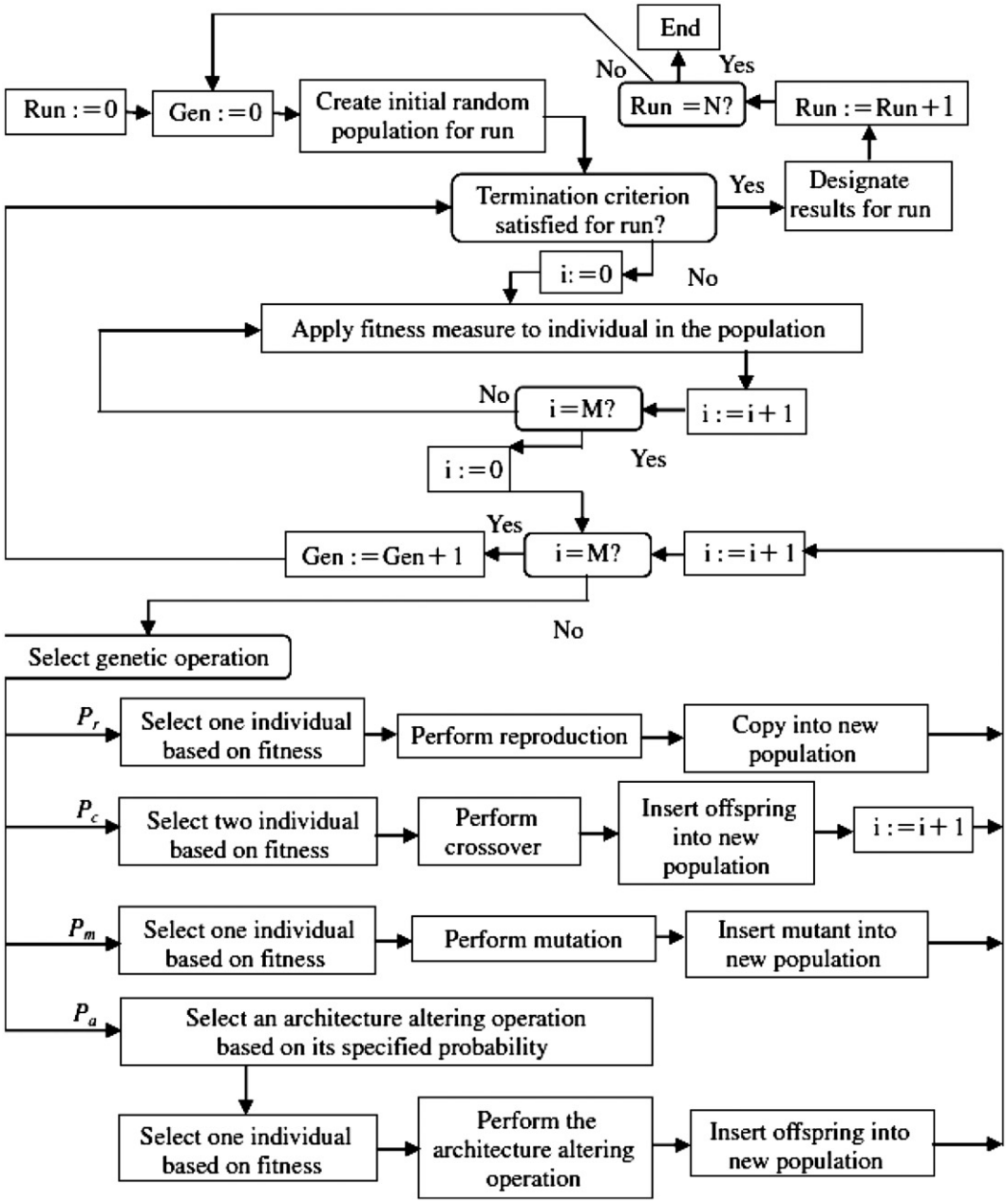

Fig. 1. Genetic programming flowchart [22].

GP approach evolves through the action of three basic genetic operators: reproduction, crossover and mutation. In the reproduction stage, a strategy must be adopted as to which programs should die. In the implementation, a small percentage of the trees with the worst fitness are killed. The population is then filled with the surviving trees according to accepted selection mechanisms, as explained following. Crossover swamps randomly selected parts of two trees to combine good information from the parents and to develop the fitness of the next generation, as shown in Fig. 2. Mutation protects the model against premature convergence and develops the non-local properties of the search, as shown in Fig. 3. Occasionally, one randomly selected node is replaced by another one from the same set, except itself [22].

In applying GP to a problem, there are five major preparatory steps. In order to solve a problem using GP Koza [22] states that it is necessary to specify the following:

(1) The set of terminals: A set of input variables or constants.
(2) The set of primitive functions: A set of domain specific functions used in conjunction with the terminal set to construct potential solutions to a given problem. For symbolic regression this could consist of a set of basic mathematical functions, while Boolean and conditional operators could be included for classification problems.

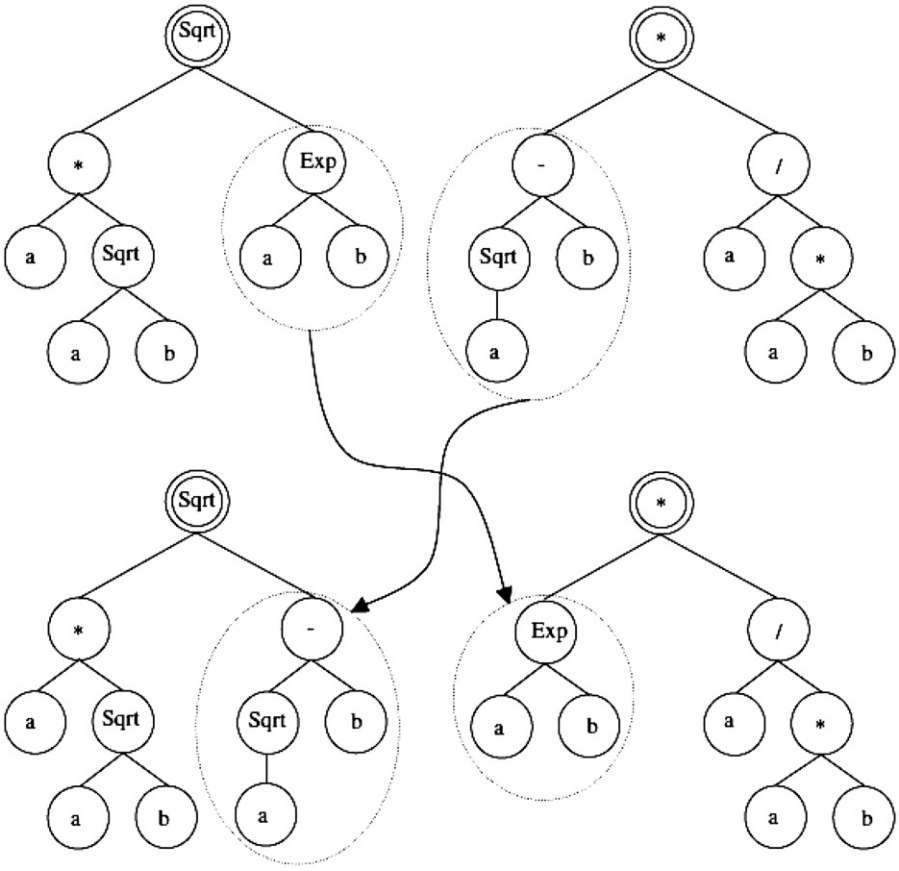

Fig. 2. Example of genetic programming crossover [22].

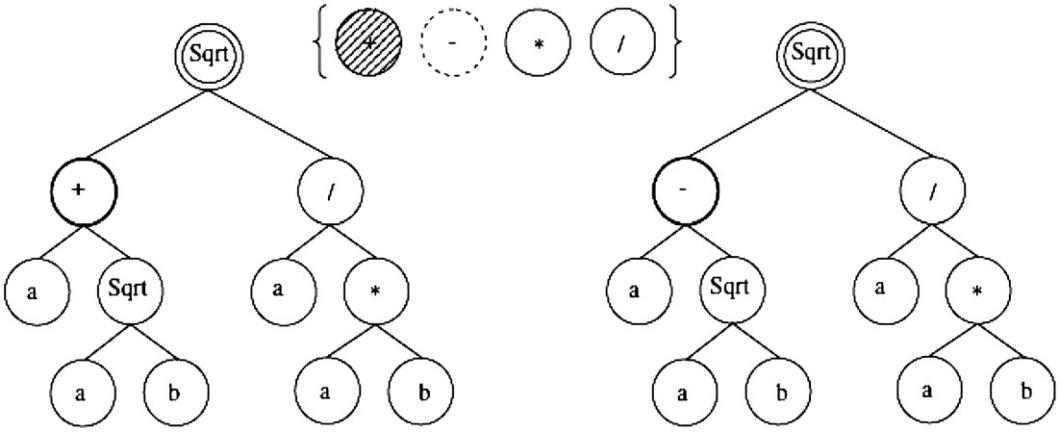

Fig. 3. Example of genetic programming mutation [22].

(3) The fitness measure: Fitness is a numeric value assigned to each member of a population to provide a measure of the appropriateness of a solution to the problem in question.
(4) The parameters for controlling the run: This includes the population size and the crossover and mutation probabilities.
(5) The method for designating a result and the criterion for terminating a run: This is generally a predefined number of generations or an error tolerance on the fitness. It should be noted that the first three components determine the algorithm search space, while the final two components affect the quality and speed of search [22].

The first major step in preparing to use GP is to identify the set of terminals. The terminals can be viewed as the inputs to the as yet-undiscovered computer program. The set of terminals (along with the set of functions) are the

ingredients from which GP attempts to construct a computer program to solve, or approximately solve, the problem [22].

The second major step in preparing to use GP is to identify the set of functions that are to be used to generate the mathematical expression that attempts to fit the given finite sample of data [22].

4. Gene expression parameters and structures

In the present work, as seen for example in Fig. 4 for GEP-5, the expression trees of eleven different GEP models named GEP-1 and GEP-10 were constructed for mean grain size (MGS) values of synthesized nanopowders. As will be described thereinafter, GEP-5 is the best proposed models and for the other models, only the obtained equation has been presented in Table 3 d0, d1, d2, d3, d4 and d5 in Fig. 4 and Table 3 represent the values for input layers which were method of determining mean grain size (M), milling time (t), annealing temperature (T), produced phases (P), vial speed (V) and ball to powder ratio (B/P), respectively, in accordance to the type of collected data from the literature. In GEP-1 to GEP-6 models, addition was used as linking function while this was multiplication for GEP-7 to GEP-11 models. In addition, the number of genes (Sub-ETs) was 3 for GEP-1 and GEP-6, 4 for GEP-2 and GEP-7, 5 for GEP-3 and GEP-8, 6 for GEP-4 and GEP-9, 7 for GEP-5 and GEP-10 and 8 for GEP-6 models. In training and testing of the GEP-1 to GEP-11 approach models constituted with different Sub-ETs and linking functions, M, t, T, P, V and B/P were used as input data and MGS as independent output data. Among 86 collected experimental

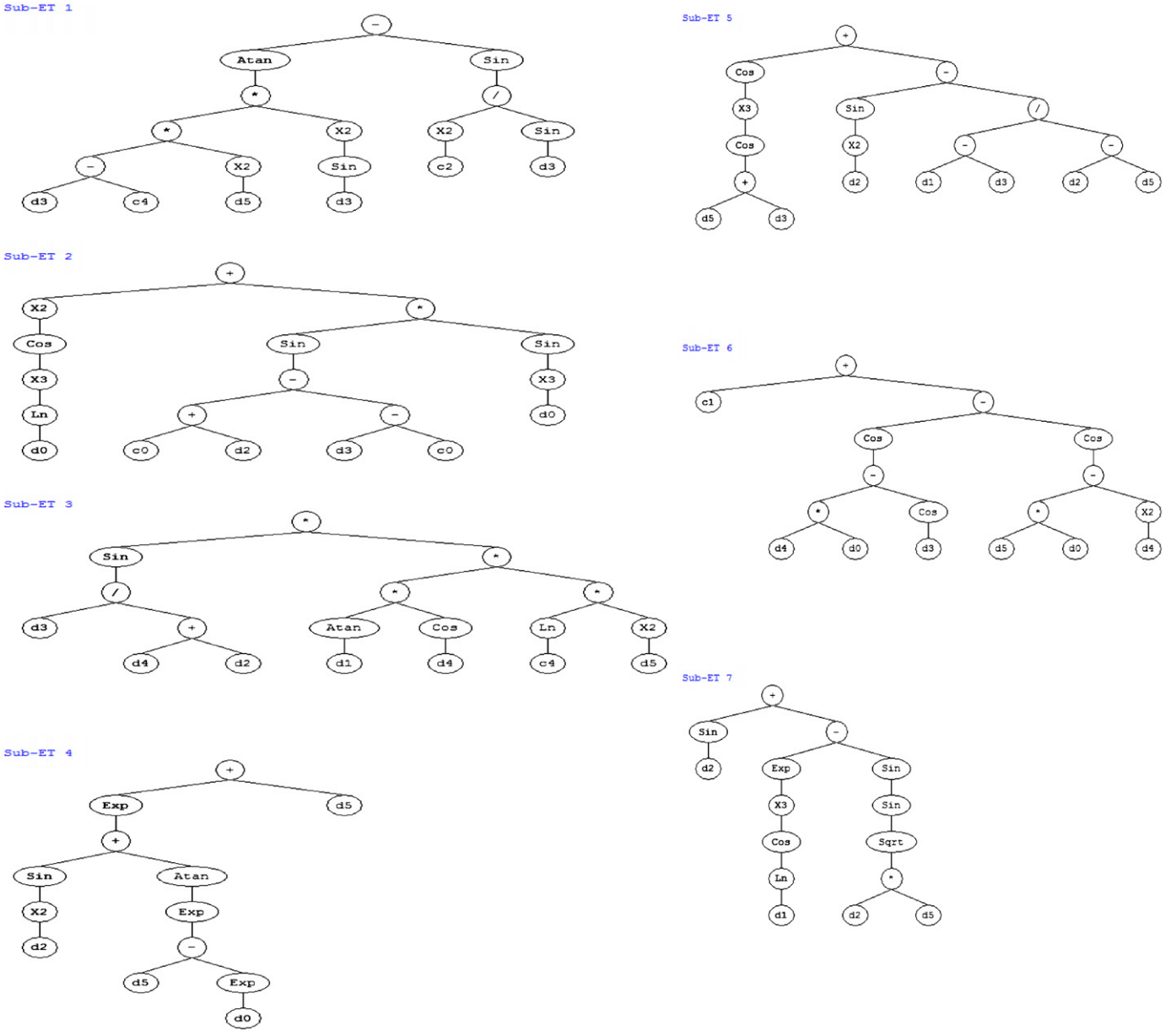

Fig. 4. Expression tree with 7 gens for predicting mean grain size of synthesized nanopowders in GEP-5 model.

Table 3
The performance of 10 suggested models in terms of R^2 and the obtained equations by the program.

Models	R^2		Predicted equation for estimation of MGS
	Training	Testing	
GEP-1	0.7992	0.5539	$MGS = 1.47 + \left(\frac{\sin(M)}{\text{Artan}(4.86t)-\sqrt[3]{M}}\right)^2 + \sqrt{\ln\left(\cos\left(\sin^2(V)(5.22d2-t)\right)^{6561}\right)} + \text{Arctan}\left(\sin\left(0.13P^9\right) \times \frac{t+V-P^2}{t}\right)$
GEP-2	0.8691	0.4147	$MGS = 2d5 + \cos\left(\ln(t) - \text{Exp}\left(B/P\right) - T - 11.6\right) + \cos(M-6.21) + 2\ln\left(\frac{T}{\left(\sin^2(P)-t\right) \times (\cos(P)-\sin(M))}\right) + \frac{M \times \text{Arctan}(\text{Exp}\left(\ln(B/P)\right)^3)}{\text{Arctan}\left(\cos\left(B/P-M-M \times B/P\right)\right)} + \cos\left(\left(16\ln(M)-0.19t^3\right) \times \sin(P+5.33)\right)$
GEP-3	0.8176	0.5500	$MGS = \ln\left(T \times P \times B/P + d4 - \frac{2.38(t-T)}{\sin(P)}\right) + \left(M \times \cos\left(\text{Exp}\left(\cos\left(\sqrt{M}-\cos^3(\cos(V))\right)\right)\right)\right)^3 + B/P + \frac{B/P}{t} + 7.36 - \frac{0.53t}{\sin(V) \times (t \times T-8.84)} + \frac{\sin^2(-3.4d3 \times V)}{\text{Arctan}(\cos(M+T)-0.58)}$
GEP-4	0.8064	0.4581	$MGS = \ln\left(B/P - \text{Arctan}(\cos(P) \times (T-960) + 2\ln(M))\right) + \frac{(T+9.9) \times M}{B/P-V} - \frac{\text{Arctan}(P)}{P-5.11} + \frac{\text{Arctan}\left(\cos\left(4.88P + \ln(B/P)\right) - (t \times P-P)^2\right)}{\sin(M)} + \left(\text{Exp}\left(\cos\left(\cos^3(V) \times (\cos(M) + \frac{t}{V})^3\right)\right)^3 + \sin\left(4.91(V+0.34)^2\right) + \text{Exp}\left(\sin^3\left(d2 - \frac{6.83}{\frac{-0.4}{B/P} + t - B/P}\right)\right)\right)$
GEP-5	0.8425	0.7683	$MGS = \text{Arctan}\left(B/P^2(P-8.14)\sin^2(P)\right) - \sin\left(\frac{36.8}{\sin(P)}\right) + \cos^2(\ln(M))^3 + \sin\left(M^3\right) \times \sin(T-P-10) + 2.07B/P^2 \sin\left(\frac{P}{T+V}\right) \times \text{Arctan}(t) \times \cos(V) + B/P + \text{Exp}\left(\begin{matrix}\sin\left(T^2\right) \\ +\text{Arctan}\left(\text{Exp}\left(B/P - \text{Exp}(M)\right)\right)\end{matrix}\right) + \cos^3\left(\cos(P+B/P)\right) + \sin\left(T^2\right) - \frac{t-P}{T-B/P} + 8.46 + \cos(M \times V - \cos(P)) - \cos\left(M \times B/P - V^2\right) + \sin(T) + \text{Exp}\left(\cos^3(\ln(t))\right) - \sin\left(\sin\left(\sqrt{T \times B/P}\right)\right)$
GEP-6	0.8436	0.3160	$MGS = \cos\left(\cos\left(\sin\left(\frac{V}{B/P} - 0.22t\right)\right) + \cos\left(\sin(V) \times \sqrt{T}\right)\right)^3 + \text{Arctan}\left(\frac{3.88}{M} + \frac{13.1}{t^3}\right)^3 + \ln(T) + \cos\left(P \times \sqrt{\text{Exp}(\text{Arctan}(M)+5.62)}\right) + \text{Exp}\left(\cos\left(\text{Arctan}(\cos(T-6.41)) + (P-6.41)^3 + M + \frac{P}{T}\right)\right) \times \text{Exp}(\sin(P)) + \left(2.26\cos^2\left(\ln(\text{Exp}(M)+1.46) - \text{Exp}\left(\frac{8.63}{B/P}\right)\right)\right)^3 + \text{Arctan}(T) + 2\ln\left(0.5\ln\left(\frac{V}{t}\right) \times \sin(P) \times (8.59-M)\right) \times \ln(\sin(M))$
GEP-7	0.7637	0.4233	$MGS = \left(B/P - \cos^3\left(V \times \text{Arctan}\left(\text{Exp}\left(\frac{\cos^3(M)}{\text{Exp}(P)}\right)\right)\right)\right) \times \left(\text{Exp}\left(\cos(M) \times \text{Arctan}\left(M + \frac{\text{Arctan}^3(7.41-B/P)}{t}\right)\right)\right) \times \left(1.58 + \sqrt{\frac{M}{\text{Exp}\left(\sin\left(\frac{-0.06(t-0.061}{P} + 8.03 \times B/P\right)\right)}}\right)$
GEP-8	0.7610	0.5399	$MGS = \left(9.76 + \cos\left(7.13 \times \text{Arctan}\left(\frac{\frac{T}{M}+9.76}{\cos(P)}\right)\right)^6\right) \times \cos\left(\cos\left(M + \text{Arctan}\left(\frac{B/P}{\text{Exp}(\cos(-6.987T))}\right)^3\right)^3\right) \times \text{Arctan}\left(\frac{T \times \left(\frac{T}{T} - \cos\left(B/P\right)\right)^3}{0.67P}\right) \times \text{Arctan}\left(\frac{d2 + \frac{\sin(\cos(P))}{\sin(V)}}{\sqrt{M \times P \times \sqrt{t}}}\right)$
GEP-9	0.8401	0.5331	$MGS = \cos\left(\text{Arctan}\left(B/P - \text{Arctan}^3(\text{Exp}(\text{Arctan}(V)) \times \cos(-5.86 \times T \times V))\right) \times \text{Exp}(\cos(M)) \times \left(P + V + \frac{\frac{P}{T}\text{Exp}(M)+27.4}{\cos\left(\frac{t}{M}\right)}\right) \times \cos^2\left(\frac{P \times \cos(V) \times \ln(t)}{(B/P-T+0.21) \times \frac{P}{M}}\right) \times \cos^2\left(\text{Exp}\left(\cos(B/P)\right)\right)\right)$
GEP-10	0.6811	0.4096	$MGS = 1.87\ln\left(\ln\left(\ln\left(B/P\right) + \frac{2.97}{V}\right)\right) - \cos(\text{Arctan}(P) - 0.98) \times \left(\frac{\text{Exp}(\cos(5.77+V)) + \text{Arctan}\left(P^2 + \cos(P)\right)}{\cos\left(\sin^3(M)\right)}\right) \times \left(\ln\left(B/P^2 - \frac{16.5}{P}\right) - B/P + 0.59P\right) \times \text{Arctan}\left(\ln\left(4.06\frac{t+8}{t}\right)\right) \times \cos\left(\frac{3.48}{t^2} - \text{Exp}\left(\frac{P-T}{P}\right)\right)^2$
GEP-11	0.7746	0.3551	$MGS = 1.68Arctan\left(2M-T+M^2+Exp\left(cos\left(B/P\right)\right) \times \left(sin(t)-5.7\right)\right) \times cos(Arctan(cos(P))) \times Arctan\left(\frac{Arctan\left(\frac{T}{B/P}\right)}{M} + M \times T - T + 5.11 - \sqrt{t}\right) \times cos(cos(sin(sin(3.85\left(B/P^2 \times (t+T)\right)^3)))) \times \left(9.31 + cos^3(t) + Exp\left(cos\left(T - \sqrt{V} + 3.62\right)\right)\right) cos\left(cos^3(M)\right)$

sets collected from the literature, 65 sets were randomly chosen as a training set for the GEP-1 to GEP-11 modeling and the remaining 21 sets were used as testing the generalization capacity of the proposed models.

For this problem, first, the fitness, f_i, of an individual program, i, is measured by [22]:

$$f_i = \sum_{j=1}^{C_t} \left(M - \left|C_{(ij)} - T_j\right|\right) \quad (1)$$

where M is the range of selection, $C_{(i,j)}$ is the value returned by the individual chromosome i for fitness case j (out of C_t fitness cases) and T_j is the target value for fitness case j. If $\left|C_{(ij)} - T_j\right|$ (the precision) is less than or equal to 0.01, then the precision is equal to zero, and $f_i = f_{\max} = C_t M$. In this case, $M = 100$ was used, therefore, $f_{\max} = 1000$. The advantage of this kind of fitness functions is that the system can find the optimal solution by itself [22]. All of the models were let to experience more than 100,000 iterations to ensure gaining maximum fitness.

Afterwards the set of terminals T and the set of functions F to create the chromosomes are preferred, namely, $T = \{M, t, T, P, V, B/P\}$ and four basic arithmetic operators (+, −, ×, /) and some basic mathematical functions (Sqrt, x^2, x^3, ln, Exp, sin, cos, Arctan) were used.

Another major step is to choose the chromosomal tree, i.e., the length of the head and the number of genes. For all of GEP-1 to GEP-11 approach models initially used single gene and two lengths of heads, and increased the number of genes and heads, one after another during each run, and monitored the training and testing sets performance of each model. In this study, for the GEP-1 to GEP-11 approach models observed the heads length of 12.

Finally, a combination of all genetic operators (mutation, transposition and crossover) was utilized as set of genetic operators. Parameters of the training of the GEP-1 to GEP-11 approach models are given in Table 4. For the GEP-1 to GEP-11 approach models, chromosome number of 40 was observed to be the best of generation individuals predicting the mean grain size of the synthesized nanopowders. Explicit formulations based on the GEP-1 to GEP-11 approach models for mean grain size were obtained by:

$$\mathrm{MGS} = f(M, t, T, P, V, B/P) \quad (2)$$

The related formulations could be obtained by the procedure shown in Fig. 5 [22].

Table 4
Parameters of GEP approach models.

Parameter definition		GEP-1 to GEP-10 models
P1	Function set	+, −, *, /, sqrt, x^2, x^3, Exp, ln, sin, cos, Arctan
P2	Chromosomes	40
P3	Head size	12
P4	Mutation rate	0.055
P5	Inversion rate	0.1
P6	One-point recombination rate	0.3
P7	Two-point recombination rate	0.3
P8	Gene recombination rate	0.1
P9	Gene transposition rate	0.1
P10	Constants per gene	5
P11	Weight of functions	7

5. Predicted results and discussion

In this study, the error arose during the training and testing in GEP-1 to GEP-11 models can be expressed as absolute fraction of variance (R^2), the absolute percentage error (MAPE) and the root mean square error (RMSE) which are calculated by Eqs. (3)–(5), respectively [22]:

$$R^2 = 1 - \left(\frac{\sum_i (t_i - o_i)^2}{\sum_i (o_i)^2}\right) \quad (3)$$

$$\mathrm{MAPE} = \frac{1}{n}\sum_i \left|\frac{t_i - o_i}{t_i}\right| \times 100 \quad (4)$$

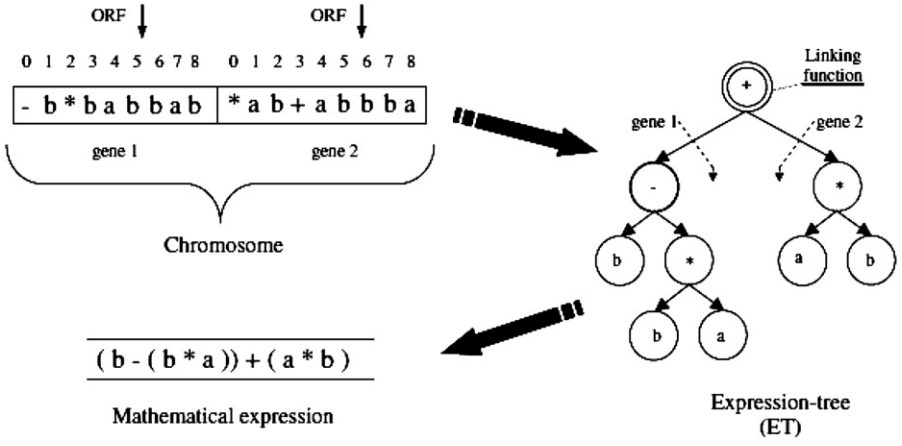

Fig. 5. Chromosome with two genes and its decoding in GEP [22].

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i}(t_i - o_i)^2} \quad (5)$$

where t is the target value, o is the output value and n is the number of data sets in each of training and testing phases.

All of the results obtained from experimental studies and predicted by using the training and testing results of GEP-5 models are given in Fig. 6(a) and (b), respectively. The linear least square fit line equation, R^2, MAPE and RMSE values were shown in the figures for the training and testing data. As it is visible in Fig. 6, the values obtained from the training and testing in GEP-5 are relatively close to the collected experimental results by an accuracy of more than 85% for training set and more than 75% for testing set.

As shown in Fig. 6(a) and (b), the predicted results from models are compared to the collected experimental results for training and testing sets, respectively. The training set results proved that the proposed model have moderately well learned the non-linear relationship between the input and the output variables with a good correlation and comparatively low error values. Comparing the GEP-5 approach model prediction with the collected experimental results for the testing and training stages demonstrates a generalization capacity of the proposed models and fairly low error values. All of these findings exhibit a successful performance of the model for predicting mean grain size values of synthesized nanopowders in training and testing stages. The result of testing phase in Fig. 6(b) shows that the GEP-5 model is capable of generalizing between input and output variables with reasonably good predictions and accuracy more than 75%.

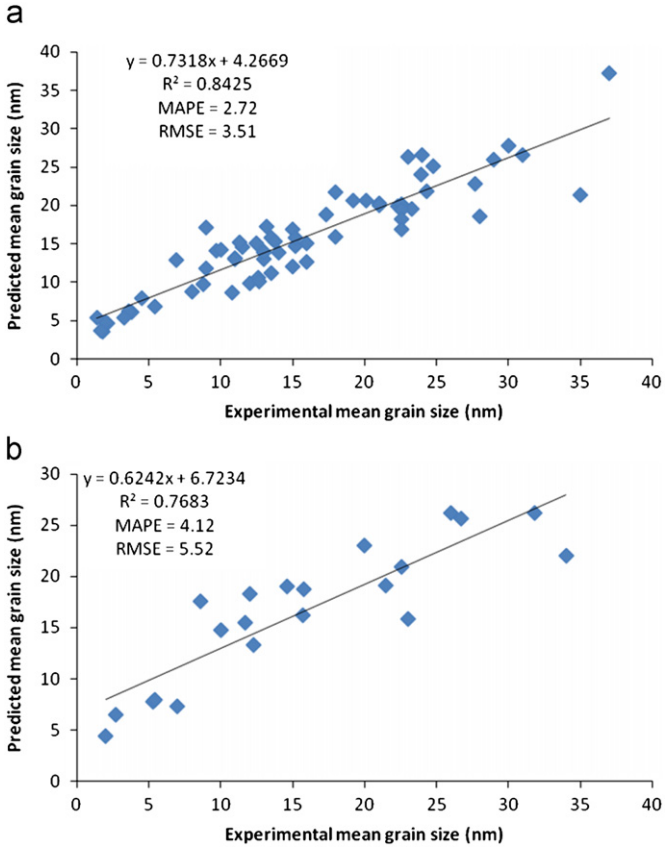

Fig. 6. The correlation of the measured and predicted mean grain size values of synthesized nanopowders in (a) training and (b) testing phase for GEP-5 model.

The performance of GEP-1 to GEP-10 models is shown in Table 3. The best value of R^2 in training sets is 0.8691 for GEP-2 model. However, its R^2 in testing phase is only 0.4147. A high performance network is achieved when its performance in terms of R^2 reaches to at least 75%. The next model with high performance is GEP-5 model with R^2 value of 0.8425 in training phase and 0.7683 in testing phase. GEP-5 is the only model that could predict the collected experimental results by accuracy of more than 75% in testing phase. Therefore, GEP-5 could be the only proposed model to predict mean grain size value of the synthesized nanopowders in the considered range of the present work. To ensure that increasing the number of sub-ETs more than 7 could improve the performance of the models, GEP-6 model was conducted with 8 Sub-ETs and addition as linking function. Although, R^2 value of GEP-6 model is more than 0.8 in training phase, its low value in testing phase make it an imprecise model for predicting mean grain size values. Finally, by selecting multiplication as linking function in GEP-7 to GEP-11 models, no accurate model was proposed to predict the mean grain size of the synthesized nanopowders.

6. Conclusions

This study reports a new and efficient approach for the formulation of mean grain size of synthesized nanopowders. Eleven different GEP-1 and GEP-11 models were proposed in order to predict mean grain size of synthesized nanopowders. The proposed models are empirical and based on experimental results collected from the previous works. The models developed in this study were used to be the number of genes 3 to 8, and the linking function multiplication and addition. The results obtained from the models showed that only by selecting 7 expression trees and linking them by addition operation could have a suitable agreement with the collected experimental results. The statistical values of R^2 in training and testing phases showed this situation. It was found that GEP can be an alternative approach for the evaluation of mean grain size of the synthesized nanopowders in the considered range.

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